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# New Insights in Prediction and Dynamic Modeling from Non-Gaussian Mixture Processing Methods 

## DOCTORAL THESIS

## by

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# New Insights in Prediction and Dynamic Modeling from Non-Gaussian Mixture Processing Methods 

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## THESIS

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To Marta
"Intelligence is nothing more than discussing things with others.
Limitless wisdom comes of this."
-Yamamoto Tsunetomo, Hagakure (In the Shadow of Leaves)


#### Abstract

This thesis considers new applications of non-Gaussian mixtures in the framework of statistical signal processing and pattern recognition. The non-Gaussian mixtures were implemented by mixtures of independent component analyzers (ICA). The fundamental hypothesis of ICA is that the observed signals can be expressed as a linear transformation of a set of hidden variables, usually referred to as sources, which are statistically independent. This independence allows factoring the original $M$-dimensional probability density function (PDF) of the data as a product of one-dimensional probability densities, greatly simplifying the modeling of the data. ICA mixture models (ICAMM) provide further flexibility by alleviating the independency requirement of ICA, thus allowing the model to obtain local projections of the data without compromising its generalization capabilities. Here are explored new possibilities of ICAMM for the purposes of estimation and classification of signals.

The thesis makes several contributions to the research in non-Gaussian mixtures: (i) a method for maximum-likelihood estimation of missing data, based on the maximization of the PDF of the data given the ICAMM; (ii) a method for Bayesian estimation of missing data that minimizes the mean squared error and can obtain the confidence interval of the prediction; (iii) a generalization of the sequential dependence model for ICAMM to semi-supervised or supervised learning and multiple chains of dependence, thus allowing the use of multimodal data; and (iv) introduction of ICAMM in diverse novel applications, both for estimation and for classification.

The developed methods were validated via an extensive number of simulations that covered multiple scenarios. These tested the sensitivity of the proposed methods with respect to the following parameters: number of values to estimate; kinds of source distributions; correspondence of the data with respect to the assumptions of the model; number of classes in the mixture model; and unsupervised, semi-supervised, and supervised learning. The performance of the proposed methods was evaluated using several figures of merit, and compared with the performance of multiple classical and state-of-the-art techniques for estimation and classification.

Aside from the simulations, the methods were also tested on several sets of real data from different types: data from seismic exploration studies; ground penetrating radar surveys; and biomedical data. These data correspond to the following applications: reconstruction of damaged or missing data from ground-penetrating radar surveys of historical walls; reconstruction of damaged or missing data from a seismic exploration survey; reconstruction of artifacted or missing electroencephalographic (EEG) data; diagnosis of sleep disorders; modeling of the brain response during memory tasks; and exploration of EEG data from subjects performing a battery of neuropsychological tests. The obtained results demonstrate the capability of the proposed methods to work on problems with real data. Furthermore, the proposed methods are general-purpose and can be used in many signal processing fields.


## Resum

Aquesta tesi considera noves aplicacions de barreges no Gaussianes dins del marc de treball del processament estadístic de senyal i del reconeixement de patrons. Les barreges no Gaussianes van ser implementades mitjançant barreges d'analitzadors de components independents (ICA). La hipòtesi fonamental d'ICA és que els senyals observats poden ser expressats com una transformació lineal d'un grup de variables ocultes, comunament anomenades fonts, que són estadísticament independents. Aquesta independència permet factoritzar la funció de densitat de probabilitat (PDF) original $M$-dimensional de les dades com un producte de densitats de probabilitat unidimensionals, simplificant àmpliament la modelització de les dades. Els models de barreges ICA (ICAMM) aporten una major flexibilitat en alleugerar el requeriment d'independència d'ICA, permetent així que el model obtinga projeccions locals de les dades sense comprometre la seva capacitat de generalització. Ací s'exploren noves possibilitats d'ICAMM pels propòsits d'estimació i classificació de senyals.

Aquesta tesi aporta diverses contribucions a la recerca en barreges no Gaussianes: (i) un mètode d'estimació de dades faltants per màxima versemblança, basat en la maximització de la PDF de les dades donat l'ICAMM; (ii) un mètode d'estimació Bayesiana de dades faltants que minimitza l'error quadràtic mitjà i pot obtenir l'interval de confiança de la predicció; (iii) una generalització del model de dependència seqüencial d'ICAMM per entrenament supervisat o semi-supervisat i múltiples cadenes de dependència, permetent així l'ús de dades multimodals; i (iv) introducció d'ICAMM en diverses noves aplicacions, tant per a estimació com per a classificació.

Els mètodes desenvolupats van ser validats mitjançant una extensa quantitat de simulacions que cobriren múltiples situacions. Aquestes van verificar la sensibilitat dels mètodes proposats amb respecte als següents paràmetres: nombre de valors per estimar; mena de distribucions de les fonts; correspondència de les dades amb respecte a les suposicions del model; nombre de classes del model de barreges; i aprenentatge supervisat, semi-supervisat i no-supervisat. El rendiment dels mètodes proposats va ser avaluat mitjançant diverses figures de mèrit, i comparat amb el rendiments de múltiples tècniques clàssiques i de l'estat de l'art per a estimació i classificació.

A banda de les simulacions, els mètodes van ser verificats també sobre diversos grups de dades reals de diferents tipus: dades d'estudis d'exploració sísmica; exploracions de radars de penetració de terra; i dades biomèdiques. Aquestes dades corresponen a les següents aplicacions: reconstrucció de dades danyades o faltants d'estudis d'exploracions de radar de penetració de terra sobre murs històrics; reconstrucció de dades danyades o faltants en un estudi d'exploració sísmica; reconstrucció de dades electroencefalogràfiques (EEG) artefactuades o faltants; diagnosi de desordres de la son; modelització de la resposta del cervell durant tasques de memòria; i exploració de dades EEG de subjectes realitzant una bateria de tests neuropsicològics. Els resultats obtinguts han demostrat la capacitat dels mètodes proposats per treballar en problemes amb dades reals. A més, els mètodes proposats són de propòsit general i poden fer-se servir en molts camps del processament de senyal.

## Resumen

Esta tesis considera nuevas aplicaciones de las mezclas no Gaussianas dentro del marco de trabajo del procesado estadístico de señal y del reconocimiento de patrones. Las mezclas no Gaussianas fueron implementadas mediante mezclas de analizadores de componentes independientes (ICA). La hipótesis fundamental de ICA es que las señales observadas pueden expresarse como una transformación lineal de un grupo de variables ocultas, normalmente llamadas fuentes, que son estadísticamente independientes. Esta independencia permite factorizar la función de densidad de probabilidad (PDF) original $M$-dimensional de los datos como un producto de densidades unidimensionales, simplificando ampliamente el modelado de los datos. Los modelos de mezclas ICA (ICAMM) aportan una mayor flexibilidad al relajar el requisito de independencia de ICA, permitiendo que el modelo obtenga proyecciones locales de los datos sin comprometer su capacidad de generalización. Aquí se exploran nuevas posibilidades de ICAMM para los propósitos de estimación y clasificación de señales.

La tesis realiza varias contribuciones a la investigación en mezclas no Gaussianas: (i) un método de estimación de datos faltantes por máxima verosimilitud, basado en la maximización de la PDF de los datos dado el ICAMM; (ii) un método de estimación Bayesiana de datos faltantes que minimiza el error cuadrático medio y puede obtener el intervalo de confianza de la predicción; (iii) una generalización del modelo de dependencia secuencial de ICAMM para aprendizaje supervisado o semi-supervisado y múltiples cadenas de dependencia, permitiendo así el uso de datos multimodales; y (iv) introducción de ICAMM en varias aplicaciones novedosas, tanto para estimación como para clasificación.

Los métodos desarrollados fueron validados mediante un número extenso de simulaciones que cubrieron múltiples escenarios. Éstos comprobaron la sensibilidad de los métodos propuestos con respecto a los siguientes parámetros: número de valores a estimar; tipo de distribuciones de las fuentes; correspondencia de los datos con respecto a las suposiciones del modelo; número de clases en el modelo de mezclas; y aprendizaje supervisado, semi-supervisado y no supervisado. El rendimiento de los métodos propuestos fue evaluado usando varias figuras de mérito, y comparado con el rendimiento de múltiples técnicas clásicas y del estado del arte para estimación y clasificación.

Además de las simulaciones, los métodos también fueron probados sobre varios grupos de datos de diferente tipo: datos de estudios de exploración sísmica; exploraciones por radar de penetración terrestre; y datos biomédicos. Estos datos corresponden a las siguientes aplicaciones: reconstrucción de datos dañados o faltantes de exploraciones de radar de penetración terrestre de muros históricos; reconstrucción de datos dañados o faltantes de un estudio de exploración sísmica; reconstrucción de datos electroencefalográficos (EEG) dañados o artefactados; diagnóstico de desórdenes del sueño; modelado de la respuesta del cerebro durante tareas de memoria; y exploración de datos EEG de sujetos durante la realización de una batería de pruebas neuropsicológicas. Los resultados obtenidos demuestran la capacidad de los métodos propuestos para trabajar en problemas con datos reales. Además, los métodos propuestos son de propósito general y pueden utilizarse en muchos campos del procesado de señal.

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## Mathematical notations

## Independent component analysis mixture models

| $K$ | number of classes (ICA models) |
| :--- | :--- |
| $k$ | one particular class within the ICAMM, $k=1, \ldots, K$ |
| $N$ | number of observations or time instants |
| $n$ | one particular time instant, $n=1, \ldots, N$ |
| $M$ | number of sources (i.e., dimensionality of the data) |
| $m$ | one particular source, $m=1, \ldots, M$ |
| $\mathbf{x}(n)$ | $n$-th observation (or observation at time $n$ ) |
| $x_{m}(n)$ | $m$-th value of $\mathbf{x}(n)$ |
| $\mathbf{s}_{k}(n)$ | source vector of class $k$ at time $n$ |
| $s_{k, m}(n)$ | $m$-th source of class $k$ at time $n$ |
| $\mathbf{A}_{k}$ | mixing matrix of class $k$ |
| $\mathbf{W}_{k}$ | de-mixing matrix of class $k$ |
| $\mathbf{b}_{k}$ | centroid of class $k$ |

## Estimation

| $\mathbf{y}(n)$ | known data at time $n$ |
| :--- | :--- |
| $\mathbf{z}(n)$ | unknown data at time $n$ |

## Sequential models

| $\mathbf{X}(n)$ | all observations up to time $n, \mathbf{X}(n)=[\mathbf{x}(1), \mathbf{x}(2), \ldots, \mathbf{x}(n)]$ |
| :--- | :--- |
| $L$ | number of chains of dependence in the model |
| $l$ | one particular chain within the model, $l=1, \ldots, L$ |
| $\mathbf{x}_{l}(n)$ | $n$-th observation of chain $l$ (or observation of chain $l$ at time $n$ ) |

## Statistics and mathematics

| $p(\cdot)$ | probability density function |
| :--- | :--- |
| $P(\cdot)$ | discrete probability function |
| $p(A \mid B)$ | conditional probability of $A$ with respect to $B$ |
| $p(A, B)$ | joint probability of $A$ and $B$ |
| $\operatorname{det} \mathbf{A}$ | determinant of matrix $\mathbf{A}$ |
| $\sigma, \sigma^{2}$ | standard deviation, variance |
| $\mathbf{A}^{-1}$ | inverse of matrix $\mathbf{A}$ |
| $\hat{a}$ | estimate of $a$ |
| $\mathbf{A}^{T}, \mathbf{a}^{T}$ | transpose of a matrix, vector |
| $\|\cdot\|$ | absolute value |
| $\operatorname{tr}(\mathbf{A})$ | trace of a matrix |
| $E[\cdot], E(\cdot)$ | expectation operator |
| $\delta$ | partial derivative operator |
| $\Delta$ | increment, gradient operator |

## Acronyms

| AIC | Akaike Information Criterion |
| :---: | :---: |
| AR | Autoregressive |
| ASI | Alpha Slow-wave Index |
| BER | Balanced Error Rate |
| BN | Bayesian Network |
| CHMM | Coupled Hidden Markov Model |
| CORR | CORRelation between true values and estimated values |
| DBN | Dynamic Bayesian Network |
| ECG | Electrocardiogram |
| EEG | Electroencephalogram |
| E-ICAMM | Expectation of ICAMM |
| EM | Expectation-Maximization |
| FastICA | FAST fixed-point algorithm for Independent Component Analysis |
| GMM | Gaussian Mixture Model |
| GPR | Ground-Penetrating Radar |
| G-SICAMM | Generalized Sequential ICAMM |
| HMM | Hidden Markov Model |
| ICA | Independent Component Analysis |
| ICAMM | Independent Component Analysis Mixture Model |
| i.i.d. | Independent and Identically Distributed |
| JADE | Joint Approximate Diagonalization of Eigenmatrices |
| KDE | Kernel Density Estimation |
| KLD | Kullback-Leibler Divergence |
| LMSE | Least Mean Square Error estimation |
| MAP | Maximum A Posteriori estimation |
| Mixca | MIXture of Component Analyzers (non-parametric density estimation) |
| ML,MLE | Maximum Likelihood, Maximum Likelihood Estimation |
| MSE | Mean Squared Error |
| PCA | Principal Component Analysis |
| PREDICAMM | Prediction using ICAMM |
| PDF | Probability Density Function |
| PSG | Polysomnogram |
| REM | Rapid Eye Movement sleep |
| SICAMM | Sequential ICAMM |
| SIR | Signal-to-Interference Ratio |
| TAVEC | From the Spanish Test de Aprendizaje Verbal España-Complutense |
| TB | Barcelona memory test (from the Spanish Test de Barcelona) |
| TICA | Topographic Independent Component Analysis |
| TSI | Theta Slow-wave Index |
| UG-SICAMM | Unsupervised Generalized Sequential ICAMM |
| WMS | Wechsler Memory Scale |
| WAIS | Wechsler Adult Intelligence Scale |
| w.r.t. | With Respect To |

## Introduction

## Chapter 1-Introduction

The human brain has a well-known ability to distinguish patterns, far in advance to what computers can reproduce nowadays. This capability turns the perceived information from the senses into much more, recognizing sets of stimuli as groups (patterns) rather than isolated events. This feature of our brains is used almost constantly in our everyday lives for a wide array of tasks, most of which would be difficult (if at all possible) for any machine but trivial for most people. Face recognition is arguably the most common of these tasks, but there are a slew of everyday tasks that are known (or thought) to be performed by pattern recognition. To cite but an interesting example, there is "subitizing:" the fast, accurate and confident determination of the number of elements in any small set (up to four elements) at a faster rate than it would be possible by counting [133]. This phenomenon is thought to be caused by the brain recognizing the shape of small groups rather than counting their elements, e.g., recognizing the shape of a group of three people instead of actually counting that there are three people in the group.

These skills are imitated in machine learning techniques, which attempt to learn general models from a limited set of experiences. However, computers cannot directly access the physical world for this kind of information. To do this learning, machine learning techniques require the simplification of the natural world into a set of quantified observations or data, i.e., a series of ones and zeros. These data are then used to fit a number of mathematical/statistical models and equations whose results can sometimes be interpreted in some fashion that relates back to the physical world. Machine learning can be used for a number of tasks, such as recovering missing values, classifying data, searching for interesting/hidden patterns... several of which will be considered in this thesis.

Far less developed that our capability for pattern recognition is our ability to measure the passage of time, and yet, it has always been one of the main motivators behind human thought and philosophy. Modern society is perhaps the best example of this, with the many deadlines, delays, timetables and the like that preoccupy most of us. Nonetheless, time and its flow have always been a constant concern for people. This is superbly presented in Julio Cortazar's short story, "El Perseguidor," a passage of which we would like to quote here:

[^0]> -Todo el mundo sabe las fechas menos yo -rezonga Johnny, tapándose hasta las orejas con la frazada-. Hubiera jurado que era esta noche, y que esta tarde había que ir a ensayar.
> -Lo mismo da -ha dicho Dédée-. La cuestión es que no tienes saxo.
> -¿Cómo lo mismo da? No es lo mismo. Pasado mañana es después de mañana, y mañana es mucho después de hoy. Y hoy mismo es bastante después de ahora, en que estamos charlando con el compañero Bruno y yo me sentiría mucho mejor si me pudiera olvidar del tiempo y beber alguna cosa caliente.
> -Ya va a hervir el agua, espera un poco.

The consideration of time is absent from most machine learning techniques, however. This omission owes, for the most part, to the increased complexities in the underlying models and equations: most models are complex enough even after considering stationarity, i.e., that the properties of the data do not change over time. Adding time to the equation (pun intended) would make them intractable, unfeasible, or simply too computationally expensive. Still, some machine learning techniques do consider time dependences or effects in the data, and several of the methods proposed in this work consider sequential dependence. As a matter of fact, it will be shown that these techniques are improved by the inclusion of time dependences, thus proving the benefit of these considerations despite the increase in complexity.

The research described in this thesis has been undertaken at the Grupo de Tratamiento de Señal (GTS, Signal Processing Group) of the Universitat Politècnica de València (UPV, Polytechnic University of Valencia). The group focuses on new theoretical analyses and novel algorithms, usually applied in diverse areas where processing of signals plays a fundamental role. More specifically, this thesis focuses in statistical signal processing methods. It is noteworthy that many concepts, methods and algorithms are shared by statistical signal processing and other related areas such as data processing, pattern recognition and machine learning. In general terms, statistical signal processing may be extended to the concept of computational intelligence. This broader scope of statistical signal processing is usually applied throughout this thesis.

Statistical signal processing has been traditionally divided into three different topics: estimation, detection and classification. Nevertheless, the optimum design of estimators, detectors or classifiers shares the need (in an explicit or implicit manner) of multidimensional probability densities (MPD) in the observation space. Thus, the essential problem in optimum statistical signal processing is ultimately that of modeling/computing MPD. Classical parametric and nonparametric methods for modeling/computing MPD have evolved towards two types of approaches. The first one considers that the MPD is a mixture of some simpler MPD [85]; the most representative example of this approach is Gaussian mixture models (GMM). The other approach is based on separating the dependence model from the marginal model. One instance of this is Copula methods [203], which consider the MPD as the product of a number of unidimensional probability densities (UPDs) of every observed vector component (i.e., as if they were statistically independent) times a factor measuring the possible dependence between the observed variables. Independent component analysis (ICA) [115] is another significant example of this second kind of approach. In ICA, some independent variables (sources) having arbitrary UPDs are assumed to be linearly combined by a parametric dependence model to conform the observed variables. This thesis concentrates in a combination of the two kinds of approaches, termed ICA mixture models (ICAMM). In ICAMM, the MPD is considered to be a mixture of simpler MPD, each modeled with a separate ICA. This approach can be considered an extension of GMM to the general case of non-Gaussian mixture models (NGMM) as ICA may incorporate an arbitrary class of MPD for every component of the mixture. ICAMM affords a large versatility to model almost any kind of MPD and it is particularly suited to scenarios with very irregular and complicated dependences in the observation space.

Relevant previous research on ICAMM has been done in the GTS. For example, a general procedure that encompasses many different options and variations for estimating the model has been proposed [231]. This procedure has been applied to different real problems of interest for the GTS. An extension of ICAMM named SICAMM [230] has also been proposed to incorporate time dependences in the model through a matrix of transition probabilities between classes in a hidden Markov model (HMM), where ICAMM was the underlying probabilistic model for the observed data. In spite of the work that has already been done, there remain many options for further development of ICAMM in order to exploit its powerful capability to model complex MPDs. In this thesis, two lines of new research on ICAMM have been considered, as explained below.

ICAMM has been applied mostly to detection and classification problems. In detection, ICAMM exploits the implicit ICA for every mixture component to transform the original domain of dependent observations to the source domain of independent components, thus simplifying the design of the subsequent detector [178]. On the other hand, a classification problem is a natural framework for ICAMM, as every mixture component can be associated to a corresponding class. In fact, most of the interest on ICAMM emanates from the classification area [153]. To the best of our knowledge, however, there is no work so far on the application of ICAMM to estimation problems. Hence, one of the foci of this thesis is the use of ICAMM for the derivation of optimum estimators. To be more specific, it will be considered for the problem of prediction/interpolation of signals, which (together with optimum filtering) is the most relevant problem of signal estimation. Maximum-likelihood (ML) and least-mean-squared-error (LMSE) optimum predictors will be obtained under the assumption of ICAMM for the underlying MPD in the observation space. The analytical derivations of these predictors, including iterative algorithms for the resulting non-linear equations and/or the maximization of the corresponding cost functions, are given in the thesis. These new predictors are compared with classical solutions on simulated and real data. Regarding the latter, the recovering of missing signals is considered in three different applications: (i) ground penetrating radar (GPR) non-destructive evaluation of historical walls; (ii) reconstruction of seismic traces; and (iii) recovering of missing EEG data. These applications come from a number of collaborations of the GTS with the Instituto de Tecnologías de la Construcción (Valencia, Spain), ECOPETROL (Colombia) and the Hospital Universitari i Politècnic La Fe (Valencia, Spain), respectively.

SICAMM was a first attempt to incorporate time dependences in ICAMM. However, it requires previous knowledge of the transition probabilities, so that only the ICAMM parameters are estimated. In this thesis, we will develop new algorithms for simultaneous estimation of the transition probabilities and the ICAMM parameters. Moreover, several HMM can be connected in parallel, every one corresponding to a different coordinate in an additional domain (e.g., the space domain). This thesis will also consider this general structure of multiple chained hidden Markov models (CHMM) and develop new algorithms for simultaneous estimation of the transition probabilities and the ICAMM parameters. The new developments will be compared with equivalent existing procedures and applied to the processing of electroencephalographic signals (EEG) to monitor the dynamics of the brain under specific tasks, which is part of different collaborative projects between the GTS and the La Fe hospital.

In conclusion, the thesis continues the intensive research of the GTS in ICAMM. Two new theoretic/algorithmic contributions are given: (i) application of ICAMM to prediction and interpolation problems; and (ii) extension to dynamic classifiers which incorporate time and space dependences in the class domain. The connection between both contributions is possible in a scenario where part of the signal information is missing and must be recovered in order to improve the feature extraction step in a possible classifier to be implemented.

Not less relevant is the application of the new methods on data coming from several areas, which involve multiple types of signals: ground-penetrating radar (reconstruction of missing traces in GPR B-Scans or radargrams); seismic data exploration (reconstruction of missing data
in seismic radargrams); and electroencephalographic data (reconstruction of missing or artifacted EEG data; automatic detection of microarousals during sleep; exploration of data from subjects performing a memory task; automatic classification of data from subjects performing neuropsychological tests and data exploration). These are very diverse signals, with ample differences in features such as: their frequency distributions, ranging from a few Hertz to the VHF band; the nature of the captured signal, be it incident EM radiation, sonic vibrations, or small electric currents; and the medium under test, which can be historical walls, underground materials, or the human brain. The successful application of the proposed methods on these data demonstrates their general aptness for most real-world problems.

### 1.1. Review of methods

The thesis explores the possibilities of non-Gaussian mixtures by way of mixtures of independent component analyzers. This exploration will revolve around two problems: data estimation and classification. We develop several theoretical concepts that require a basic working knowledge of Calculus and Statistics. To make the thesis more accessible to the reader, this section includes a brief review on several concepts that are of importance for the methods presented in later chapters.

### 1.1.1. Estimation

Estimation theory is concerned with the determination of the value of a vector of unknown parameters from related observations [266]. For instance, given some noisy observations generated by a model from a known family of models, but whose parameters are actually unknown, one might be interested in estimating the parameters of the underlying model, or recovering the clean observations without noise. The estimation problem is summarized in Figure 1.1, where it is assumed that we want to estimate some parameter $\alpha$ from an observation vector, $\mathbf{x}$. The parameter space, which can be deterministic or stochastic, cannot be directly accessed or measured. Instead, only the observation space can be measured to obtain stochastic observations, $\mathbf{x}$, that are assumed to have some sort of dependence on the unknown parameter, $\alpha$. This dependence is usually modeled through a probability density function $p(\mathbf{x}, \alpha)$, but it can be expressed as a deterministic equation (with noise) in some cases. Estimation consists in obtaining estimates of $\alpha$ from the observations $\mathbf{x}(\alpha)$, thus creating a mapping from the observation space to the estimation space, $\hat{\alpha}=f(\mathbf{x}(\alpha))$. If the estimation were perfect, the estimation space would overlap with the parameter space. In practice, however, there is a difference between the estimate, $\hat{\alpha}$, and the true value, $\alpha$. Estimation methods optimize some kind of error or cost function to minimize this difference and obtain the "best" estimate (in the sense of the optimized function).



Figure 1.1. Diagram explaining the estimation problem.

Estimation theory [266] gives us well-known optimization criteria and their corresponding solutions. The two criteria that have been most commonly considered in practice are the maximum a posteriori criterion and the Bayesian least mean squared error criterion. Both criteria are considered in Chapter 3 (for data estimation) and Chapter 4 (for estimation of model parameters) of this thesis.

### 1.1.1.a. Maximum a posteriori estimation

Let us assume that the parameter to estimate, $\alpha$, is a random value with known probability density $p(\alpha)$. Intuitively, one possible way to estimate $\alpha$ is searching for the most probable value given the information we already have, i.e., observation vector $\mathbf{x}$. This is known as maximum a posteriori (MAP) estimation. More formally, MAP estimation consists in seeking the value $\hat{\alpha}$ that maximizes the posterior probability of the parameter with respect to the observation, $\hat{\alpha}_{\text {MAP }}(\mathbf{x})=\underbrace{\arg \max } p(\alpha \mid \mathbf{x})$. In practice, however, $p(\alpha \mid \mathbf{x})$ is unknown and difficult to estimate. Since the observation vector is fixed and does not change during the maximization procedure, $\underbrace{\arg \max } p(\alpha \mid \mathbf{x}) \quad$ and $\underbrace{\arg \max } p(\alpha \mid \mathbf{x}) \cdot p(\mathbf{x})$ are equivalent. Therefore, by using the Bayes rule several times:

$$
\begin{align*}
\hat{\alpha}_{M A P}(\mathbf{x}) & =\underbrace{\arg \max }_{\alpha} p(\alpha \mid \mathbf{x})=\underbrace{\arg \max }_{\alpha} p(\alpha \mid \mathbf{x}) \cdot p(\mathbf{x})=  \tag{1.1}\\
& =\underbrace{\arg \max }_{\alpha} p(\mathbf{x} \mid \alpha) \cdot p(\alpha)=\underbrace{\arg \max }_{\alpha} p(\mathbf{x}, \alpha)
\end{align*}
$$

Thus, maximizing $p(\mathbf{x}, \alpha)=p(\mathbf{x} \mid \alpha) \cdot p(\alpha)$ is equivalent to maximizing the posterior probability. The conditional density $p(\mathbf{x} \mid \alpha)$, also known as the likelihood, indicates the prior conditional probability that the observation $\mathbf{x}$ was generated, given the (unknown) parameter $\alpha$. The likelihood is usually easier to obtain than the posterior probability, and is therefore more commonly used for MAP estimation.

If we assume that $\alpha$ is deterministic or is uniformly distributed, $p(\alpha)$ does not affect the maximization procedure and (1.1) becomes the maximum likelihood (ML) criterion:

$$
\begin{equation*}
\hat{\alpha}_{M L}(\mathbf{x})=\underbrace{\arg \max }_{\alpha} p(\mathbf{x} \mid \alpha) \cdot p(\alpha)=\underbrace{\arg \max }_{\alpha} p(\mathbf{x} \mid \alpha) \tag{1.2}
\end{equation*}
$$

Figure 1.2 shows a toy example that displays the difference between MAP and ML estimation. The joint density is shown as a series of lines of equal density, with lines of higher densities being more yellow. The solution to the MAP criterion, denoted by the the dashed lines, is the maximum of the joint density $p(\mathbf{x}, \alpha)$, as indicated by (1.1). The lines have been extended to the side plots for comparison. Note that this maximum returns two solutions, the optimum values of $x$ and $\alpha$. Conversely, the solution to the ML criterion, denoted by the red square, is the maximum of the likelihood function. The solutions for $x$ and $\alpha$ are not linked. Furthermore, note that the ML solution for $x$ is different from the MAP solution. Should the parameter, $\alpha$, be uniformly distributed, both solutions would be identical.


Figure 1.2. Comparison of the joint density of one-dimensional observations, $x$, with respect to a parameter $\alpha$. The concentrical ovals denote points of equal density, with higher PDF being more yellow. The plots on the side of the joint density show the PDF of $\alpha$ and the likelihood of $x$ for the most common value of $\alpha$. Note that the maximum of the joint density (denoted by the two dashed lines) yields a different solution than the maximum of the likelihood function (denoted by the red square), particularly for $x$.

The MAP and ML criteria involve seeking the global maximum in a multidimensional function, which can only be done by means of iterative algorithms like gradient methods. Hence, problems of initialization and convergence to local maxima typically emerge in these solutions. This has been considered in the applications of the ML criterion in this thesis in Chapter 3 and Chapter 4.

### 1.1.1.b. Bayesian LMSE estimation

Another way to estimate the unknown parameter is by minimizing the "distance" between its true value and the estimated value $\hat{\alpha}(\mathbf{x})$, as defined by an cost (or cost) function $\varepsilon(\alpha, \hat{\alpha}(\mathbf{x}))$. Since $\alpha$ and $\hat{\alpha}(\mathbf{x})$ are usually random variables, this error function is a random variable as well. The Bayesian estimator is defined as the estimator that minimizes the average error function of the estimate, $E[\varepsilon(\alpha, \hat{\alpha}(\mathbf{x}))]$. More explicitly, this average error function is:

$$
\begin{align*}
E[\varepsilon(\alpha, \hat{\alpha}(\mathbf{x}))] & =\iint \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha, \mathbf{x}) \cdot d \alpha \cdot d \mathbf{x}=  \tag{1.3}\\
& =\iint \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha \mid \mathbf{x}) \cdot p(\mathbf{x}) \cdot d \alpha \cdot d \mathbf{x}
\end{align*}
$$

The minimum average error can be obtained by setting the derivative of (1.3) to zero:

$$
\begin{align*}
& 0= \frac{d}{d \hat{\alpha}} \iint \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha, \mathbf{x}) \cdot d \alpha \cdot d \mathbf{x}= \\
&=\int\left[\frac{d}{d \hat{\alpha}} \int \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha\right\rceil \cdot p(\mathbf{x}) \cdot d \mathbf{x}  \tag{1.4.a}\\
& 0=\frac{d}{d \hat{\alpha}} \int \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha \tag{1.4.b}
\end{align*}
$$

The solution to (1.4.b) depends on the shape of the error function, $\varepsilon(\cdot)$. In least mean squared error estimation, the error function is set to the squared error: $\varepsilon(\alpha, \hat{\alpha}(\mathbf{x}))=(\alpha-\hat{\alpha}(\mathbf{x}))^{2}$. Substituting this error function in (1.4.b) results in

$$
\begin{align*}
& 0=\frac{d}{d \hat{\alpha}} \int \varepsilon(\alpha, \hat{\alpha}(\mathbf{x})) \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha=\frac{d}{d \hat{\alpha}} \int(\alpha-\hat{\alpha}(\mathbf{x}))^{2} \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha= \\
&= 2 \int(\alpha-\hat{\alpha}(\mathbf{x})) \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha=2 \int \alpha \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha-2 \hat{\alpha}(\mathbf{x}) \cdot \int p(\alpha \mid \mathbf{x}) \cdot d \alpha=  \tag{1.5}\\
&= 2 \int \alpha \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha-2 \hat{\alpha}(\mathbf{x}) \\
& \hat{\alpha}(\mathbf{x})=\int \alpha \cdot p(\alpha \mid \mathbf{x}) \cdot d \alpha=E[\alpha \mid \mathbf{x}] \tag{1.6}
\end{align*}
$$

Thus, the solution to the LMSE criterion is the conditional expectation of the unknown parameter with respect to the observation $\mathbf{x}$.

In practice, the expectation cannot be formulated in closed form in most cases. Without a closed form for $E[\alpha \mid \mathbf{x}]$, the only way to solve (1.6) is through numerical methods such as Monte Carlo numerical integration. In some cases, a solution can be obtained by finding a non-linear function that can reasonably approximate the expectation. The simplest form of LMSE estimation, however, is to assume that a linear approximation is sufficient, thus reaching the solution of the linear LMSE (LLMSE) criterion. The advantage of the LLMSE criterion is that the linear operator can be obtained by solving a system of linear equations (the Wiener-Hopf equations [236]). Moreover, only second-order statistics are necessary to define this system. When the model cannot be simplified by a linear approximation, however, the solution to the LLMSE criterion is no longer optimal. This is demonstrated in Chapter 3 and Chapter 5, where we compared our proposed ML and LMSE estimators with (among other methods) a classical LLMSE estimator, Ordinary Kriging. The comparison is performed on sets of simulated (Chapter 3) and real (Chapter 5) data.

### 1.1.2. Probability density estimation

The probability density is one of the main concepts in statistics. The probability density function (PDF) $p$ of a random variable $x$ at value $a$, also written as $p_{x}(x=a)$ or $p_{x}(a)$, is defined as the likelihood that the random value takes the value $a$ during any given realization. The PDF allows to determine the probability of any realization of $x$ falling within the interval $[a, b]$ :

$$
\begin{equation*}
P(a<x<b)=\int_{a}^{b} p_{x}(x) \cdot d x \tag{1.7}
\end{equation*}
$$

In practice, however, the probability density of the data is unknown. More typically, we have a limited set of samples from some unknown density that we want to know. This is known as probability density estimation. There are two main approaches to density estimation, parametric estimation and non-parametric estimation. In parametric estimation, it is assumed that the data, $x$, are drawn from a given density distribution or family of distributions (e.g., Gaussian or Laplacian). The data are then used to estimate the parameters of the assumed distribution, e.g., the mean and standard deviation of the Gaussian distribution, or the mean and scale parameter of the Laplacian distribution. Non-parametric estimation, on the other hand, assumes no explicit distribution; only that the data follow some probability density function $p$. The data are used to "build" a general probability density that can have almost any shape. There are many methods for non-parametric density estimation, such as: histograms; naive estimator; nearest neighbors; variable kernel; orthogonal series; maximum penalized likelihood; general weight function; and bounded domains and directional data [75,244]. In this thesis, non-parametric kernel density estimation (KDE) will be used. Thus, a brief review on KDE is included in this section.

In kernel density estimation, the underlying probability density $p$ of the data is estimated by the application of a kernel function to smooth the known samples. The KDE of the density at any given sample $x$ is

$$
\begin{equation*}
\hat{p}(x \mid h)=\frac{1}{N \cdot h} \sum_{n=1}^{N} K\left(\frac{x-x_{n}}{h}\right) \tag{1.8}
\end{equation*}
$$

where $K$ is the kernel function; $h$ is the smoothing parameter, window size or "bandwidth;" and $x_{n}, n=1, \ldots, N$ are the available samples. The kernel must be a non-negative function that integrates to one, $\int_{-\infty}^{\infty} K(x) \cdot d x=1$, and has mean zero. There is a number of functions that are commonly used as kernels, such as uniform, triangular, Epanechnikov, and normal kernels (see Table 1.1). The selection of one particular kernel or another has been found to barely affect the performance of the estimator. However, the estimated density $\hat{p}$ will inherit the continuity and differentiability properties of this kernel (e.g., infinitely differentiable for normal kernels). Therefore, the selection of the kernel is usually based on the desired properties and computational cost of the estimation, rather than performance consideration. The normal kernel is most commonly used, owing to its rather convenient mathematical properties.

Contrary to kernel selection, the selection of the bandwidth does affect the performance of the kernel estimator. Intuitively, one might attempt to use a small a bandwidth as possible in order to improve the resolution of the density estimation. In practice, however, the bandwidth is a compromise between precision and estimator variance. As illustrated in Figure 1.3, overly small bandwidths will under-smooth the data, thus obtaining a "spiky" density that might contain spurious artifacts. Conversely, overly large bandwidths will over-smooth the data and result in a density that changes too slowly to fit the data. There are many techniques for bandwidth estimation, such as subjective choice, cross-validation, or the test graph method [244]. If the shape of the underlying distribution $p$ is known and the kernel function is set, the bandwidth can be calculated directly to minimize some value, e.g., the average error. For instance, the optimal bandwidth (least average squared error) to estimate a Gaussian distribution using the normal kernel is $h_{\text {opt }}=\left(4 \hat{\sigma}^{5} / 3 N\right)^{1 / 5}$, where $\hat{\sigma}$ is the standard deviation of the samples.

| Kernel name | Kernel function $K(\boldsymbol{x})$ |
| :---: | :---: |
| Uniform | $1 / 2$ if $-1 \leq x \leq 1,0$ otherwise |
| Triangular | $1-\|x\|$ if $-1 \leq x \leq 1,0$ otherwise |
| Epanechnikov | $0.75 \cdot\left(1-x^{2}\right)$ if $-1 \leq x \leq 1$, |
| 0 otherwise |  |
| Normal | $(2 \pi)^{-1 / 2} \cdot \exp \left(-x^{2} / 2\right)$ |

Table 1.1. Typical kernel functions used for kernel density estimation.


Figure 1.3. Illustrative example of the effect of bandwidth selection on kernel density estimation.
Throughout this thesis, source densities have been modeled with non-parametric density estimation. More specifically, we have considered KDE estimation with normal kernels, and the bandwidth was always set to the optimal value for Gaussian data shown above.

### 1.1.3. Statistical classification

Pattern recognition is a branch of machine learning that has accepted multiple definitions over time [267]. In this thesis, we will assume a common accepted explanation of pattern recognition as a search for structure in data [25]. We are concerned in particular with one of the most common tasks in pattern recognition, the identification of a set of categories to which the data belong. The meaning of these categories -also known as sub-populations or classes) is dependent on the application, e.g., different approaches to e-learning, the diagnosis of a given disease, or the identity of a subject for access control purposes. There are four main approaches to pattern recognition: (i) template matching, (ii) statistical classification, (iii) syntactic or structural matching, and (iv) neural networks [118]. This thesis considers the second approach, statistical classification, in Chapter 4 and Chapter 6.

Statistical classification procedures typically include the following stages: (i) data preprocessing, (ii) mapping to the feature space, (iii) model learning, and (iv) decision making. The data pre-processing step de-noises the input data and improves their representation (normalization, de-trending...). These cleaned data are usually projected on a $D$-dimensional feature space defined by a number of "features," i.e., transforms of the data. The point of this representation is choosing a set of features that enhances the effectiveness of the classification. The model learning stage stablishes a set of decision boundaries (or regions) in the feature space that divide the data into classes. These boundaries are used for decision making purposes, classifying new data into the classes considered in the previous stages. This process is illustrated on a set of sample data in Figure 1.4. The pre-processing and feature extraction stages are identical for both sets of data, and the model learning stage determines the boundaries and methods that will be used during the decision making stage. An algorithm that implements this process is usually known as a "classifier." Some classifiers, however, only consider the last two stages (model learning and decision making). Another way to define a classifier is as a mapping from the observation/feature space to categories.

The feature extraction stage is expected to provide an adequate set of features for the following stages. The selection of the best set of features, which is known as feature selection, is a classical problem in pattern recognition. There have been many methods proposed to solve this problem, such as heuristic selection, information gain, and weight-based methods [106]. If the
number of selected features $(D)$ is large, the feature extraction stage is usually completed by a dimensionality-reduction method that alleviates the cost and complexity of the subsequent stages of the classifier. Many methods have been proposed for dimensionality reduction, although the most commonly used is principal component analysis (PCA, [124]).

The model learning stage estimates the boundaries between classes in the feature space, which are then used in the decision making stage to classify new data (i.e., assign each input observation to one of the classes). In this regard, classification can be thought of as an estimation problem (see Section 1.1.1): the parameters of the method or boundaries are estimated during the model learning stage, and the class of each new observation is estimated as well during decision making.

In statistical classification, the decision making process can be summarized as follows. A given observation $\mathbf{y}$ can be assigned to one of $K$ classes $C_{1}, \ldots, C_{K}$ depending on the $D$ feature values, grouped in feature vector $\mathbf{f}=\left[f_{1}, \ldots, f_{D}\right]^{T}$. The features are assumed to have a conditional probability density with respect to the classes, $p\left(\mathbf{f} \mid C_{k}\right), k=1, \ldots, K$. Therefore, each feature vector is treated as a realization of one of these conditional densities. Given these conditions, there are several possible decision rules to define the boundaries. Let us consider the Bayes decision rule, since it is the rule that will be considered in this work. The "optimal" Bayes decision rule for minimizing the conditional risk $R$ can be stated as

$$
\begin{equation*}
R\left(C_{k} \mid \mathbf{f}\right)=\sum_{j=1}^{K} L\left(C_{k}, C_{j}\right) \cdot P\left(C_{j} \mid \mathbf{f}\right) \tag{1.9}
\end{equation*}
$$

where $L\left(C_{i}, C_{j}\right)$ is the loss function associated with misclassifying an observation from class $C_{j}$ as pertaining to class $C_{i}$, and $P\left(C_{k} \mid \mathbf{f}\right)$ is the posterior probability of class $C_{k}$. If $L$ is replaced by the $0 / 1$ loss function (i.e., $L\left(C_{i}, C_{j}\right)=1$ if $i \neq j, 0$ otherwise), then the Bayes decision rule is simplified to selecting the class with highest posterior probability.

There have been multiples approaches to designing classifiers, depending on issues such as: (i) the knowledge of the posterior probabilities; (ii) the amount of labeled data; and (iii) if $P\left(C_{k} \mid \mathbf{f}\right)$ are unknown, the type of estimation of the densities. Figure 1.5 shows a classical classification of the most common approaches to statistical classification. The boxes shadowed in green indicate the approaches considered in Chapter 4 and Chapter 6 of this work.


Figure 1.4. Statistical classification process.


Figure 1.5. Approaches to statistical classification. Shadowed boxes indicate the approaches considered in this work.

### 1.1.3.a. Semi-supervised learning and classification

Traditionally, the statistical classification methods that assume no knowledge about the posterior probabilities have considered two types of learning: supervised or unsupervised.

Supervised learning assumes that all the observations used for model learning are labeled, i.e., we know to which class or category they belong. More formally, supervised learning assumes that there are $N$ independent and identically distributed (i.i.d.) observations $\mathbf{x}_{1}, \ldots, \mathbf{x}_{N}$, each one with their corresponding label $y_{1}, \ldots, y_{N}$. Within the context of statistical classification, the goal of supervised learning is estimating the posterior probabilities $P\left(C_{k} \mid \mathbf{f}\right)$ from the data, in order to solve (1.9). The knowledge of the labels simplifies the process, since a mapping can be evaluated through its predictive performance. In some applications, however, reliable data labeling is a costly and difficult task.

Unsupervised learning, on the other hand, determines decision boundaries based on unlabeled data. This is a much more difficult problem than supervised learning, however, since the data can reveal classes with different shapes and sizes, whose separation might not be trivial. Furthermore, the lack of labels means that there is no risk or error function that can be optimized for classification. In unsupervised learning, the estimated labels are used for modeling purposes (e.g., the hidden states of a hidden Markov model), rather than for any purpose that is observable in reality [50]. This makes it more similar to density estimation problems than to classification [126].

Semi-supervised learning (SSL) falls between supervised and unsupervised learning. As with supervised learning, it is assumed that there are $N$ i.i.d. observations $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}$, each one with their corresponding label $y_{1}, \ldots, y_{N}$. However, SSL also assumes that there are $N_{u}$ observations $\mathbf{x}_{N+1}, \ldots, \mathbf{x}_{N+N_{u}}$ whose labels are unknown. In order to use the information from unlabeled observations (i.e., generalize the information gained from labeled observations onto unlabeled ones), there must be some structure or smoothness to the data. If that is not the case, the performance of the classifier might degrade because of the unlabeled data. There are three main approaches to the structure assumption: (i) assume that if two points in a high-density region are close, so will their labels (smoothness assumption); (ii) assume that points tend to aggregate in clusters in such a way that points of the same cluster tend to be of the same class (cluster
assumption); and (iii) assume that the high-dimensional data lie on a lower-dimensional manifold, thus avoiding the curse of dimensionality that plagues many statistical estimation tasks (manifold assumption). These assumptions are rarely explicitly stated by SSL methods, and instead, they are usually implicit assumptions or consequences of the particular algorithm.

SSL methods can roughly be classified in four classes, depending on which assumptions they take: (i) generative models, which use the unlabeled observations as additional information for the marginal density of the observations (e.g., the EM algorithm); (ii) low-density separation methods, which "push" the decision boundaries away from unlabeled observations, thus considering the smoothness assumption or the clustering assumption (e.g., transductive SVM); (iii) graph-based methods, which employ the manifold assumption (e.g., mincut); and (iv) change of representation methods, which perform two-step learning (unsupervised with all observations, then supervised with only the labeled observations) in an application of the smoothness assumption (e.g., graph kernel by spectral transforms).

SSL is most useful in applications where there are far more unlabeled than labeled data. This is likely to occur if taking an observation is cheap, but labeling it costs a lot of time, effort, or money. There are many recent applications that follow this pattern, such as text on websites, speech samples, or protein sequences [290]. In this work, we apply semi-supervised learning on simulated data (Chapter 4) and on several sets of biomedical data (Chapter 6).

### 1.1.4. Non-linear dynamic modeling

Dynamic modeling is based on the assumption that there are hidden (stochastic) states that control the generating process behind the data that correspond to a non-stationary model. The states of the model could be continuous, as in Kalman filters, or discrete, as in hidden Markov models. We will center on the latter type, since the contributions in this work consider discrete states. Figure 1.6 shows a general dynamic model with discrete states, considering observations $\mathbf{x}_{t}$ and (hidden) states $y_{t}$. Such a system is characterized by the probabilities of emission of each observation, $p\left(\mathbf{x}_{t} \mid y_{t}\right)$, and the probabilities of transition between states, $p\left(y_{t+1} \mid y_{t}\right)$. This model could be considered a generalization of a mixture model where the classes are related to each other by some non-stationary process instead of being independent.

The dynamic model can be used to predict the future state of the process by estimating the probability density of the next state, $y_{t+1}$, with respect to the $t$ previous states and their corresponding observations $\mathbf{X}_{1: t}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{t}\right\}$. Assuming that the model has the Markov property $\left(P\left(y_{t+1} \mid y_{t}, y_{t-1}, \ldots, y_{1}\right)=P\left(y_{t+1} \mid y_{t}\right)\right)$, then:

$$
\begin{equation*}
P\left(y_{t+1} \mid \mathbf{X}_{1: t}\right)=\sum_{y_{t}} P\left(y_{t+1} \mid y_{t}\right) \cdot p\left(y_{t} \mid \mathbf{X}_{1: t}\right) \tag{1.10}
\end{equation*}
$$

Due to the Markov assumption, each state depends only on the immediately previous state. Therefore, the probability of future observations is


Figure 1.6. A basic dynamic model that relates hidden states, $y_{t}$, with observation vectors, $\mathbf{x}_{t}$.

$$
\begin{equation*}
P\left(\mathbf{x}_{t+1}, \ldots, \mathbf{x}_{t+k} \mid \mathbf{X}_{1: t}\right) \propto \sum_{y_{t+1}} p\left(\mathbf{x}_{t+1}, \ldots, \mathbf{x}_{t+k} \mid y_{t+1}\right) \cdot P\left(y_{t+1} \mid \mathbf{X}_{1: t}\right) \tag{1.11}
\end{equation*}
$$

for any $k>0$. Thus, calculating the probability of the observations at times $t+1$ through $t+k$ does not require knowledge of the previous observations $\mathbf{X}_{1: t}$, but only of the state of the system at time $t$. In order to incorporate higher order dependences, a representation of the form $\mathbf{Y}_{t}=\left[y_{t}, y_{t+1}, \ldots, y_{t+k}\right]^{T}$ can be considered. This expanded representation is considered throughout Chapter 4 of this thesis, where we consider the dependences between multiple Markov chains.

The dynamics of the system (transition probabilities and probability densities of the observations) can be used to implement linear or non-linear models. Linear models can be estimated using techniques such as expectation maximization (EM). In particular, HMM are most commonly estimated using the Baum-Welch algorithm [17], a particular implementation of the EM algorithm for hidden Markov models. The Baum-Welch algorithm uses dynamic programming to estimate the dynamics of the system in a fast manner. Nevertheless, system dynamics cannot be approximated linearly in many real problems, thus motivating the inclusion of non-linearities. There have been a number of approaches to non-linear dynamic models: using probabilistic priors plus parametric models [207]; particle filtering using a finite number of samples to represent the posterior distribution that are updated with new observation arrivals [37]; and approximating the posterior $P\left(\mathbf{y}_{t} \mid \mathbf{X}_{1: t}\right)$ by means of a mixture of distributions such as mixture of Gaussians (MoG, also known as GMM) [53]. Recent works by the GTS have proposed the use of non-Gaussian mixture models, using ICAMM in order to model the nonlinear part of the system dynamics [230]. Chapter 4 introduces a non-Gaussian mixture model that is extended to consider multiple chains of dependence.

There is an extensive range of applications for hidden state-based dynamic models. The objective is to exploit the sequential dependence of the data, which is inherent in many realworld problems, in a scheme of sequential pattern recognition. Some of the applications of HMM (the most common dynamic model) are the following: speech recognition [174], video event classification and image segmentation [166], people recognition [167], and human motion for robotics [145]. Of particular relevance is the application of HMM in event-related dynamics of brain oscillations [183] and, in general, in causality analysis of physiological phenomena. One example of these analyses is sleep staging, which is approached using radial basis function (RBF) networks and HMM for the classification of EEG recordings measured during afternoon naps in [139]. In Chapter 6, we address the sleep staging problem focusing on the analysis of arousal provoked by apnea.

### 1.2. Scope

The scope of this work is the exploration of new possibilities of non-Gaussian mixtures. Thus, new algorithms based on these mixtures will be designed for data estimation, feature extraction, semi-supervised or unsupervised learning, and sequential dynamic modeling. The interpolation algorithms will consider the use of non-Gaussian mixtures for the interpolation itself, unlike other works where it was used as a pre-processing step. Two criterions will be considered for this estimation: maximum likelihood and least mean square error. The modeling algorithms will consider sequential dynamic modeling, which can in turn be used for unsupervised (or semisupervised) learning and feature extraction. The proposed methods will expand on previous works and obtain general methods that combine several synchronized sets of data. The resulting methods will be thoroughly explained using appropriate and demonstrative examples. Results come from a large number of sets of synthetic and real data. Quantifiable evaluation will be obtained for synthetic data where the underlying patterns and distributions are known.

In addition to its theoretical developments, this works intends to demonstrate the suitability of the developed algorithms for real-world problems. The research carried out in this thesis is framed within the following projects of the Grupo de Tratamiento de Señal of the Universitat Politècnica de València:

- "Técnicas Avanzadas de Procesado de Señales EEG para el Estudio de Estructuras de Conectividad Cerebral," supported by Generalitat Valenciana (Regional Administration) under grant GV/2014/034.
- "Clasificación de Señales Multimodales: Algoritmos y Aplicaciones," supported by Universitat Politècnica de València under grant SP20120646.
- "Algoritmos para el Análisis de Modalidad de Señal: Aplicación en el Procesado Avanzado de Señales Acústicas," supported by the Spanish Administration under grant TEC2011-23403.
- "Procesador No-Lineal de Mezclas con Aplicación de Detección, Clasificación, Filtrado y Predicción," supported by the Spanish Administration under grant TEC2008-02975.
- "Muros: Desarrollo de Metodologías No Destructivas de Aplicación a Muros Históricos," supported by IMPIVA and Universitat Politècnica de València under grant IMIDIN/2008/7.

The aforementioned projects were concerned with developing software and applications for the purposes of: (i) brain analysis and diagnosis on neurology patients; and (ii) characterization of historical walls. In the first group, the non-Gaussian mixture techniques are used to detect changes in the electroencephalographic signal captured during a battery of neuropsychological tests. This system might be used to perform automatic diagnosis and evaluation of the subject's mental proficiency. In the second group of projects, the non-Gaussian mixtures are used to reconstruct damaged data or estimate data at uncaptured positions, thus increasing the capabilities of subsequent methods. Missing data is an important problem in several nondestructive testing applications (e.g., in GPR [43]), and these techniques could help to improve data.

### 1.3. Contributions

This thesis makes a number of contributions to the research in non-Gaussian mixtures. The three main contributions are: two novel methods for data estimation based on ICA mixture models; the introduction of a generalized model for sequential dependence in ICA mixture models; and the introduction of ICA and ICA mixture models in diverse novel applications. These applications are: reconstruction of damaged or missing ground-penetrating radar, reconstruction of damaged or missing seismic data, reconstruction of artifacted or missing EEG data, diagnosis of sleep disorders, and modeling of brain response during memory tasks. This work has inspired several publications, including conference and journal papers and a book chapter (see the publication list at the end of the thesis).

### 1.3.1. Interpolation based on ICA and ICA mixture models

Two novel methods based on ICA mixture models are proposed for the interpolation of missing values in the observation record. Although ICA has been used for data interpolation applications, it has been limited to the pre-processing stages of the interpolation process, to the best of our knowledge (e.g., [164]). The methods proposed in this thesis, however, consider the non-Gaussian mixture model as an integral part of the interpolation algorithm. These methods were obtained by considering two commonly-used estimation criteria: (i) maximum likelihood; (ii) least mean square error. The resulting methods were respectively named PREDICAMM (Prediction using ICAMM) and E-ICAMM (Expectation assuming ICAMM), respectively.

PREDICAMM performs estimation by maximizing the conditional likelihood of the data to be estimated, $\mathbf{z}$, with respect to known data, $\mathbf{y}$, and the model. In practice, this probability is
replaced by the joint likelihood, $p(\mathbf{z}, \mathbf{y})$, which can be found from the ICAMM. The maximization of any of these probabilities is equivalent and leads to the same solution (as explained in Section 1.1.1.a). This maximization is performed using a gradient ascent method. The resulting interpolation is robust with respect to the number of missing data in $\mathbf{z}$, although the initial point of the gradient must be selected carefully.

The second method, E-ICAMM, estimates missing data by minimizing the mean square error of the interpolation. This is done by calculating the optimal solution for this case, the conditional expectation of unknown data with respect to known data, $E[\mathbf{z |} \mid \mathbf{y}]$. Given the ICA mixture model, a closed-form solution can be obtained for this conditional expectation. The method is relatively fast and the solution is robust with respect to the number of missing data in $\mathbf{z}$. Furthermore, since both methods make the same assumptions and consider the same model, EICAMM can be used to obtain a starting point for the gradient step in PREDICAMM.

### 1.3.2. Sequential dynamic modeling

Previous works have presented a method that extends non-Gaussian mixtures to consider sequential dependence, SICAMM (Sequential ICAMM, [230]). This method consists of a sequential Bayes processor formulated from HMM theory, in which the ICAMM parameters and the class transition probabilities are used for classification. This thesis extends the method to consider several Markov chains in a coupled Hidden Markov model, with each class considering a (potentially different) ICA mixture model. This allows for greater generalization capabilities and the possibility to process multimodal data. We have named the resulting model G-SICAMM (Generalized SICAMM). Furthermore, we adapt two classical HMM classification algorithms, Baum-Welch [17] and Viterbi [270], for use with G-SICAMM.

Furthermore, this thesis presents a method for semi-supervised or unsupervised learning of the G-SICAMM parameters, which we have named UG-SICAMM. This allows estimating the model parameters using unlabeled data. Semi-supervised learning has been extensively studied for different classification frameworks and classical generative models such as transductive support vector machines, graph-based methods, hidden Markov random fields and Bayesian classifiers [50], and in the context of information-theoretic learning [121,77].

### 1.3.3. New applications of ICA and ICAMM

The contributions described in Section 1.3.1 and 1.3.2 are general-purpose, and therefore, can be applied to a wide range of applications. The design of an accurate model to "explain" a real physical phenomenon is a complex work. Indeed, such a work could become the focus of a thesis by and of itself. With this work, however, we intended to explore the possibilities of the extensions of non-Gaussian mixtures in several different fields. Thus, we have applied the developed methods to five real-world applications. The novelty and usefulness of the explored applications are guaranteed since they arise from the development of research and engineering projects (see Section 1.2). The contributions of this thesis for these real-world problems are explained below.

### 1.3.3.a. Reconstruction of data from a GPR survey of historical walls

In ground-penetrating radar surveys, the GPR device emits high-frequency waves into the medium under test at different locations and captures the reflections produced by discontinuities in the material (e.g., air-to-material interfaces) [68]. The resulting data form a B-Scan or radargram. The problem considered is the reconstruction of missing traces from the GPR BScan. Missing traces are a classical problem in GPR, and can occur for a number of reasons [68]. For this purpose, the B-Scan is transformed into a low-dimensional signal by preprocessing and an ICA mixture model is obtained. Then, E-ICAMM and PREDICAMM are
used to reconstruct the missing data in the radargram. This contribution presents the first application of ICAMM to the reconstruction of GPR data.

### 1.3.3.b. Reconstruction of seismic data from a seismic exploration survey

Seismic exploration is somewhat similar to GPR exploration. A typical reflection seismology survey, however, has a single source event or "shot" that emits low-frequency waves. Once the shot is generated, the reflections are then captured at the surface by groups of receivers, resulting in a B-Scan or seismogram [241]. The problem considered is the reconstruction of missing traces from the seismogram. Missing traces are a classical problem in seismic exploration, chiefly due to the large distances involved and the hostile terrain [241]. For this purpose, the B-Scan is transformed into a low-dimensional signal by pre-processing and an ICA mixture model is obtained. Then, E-ICAMM and PREDICAMM are used to reconstruct the missing data in the seismogram. This contribution presents the first application of ICAMM to the reconstruction of seismic data.

### 1.3.3.c. Reconstruction of EEG data

The problem in this application is the reconstruction of missing values from EEG data from subjects performing the Sternberg memory task. This can be used to reconstruct missing or artifacted data. ICA methods have been used in many applications on EEG data, such as removing artifacts [127]. However, the contributions of this thesis are unique in both the use of an ICA mixture model and the way in which the data are recovered. Results show the potential of E-ICAMM and PREDICAMM for the interpolation of EEG data. Furthermore, both methods show a large robustness with respect to the number of missing data, and can correctly interpolate a large number of missing or artifacted EEG channels at once.

### 1.3.3.d. Diagnosis of microarousals in sleeping subjects

The problem in this application is the detection of microarousals that occur during sleep due to apneas. The data consist of processing features extracted from 8-hour EEG signals from several subjects to estimate a two-class (wake-sleep) hypnogram. This work was initiated in [230,225], but this thesis extends previous works by considering several subjects and the contributions considered in Section 1.3.2. Results show the potential application of G-SICAMM for the implementation of an automatic classifier of EEG data from sleeping subjects. A more accurate detection of microarousals in the hypnogram will help to the medical diagnosis of sleep disorders [225].

### 1.3.3.e. Analysis of the brain memory function

This application introduces the use of the sequential dependence model in G-SICAMM to model the dynamic behavior of EEG signals during memory tasks. Aside from the contributions commented in Section 1.3.3.c, G-SICAMM is used to separate the data into two states (stimulus-answer) during each one of a battery of neuropsychological tests. The methods are tested on real data from several subjects, and they are shown to differentiate well between the two suggested states for all tests. In addition, the parameters of G-SICAMM show activations of several brain regions in consistence with the expected activations due to the neuropsychological tests. Therefore, it is proven that the estimated G-SICAMM parameters are able to determine brain connectivity patterns.

### 1.4. Overview

This thesis comprises seven chapters. Broadly speaking, they can be divided into introduction (Chapter 1), background (Chapter 2), theoretical contributions (Chapters 3 and 4), applications to real data (Chapters 5 and 6), and conclusions (Chapter 7). Chapter 2 deals with the theoretical foundations of non-Gaussian mixture processing methods. Since this work expands on the possible applications of these mixture models, a review of many different types of models is presented in this chapter. Some of the methods presented in this chapter are then compared with the methods proposed in this thesis.

The theoretical contributions of this thesis can be split into two categories, interpolation algorithms (Chapter 3) and dynamic modeling methods (Chapter 4). Chapter 3 introduces two novel non-linear interpolation methods that are based on ICA mixture models, named PREDICAMM and E-ICAMM. In ICAMM, observations are partitioned into several mutuallyexclusive classes, each one modeled by a different ICA model. This underlying model is used to interpolate unknown (or missing) values of the observation vector from the remaining known values of the same vector. Each of the proposed interpolation methods approached this problem in a different way. PREDICAMM seeks the maximum likelihood criterion, i.e., the reconstruction that maximizes the conditional probability density of unknown data with respect to known data. E-ICAMM, on the other hand, seeks the least mean square error criterion, i.e., minimizing the mean squared error of the reconstruction. Both methods are tested with an extensive set of experiments. These experiments consider their performance on data generated by an ICAMM, but also the reduction or alteration in performance incurred by any alterations of this underlying model. Results are discussed and compared with those of other interpolation methods, both classical and state-of-the-art.

Chapter 4 describes two new procedures for dynamic non-Gaussian modeling which are based on synchronized ICAMM. The starting point of this work is SICAMM, a method that incorporated a hidden Markov model to extend ICAMM to consider sequential dependence in the observations [230]. The proposed methods in this chapter extend the one Markov chain featured in SICAMM to a general framework to characterize the joint behavior of a number of synchronized dynamic models or "chains." We have named these methods G-SICAMM and UG-SICAMM. The latter maximizes the log-likelihood of the model with respect to all of the available training data and the parameters of the model, and can work with unsupervised or semi-supervised data. The methods are validated using several experiments on simulated data. These experiments consider both stationary and dynamically-changing data, thus testing the limitations of the proposed methods and performing sensitivity analysis. Results are discussed and compared with those of a commonly-used modeling method, Bayesian networks.

The methods developed in Chapters 3 and 4 are considered for real applications in Chapters 5 and 6 , respectively. Chapter 5 shows the application of E-ICAMM and PREDICAMM for reconstruction of three types of data. The first application is based on non-destructive testing signals from ground-penetrating radar experiments. These signals are usually B-Scans, so they are first converted to low-dimensional signals using a process common in applications of ICA to image processing (e.g., [111]). The performance of the proposed methods is tested on simulated data and on real GPR data from a survey on replicas of historical walls, and compared with that of Kriging, Wiener structures, and splines. The second application considers the reconstruction of seismic data from a reflection seismology survey. These signals are somewhat similar to GPR, but they are more complex because they cover a larger area and the terrain is more hostile. As with GPR, the signals are converted to low-dimensional signals and then used for the interpolation experiment. The performance of E-ICAMM and PREDICAMM is compared with that of Kriging, Wiener structures and splines. In the third application, the proposed methods are used to reconstruct missing data from an electroencephalogram, a recording of the brain electrical activity on the scalp. The EEG were captured from subjects that were performing the Sternberg memory task. The proposed methods were compared with spherical splines, a
commonly-used method for interpolating EEG data. In all three applications, E-ICAMM and PREDICAMM outperform the methods with which they are compared. Furthermore, it is shown that both methods are highly resistant with respect to the number of missing data, and can perform well even if a high number of values are missing from each observation.

Chapter 6 includes three applications of the methods developed in Chapter 4 to the modeling of real EEG data. The first application considers the use of dynamic models for detection of microarousals caused by apneas during sleep. These abrupt changes are registered in a diagram known as "hypnogram," which shows the different sleep stages during the night. Long EEG records from apnea patients are analyzed, with the intention of detecting microarousals. The classification obtained by the proposed methods outperforms that of dynamic Bayesian networks. The second application analyzes EEG data taken from subjects performing the Sternberg memory task. The proposed methods are used to model the transitions in the EEG during the stages of the experiment. Results show the sensitivity of the G-SICAMM parameters to the stages of the experiment, which allow for accurate detection. The third application considers EEG data taken from epilepsy patients during a battery of neuropsychological tests.
The proposed methods are used to differentiate EEG taken during stimulus presentation from data taken during the responses of the subjects. The methods from Chapter 4 are shown to overperform dynamic Bayesian networks for this task. Furthermore, the G-SICAMM parameters are used to model the EEG and analyze the behavior of the brain during these experiments.

Chapter 7 completes the thesis with the conclusions and findings, as well as discussion of the remaining open questions and future directions of research.

Finite mixture models with non-Gaussian components

## Chapter 2 - Finite mixture models with non-Gaussian components

### 2.1. Introduction

This chapter presents theoretical foundations on data modeling using finite mixture models (FMM) of non-Gaussian distributions. Particularly, the independent component analysis mixture model that is used in the developments of this work is reviewed in detail. A FMM is a convex combination of two or more probability density functions. Thus, the combination of the individual PDF properties allows for the approximation of arbitrary distributions. FMM has been used in many fields of statistical analysis and machine learning such as modeling, clustering, and classification. There exists an extensive literature of FMM and its applications from the first known work in modern statistical literature [184] until today [170,88,171]. The flexibility of using different kinds of basic PDFs makes FMM suitable for modeling the geometry of complex data. A mixture model is able to model quite different complex distributions through an appropriate choice of its components to accurately represent the local areas of the true distribution. It can handle situations where a single parametric family is unable to provide a satisfactory model for local variations in the observed data. Depending on the application field, the geometry of the data can be defined using one (univariate) or several (multivariate) random variables.

Briefly, let $X=\left[X_{1}, \ldots, X_{L}\right]$ be an $L$-dimensional continuous random variable and $\mathbf{x}=\left[x_{1}, \cdots, x_{L}\right]^{T}$ be an observation vector of $X$, where $T$ means transposition. The PDF of a mixture model is defined by a convex combination of $K$ component PDFs [170],

$$
\begin{equation*}
p_{k}(\mathbf{x} \mid \boldsymbol{\Theta})=\sum_{k=1}^{K} \alpha_{k} p_{k}\left(\mathbf{x} \mid \boldsymbol{\theta}_{k}\right) \tag{2.1}
\end{equation*}
$$

where $p_{k}(\mathbf{x} \mid \boldsymbol{\Theta})$ is the PDF of the $k$-th component, $\alpha_{k}$ is the corresponding mixing proportion (or component prior), and $\boldsymbol{\Theta}=\left[\alpha_{1}, \ldots, \alpha_{K}, \theta_{1}, \ldots, \theta_{K}\right]^{T}$ is the vector of set of parameters. We assume that $\alpha_{k} \geq 0$, for $k \in\{1, \ldots, K\}$, and $\sum_{k=1}^{K} \alpha_{k}=1$. By the property of convexity, given that each $p_{k}\left(\mathbf{x} \mid \boldsymbol{\theta}_{k}\right)$ defines a PDF, $p(\mathbf{x} \mid \boldsymbol{\Theta})$ will also be a PDF.

The intuitive interpretation of mixture models is that the random variable $X$ is produced from $K$ distinct random generators. Each of these generators is modeled by the density $p_{k}\left(x \mid \theta_{k}\right)$, and $\alpha_{k}$ represents the proportion of observations from this particular generator. In practice, an obvious application of FMM is identifying each of the components of the mixture with real existing groups whose corresponding data follow different distributions. Nevertheless, there are many examples where the components cannot be identified as above. In this situation, the components are introduced to allow for greater flexibility in modeling a heterogeneous population, in other words to model arbitrarily complex PDFs.

The most popular mixture model is the one consisting of Gaussian components, GMM (see for instance [170]). The power of GMM to approximate different kind of data is sufficiently demonstrated. However, there are no statistical characteristics in GMM that allow differentiating one component from each other and even relating them with the observed phenomenon where the data come from. Considering this, we have selected ICAMM for data modeling [225]. There are many applications of non-Gaussian models for the univariate case, such as: applying parametric models such as mixture of Poisson distributions used in positron emission tomography [265] and document classification in information retrieval [158]; considering von Mises-Fisher distributions for the analysis of text and gene expressions [14]; handling outliers applied to measurements of geyser eruption lengths using mixtures of $t$ distributions [170]; and using mixtures of truncated exponential potentials as an alternative to discretization and Monte Carlo methods for solving hybrid Bayesian networks [57].

When $X$ is heterogeneous across and homogeneous within the $K$ components, i.e., $X$ has a different probability distribution in each component, it can be assumed that data arise from the same parametric family $p(\mathbf{x} \mid \boldsymbol{\Theta})$, with the parameter $\boldsymbol{\Theta}$ differing between components.
Another potential assumption is to consider a hybrid situation where the components arise from different parametric distributions [88]. In addition, a parametric approach could be unable to model the heterogeneity of the data, and thus a nonparametric kernel estimate could be proposed [239].

The extension of univariate FMM to the multivariate case has to deal with two problems: (i) to model the relationship between the variables (dependence), and (ii) to preserve the individual statistical characteristics (namely, the marginal PDFs) of the components. In addition, the use of different kinds of basic distributions to form the components also has to be considered for total generalization. Figure 2.1 shows a scheme of different approaches to design multivariate nonGaussian mixture models. There are two main options. The first one consists of modeling each of the components independently using univariate non-Gaussian mixture modeling based on a specific kind of distribution. Thus, dependences or associations between the variables are not considered and the multivariate PDF will simply be the product of all the univariate PDFs,

$$
\begin{equation*}
p(\mathbf{x} \mid \boldsymbol{\Theta})=\sum_{k_{1}=1}^{K_{1}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L}=1}^{K_{L}} \alpha_{k_{1}} \cdot \alpha_{k_{2}} \cdots \alpha_{k_{k_{L}}} \cdot p_{k_{1}}\left(\mathbf{x}_{1} \mid \boldsymbol{\theta}_{k_{1}}\right) \cdot p_{k_{2}}\left(\mathbf{x}_{2} \mid \boldsymbol{\theta}_{k_{2}}\right) \cdots p_{k_{L}}\left(\mathbf{x}_{L} \mid \boldsymbol{\theta}_{k_{L}}\right) \tag{2.2}
\end{equation*}
$$

In the second option, when statistical independence cannot be assumed, there are two main approaches (see Figure 2.1) that generally follow a transformation $\zeta$ of some latent variables $\mathbf{s}$ derived from the explicit variables $\mathbf{x}$,

$$
\begin{equation*}
p(\mathbf{x} \mid \boldsymbol{\Theta}) \propto p(\zeta(\mathbf{s}) \mid \boldsymbol{\Theta}) \tag{2.3}
\end{equation*}
$$

The first approach is based on theory of copulas [182]. A copula is a multivariate PDF of uniform variables derived from the explicit variables that is used to model the dependence. There are many possibilities to define a multidimensional function that has the required
properties to be a copula. For instance, the multivariate PDF can be factorized into a copula function multiplied by the marginals (see Sklar's theorem [245]). The second approach assumes that the explicit variables are obtained by a transformation of some independent latent (hidden) variables. A relevant example of latent variable modeling is independent component analysis, which allows different kinds of distributions to be mixed in the model components. Mixtures of ICAs enhance the versatility of using only one ICA for multivariate non-Gaussian mixture modeling and will be the base for this work. In addition, there are other models that consider statistical dependence that are constrained to specific kinds of variables, for example FMM for multivariate binary and categorical data [88].

Several methods have been proposed to estimate the parameters of a FMM. They can be roughly organized into five classes depending on the assumptions considered: graphical methods, method of moments, minimum-distance methods, maximum likelihood, and Bayesian approaches. It is well known that explicit formulas for parameter estimation are typically not available. For example, there is not a closed-form expression of the maximum likelihood estimate of the mixing proportions and the component means and variances/covariances for GMM. Thus, the estimation of these parameters has to be computed iteratively; for instance, using the expectation-maximization algorithm [72].

Besides parameter estimation, there are several issues related with FMM that can be of much theoretical and practical importance, including the following: modeling of asymmetrical data; testing the number of components; identifiability of the mixture distributions; extending mixture models to the analysis of dependent data using hidden Markov models; dealing with incomplete-data structure of mixture problem; and semi-parametric formulation of the mixture model. For a comprehensive survey of the results and developments in FMM we refer the readers to $[170,88,171]$ and the references therein. In this thesis, we will focus on parameter estimation for new ICAMM-based methods applied to the problems of prediction and dynamic analysis modeling.

The rest of the chapter is organized as follows. Section 2.2 includes a review of some of the most relevant parametric univariate non-Gaussian mixtures. Section 2.3 explains the basis of the latent variable modeling and the different approaches employed for ICA. Section 2.4 deals with the principal ICAMM methods that are currently in use. Finally, Section 2.5 includes the conclusions of the chapter.


Figure 2.1. Scheme of multivariate finite mixture models.

### 2.2. Univariate non-Gaussian mixtures

Figure 2.2 shows some examples of univariate non-Gaussian mixtures where each mixture is composed by three components of the same kind of distribution. It can be seen that the mixture is able to suit data with different shapes of distributions than the original components. In this section exponentials, Poisson, binomial, and multinomial univariate mixtures are reviewed.

### 2.2.1. Mixtures of Exponential Distributions

The exponential distribution, $x \sim \varepsilon(\beta)$ with $\beta>0$, is a univariate distribution defined on the positive real line $x \geq 0$ and is mainly used as a sampling distribution in the context of finite mixture models. There exist different ways to parameterize this distribution, e.g., by defining the density as [22]

$$
\begin{equation*}
p_{\varepsilon}(x ; \beta)=\beta e^{-\beta x} \tag{2.4}
\end{equation*}
$$

where mean and variance are given by $E(X)=\operatorname{Var}(X)=1 / \beta$. In this parameterization, the exponential distribution is equal to the Gamma distribution $X \sim G(\delta, \beta)$ with $\delta=1$, which is defined as $p_{G}(x ; \delta, \beta)=\frac{\beta^{\delta}}{\Gamma(\delta)} x^{\delta-1} e^{-\beta x}$ and $\mathrm{E}(X)=\frac{\delta}{\beta}, \operatorname{Var}(X)=\frac{\delta}{\beta^{2}}$ for $\delta>0$ and $\beta>0$.

Thus, nonnegative observations can be assumed as realizations of a random variable $X$ arising from a finite mixture of exponential distributions (MED):


Figure 2.2. Examples of univariate non-Gausian mixtures.

$$
\begin{equation*}
X \sim \alpha_{1} \varepsilon\left(\beta_{1}\right)+\cdots+\alpha_{K} \varepsilon\left(\beta_{K}\right) \tag{2.5}
\end{equation*}
$$

where $\varepsilon\left(\lambda_{k}\right)$ is parameterized as (2.4). Thus, this mixture is parameterized in terms of the parameters $\boldsymbol{\Theta}=\left[\beta_{1}, \cdots, \beta_{K}, \boldsymbol{\alpha}^{T}\right]^{T}$.

The parameters of a MED can be estimated by methods such as moments, Bayesian, and classical tests. For instance, Bayesian estimation using data augmentation and Markov chain Monte Carlo methods can be easily implemented based on the prior $\lambda_{k} \sim G\left(a_{0}, b_{0}\right)$, the complete-data posterior $p\left(\lambda_{k} \mid \mathbf{x}, \mathbf{S}\right)$ ( $\mathbf{S}$ is a vector with the component labels) is given by $\lambda_{k} \mid \mathbf{x}, \mathbf{S} \sim G\left(a_{k}(\mathbf{S}), b_{k}(\mathbf{S})\right), \quad$ where: $\quad a_{k}(\mathbf{S})=a_{0}+N_{k}(\mathbf{S}), \quad$ and $\quad b_{k}(\mathbf{S})=b_{0}+\sum_{i: S} x_{i} x_{i}$. Several
theoretical and application issues of mixtures of exponential distributions are currently finding the best bounds for mixtures of order statistics from independent heterogeneous exponential random variables [196]; inference about the number of components [173]; and general probabilistic interpretation of the exponential mixture [134].

Recently, mixtures of truncated exponentials (MTE) were introduced as a model for dealing with discrete and continuous variables simultaneously in Bayesian networks without imposing any restriction on the network topology and avoiding the rough approximations of methods based on the discretization of the continuous variables [148]. The MTE model is defined by its corresponding potential and density [148].

MTE potential: Let $\mathbf{X}$ be a mixed $n$-dimensional random vector. We say that a function $f: \Omega_{\mathrm{x}} \rightarrow \mathrm{R}_{0}^{+}$is an MTE potential if one of two conditions holds: (i) $f$ can be written as $f(\mathbf{x})=a_{0}+\sum_{i=1}^{m} a_{i} \exp \left\{\sum_{j=1}^{n} b_{i}^{(j)} x_{j}\right\}$ for all $\mathbf{x} \in \Omega_{\mathbf{x}}$, where $a_{i}, i=0, \ldots, m$ and $b_{i}^{(j)}, j=1, \ldots, n$ are real numbers; (ii) there is a partition $\Omega_{1}, \cdots, \Omega_{k}$ of $\Omega_{\mathrm{x}}$ verifying that the domain of the continuous variables in $\mathbf{X}$ is divided into hypercubes and such that $f$ is defined as $f(\mathbf{x})=f_{i}(\mathbf{x})$ if $\mathbf{x} \in \Omega_{i}$.

MTE density: an MTE potential $f$ is an MTE density if $\sum_{y \in \Omega_{\mathbf{y}}} \int_{\Omega_{\mathbf{z}}} f(\mathbf{y}, \mathbf{z}) d \mathbf{z}=1$, where $\mathbf{Y}$ and $\mathbf{Z}$ are the discrete and continuous coordinates of $\mathbf{X}$, respectively.

A practical example of application of this mixture is the assessment of groundwater quality through probabilistic clustering based on hybrid Bayesian networks with MTEs [3].

### 2.2.2. Mixtures of Poisson distributions

The Poisson distribution, $X \sim P(\mu)$ with $\mu>0$, is defined for $x \in\{0,1,2, \ldots\}$, making it a standard distribution to model a random count variable. Density, mean, and variance are given by $p_{\mathrm{P}}(x ; \mu)=\frac{\mu^{x}}{x!} e^{-\mu}, E(X)=\operatorname{Var}(X)=\mu$. Thus, a model for describing the distribution of count data can be defined assuming $x_{1}, \ldots, x_{N}$ independent realizations of a random variable $X$ from a mixture of Poisson distributions (MPD):

$$
\begin{equation*}
X \sim \alpha_{1} \mathrm{P}\left(\mu_{1}\right)+\cdots+\alpha_{K} \mathrm{P}\left(\mu_{K}\right) \tag{2.6}
\end{equation*}
$$

This mixture is parameterized in terms of $2 K-1$ distinct model parameters $\boldsymbol{\Theta}=\left[\mu_{1}, \ldots, \mu_{K}, \boldsymbol{\alpha}^{T}\right]^{T}$. For an MPD is easy to verify that the complete-data maximum likelihood estimator of $\mu_{k}$ is equal to the sample mean in group $k, \hat{\mu}_{k}=\bar{x}_{k}(\mathbf{S})$, under the assumption that the allocations (group indicators, variables that take values in the set $1, \ldots, K$ ) $\mathbf{S}=\left[S_{1}, \ldots, S_{N}\right]^{T}$ are observed as well. The complete-data ML estimator lies in the interior of the parameter space, if each group is nonempty $\left(N_{k}(S)>0\right)$ and contains at least one nonzero observation. Asymptotic $95 \%$ confidence intervals for $\mu_{k}$ are equal to $\bar{x}_{k}(\mathbf{S}) \pm 1.96 \sqrt{\bar{x}_{k}(\mathbf{S}) / N_{k}(\mathbf{S})}$, where the expected Fischer information has been evaluated at $\mu_{k}=\bar{x}_{k}(\mathbf{S})$. The effective coverage probability may be considerable smaller, if the sample size $N$ and the true values of $\mu_{k}$ and $\alpha_{k}$ are very small where asymptotic $95 \%$ confidence intervals are compared with Bayesian confidence intervals. Also the parameters of a MPD can be estimated by moments, data augmentation and Markov chain Monte Carlo, and distance-based methods.

The applications of MPDs include quite different issues such as counts of fish species abundant in a lake [237] and representation of protein abundance levels [141].

### 2.2.3. Mixtures of binomial distributions

For binomial mixtures, the component densities arise from BiNom $(T, \pi)$ distributions, where $T$ is commonly assumed to be known, whereas the component-specific probabilities $\pi$ are unknown and heterogeneous:

$$
\begin{equation*}
X \sim \alpha_{1} \operatorname{BiNom}\left(T, \pi_{1}\right)+\ldots+\alpha_{K} \operatorname{BiNom}\left(T, \pi_{K}\right) \tag{2.7}
\end{equation*}
$$

The density of this mixture is given by

$$
\begin{equation*}
p(x \mid \boldsymbol{\Theta})=\sum_{k=1}^{K} \alpha_{k}\binom{T}{x} \pi_{k}^{x}\left(1-\pi_{k}\right)^{T-x} \tag{2.8}
\end{equation*}
$$

with $\boldsymbol{\Theta}=\left[\pi_{1}, \ldots, \pi_{K}, \boldsymbol{a}^{T}\right]^{T}$. Mixtures of binomial distributions (MBD) are not necessarily identifiable; a necessary and sufficient condition is $T \geq 2 K-1$. MBD may be extended to the case where $T_{i}$ varies between the realizations $x_{1}, \ldots, x_{N}$ as follows:

$$
\begin{equation*}
p\left(x_{i} \mid \boldsymbol{\Theta}\right)=\sum_{k=1}^{K} \alpha_{k}\binom{T_{i}}{x_{i}} \pi_{k}^{y_{i}}\left(1-\pi_{k}\right)^{T_{i}-x_{i}} \tag{2.9}
\end{equation*}
$$

Bayesian inference for MBD is considered in [33] by applying a Metropolis-Hastings algorithm. Bayesian estimation using data augmentation and Markov chain Monte Carlo can be implemented to estimate an MBD by using the conjugate Beta prior $\pi_{k} \sim B\left(a_{k}(\mathbf{S}), b_{k}(\mathbf{S})\right)$, and the posterior $p\left(\pi_{k} \mid \mathbf{x}, \mathbf{S}\right)$ is again a Beta distribution, $\pi_{k} \mid \mathbf{x}, \mathbf{S} \sim B\left(a_{k}(\mathbf{S}), b_{k}(\mathbf{S})\right)$, where $a_{k}(\mathbf{S})=a_{0}+\sum_{i: S_{i}=k} x_{i}, b_{k}(\mathbf{S})=b_{0}+\sum_{i: S_{i}=k}\left(T-x_{i}\right)$.

MBD has been applied to problems involving binary data, e.g., estimating the trend of extreme weather from rain data using a global climate model [38] and improving aquatic warbler population assessment by accounting for imperfect detection [191].

### 2.2.4. Mixtures of multinomial distributions

Consider a categorical variable of more than two categories $\{1, \ldots, D\}$. Let $X_{l}$, for $l=1, \ldots, D$, be the number of occurrences of category $l$ among $T$ trials. If the occurrence probability distribution $\pi=\left[\pi_{1}, \ldots, \pi_{D}\right]^{T}$ of each category is homogeneous among the observed data vectors, then

$$
\begin{equation*}
\mathbf{x}=\left[X_{1}, \ldots, X_{D}\right] \sim \operatorname{MulNom}(T, \boldsymbol{\pi}) \tag{2.10}
\end{equation*}
$$

To deal with unobserved heterogeneity in the occurrence probability of the various categories, $\mathbf{x}=\left[X_{1}, \ldots, X_{D}\right]$ can be assumed to follow a finite mixture of multinomial distributions (MMD),

$$
\begin{equation*}
X \sim \alpha_{1} \operatorname{MulNom}\left(T, \boldsymbol{\pi}_{1}\right)+\cdots+\alpha_{\kappa} \operatorname{MulNom}\left(T, \boldsymbol{\pi}_{\kappa}\right) \tag{2.11}
\end{equation*}
$$

with $\pi_{k}=\left[\pi_{k, 1}, \ldots, \pi_{k, D}\right]^{T}$ being the unknown occurrence probability in group $k$. The density is given by

$$
\begin{equation*}
p(\mathbf{x} \mid \boldsymbol{\Theta})=\sum_{k=1}^{K} \alpha_{k}\binom{T}{\alpha_{1} \cdots \alpha_{D}} \prod_{l=1}^{D} \pi_{k, l}^{x_{i}} \tag{2.12}
\end{equation*}
$$

where $\boldsymbol{\Theta}=\left[\boldsymbol{\pi}^{T}, \ldots, \boldsymbol{\pi}^{T}{ }^{T}, \boldsymbol{a}^{T}\right]^{T}$ are the parameters of the mixture.
Bayesian estimation of the MMD parameters can be implemented based on the Dirichlet prior $\pi_{k} \sim D\left(a_{0,1}, \ldots, a_{0, D}\right)$, and the posterior $p\left(\boldsymbol{\pi}_{k} \mid \mathbf{x}, \mathbf{S}\right)$ is again a Dirichlet distribution $\pi_{k} \mid \mathbf{x}, \mathbf{S} \sim D\left(a_{0,1}(\mathbf{S}), \ldots, a_{0, D}(\mathbf{S})\right)$, where $a_{k, l}(\mathbf{S})=a_{0, l}+\sum_{i, S=k} x_{i i}, l=1, \ldots, D$.
Some of the recent applications of MMD include the following: learning multinomial mixture models for text document classification based on the large margin criterion [122] and solving the problem of age-invariant face recognition [29].

### 2.3. Multivariate non-Gaussian

In this section, the main definitions and applications of the copula method and latent variable modeling are reviewed. These techniques are flexible tools for PDF modeling. They allow both independence and dependence among variables to be jointly modeled for multivariate nonGaussian distribution mixtures. In particular, the principles of the LVM method called independent component analysis are explained and discussed, since they will be used to derive the theoretical contributions of this thesis.

### 2.3.1. Copula functions

The first reference to copula functions is included in [245] as a link between multidimensional PDFs and marginal PDFs. The copula represents multivariate PDFs whose univariate marginal PDFs are uniform in the interval $[0,1]$. Copula functions can be used to describe the dependence between random variables, i.e., the manner in which the variables covariate. The marginal PDFs describe the behaviour of each of the components separately and the copula function describes the dependence structure among these components. Several kinds of copulas are defined in the literature to describe different kind of dependence [165]. The copulas have
been extensively used in the field of econometrics and finance (see [203] and the references therein), and there are also a few applications in signal processing [117,256,254].

The copula function is defined by Sklar's theorem [245] considering the following. The joint probability distribution $F\left(x_{1}, x_{2}, \ldots, x_{D}\right)$ of a number of random variables $X_{1}, X_{2}, \ldots, X_{D}$ can be expressed from the marginal probability distributions associated to each of the random variables $F_{i}\left(x_{i}\right), i=1, \ldots, D$, as follows:

$$
\begin{equation*}
F\left(x_{1}, x_{2}, \cdots, x_{D}\right)=C\left(F_{1}\left(x_{1}\right), F_{2}\left(x_{2}\right), \cdots, F_{D}\left(x_{D}\right)\right)=C\left(U_{1}, \cdots, U_{D}\right) \tag{2.13}
\end{equation*}
$$

By applying the probability integral transform to each original variable, uniformly distributed marginals $U_{1}, \ldots, U_{D}$ are obtained, which are random variables with components $u_{i}$ defined as $u_{i}=F_{i}\left(x_{i}\right)$, where $F_{i}$ is the probability distribution function of $x_{i}$.

The function $C$ is termed the copula function, which is a joint PDF of uniformly distributed random variables in the interval $[0,1]$. Thus, the copula function is defined in the unitary cube $C: U\left(\begin{array}{ll}0 & 1\end{array}\right)^{D} \rightarrow\left(\begin{array}{ll}0 & 1\end{array}\right)$. The details of this theorem and the properties of copula functions can be found in [245,203].

If the copula function $C$ and the marginal distributions $F_{i}$ are sufficiently differentiable, the joint multivariate PDF can be obtained as the product of the marginals $f_{i}$ (independence) and the copula function of density $c$ (dependence) derived from $c$. For continuous distributions, the joint PDF is obtained as

$$
f\left(x_{1}, x_{2}, \cdots, x_{D}\right)=\underbrace{f_{1}}_{\begin{array}{c}
\text { independence (marginal distributions) }  \tag{2.14}\\
\text { complementary information }
\end{array}} \underline{x}_{1}) \cdot f_{2}\left(x_{2}\right) \cdots \cdots f_{D} f_{D}) \cdot \underbrace{c\left(F_{1}\left(x_{1}\right), F_{2}\left(x_{2}\right), \cdots, F_{D}\left(x_{D}\right)\right)}_{\begin{array}{c}
\text { dependence (copula function) } \\
\text { common information }
\end{array}}
$$

where $c(\mathbf{u})=\frac{\partial^{D}\left(c\left(u_{1}, u_{2}, \cdots, u_{D}\right)\right)}{\partial u_{1} \partial u_{2}, \cdots, \partial u_{D}}, u_{i}=F_{i}\left(x_{i}\right)$. The copula function of density $c(\cdot)$, in this case, is a PDF of uniformly distributed random variables. If the random variables were independent, the joint PDF would be the product of the marginal densities:

$$
f\left(z_{1}, z_{2}, \cdots, z_{D}\right)_{\text {inderependent }}=\prod_{i=1}^{D} f_{i}\left(z_{i}\right) .
$$

In order to parameterize the joint PDF defined as in (2.14), we have to find two sets of parameters, those related with the marginals and those related with the copula function (the parameters that model the dependence):

$$
\begin{equation*}
f\left(x_{1}, x_{2}, \cdots, x_{D} \mid \boldsymbol{\Theta}\right)=\left(\prod_{i=1}^{D} f_{i}\left(\mathbf{x}_{i} ; \boldsymbol{\varphi}_{i}\right)\right) \cdot c\left(F_{1}\left(x_{1} / \boldsymbol{\varphi}_{i}\right), F_{2}\left(x_{2} / \boldsymbol{\varphi}_{2}\right), \cdots, F_{D}\left(x_{D} / \boldsymbol{\varphi}_{D}\right) / \boldsymbol{\Lambda}\right) \tag{2.15}
\end{equation*}
$$

Thus, the multivariate model is parameterized by the set of parameters $\boldsymbol{\Theta}$, which can be divided in two subsets: $\varphi$ to model the marginals and $\boldsymbol{\Lambda}$ to model the structure of the dependence. Assuming that $x_{i}=F_{i}^{-1}\left(u_{i} \mid \boldsymbol{\varphi}_{i}\right)$, the copula function for the multivariate model $f\left(x_{1}, \ldots, x_{D} \mid \boldsymbol{\Theta}\right)$ can be estimated as

$$
\begin{equation*}
c\left(u_{1}, \cdots, u_{D} \mid \boldsymbol{\Lambda}\right)=\frac{f\left(F_{1}^{-1}\left(u_{1} \mid \boldsymbol{\varphi}_{1}\right), \cdots, F_{D}^{-1}\left(u_{D} \mid \boldsymbol{\varphi}_{1}\right) \mid \boldsymbol{\Theta}\right)}{\left(\prod_{i=1}^{D} f_{i}\left(F_{i}^{-1}\left(u_{i} \mid \boldsymbol{\varphi}_{i}\right) \mid \boldsymbol{\varphi}_{i}\right)\right)} \tag{2.16}
\end{equation*}
$$

Let us consider a set of random variables $X_{1}, X_{2}, \cdots, X_{D}$, with unknown joint PDF $f\left(x_{1}, x_{2}, \ldots, x_{D}\right)$. Since the real multivariate model expression that suits the set of variables is unknown, the expression for the copula density $c(\cdot)$ is unknown. Let us assume that the marginals PDFs associated to each of the random variables are known and $f\left(x_{1}, x_{2}, \ldots, x_{D}\right)$ has the same properties of dependence between the random variables as another known model $f\left(x_{m_{1}}, x_{m_{2}}, \ldots, x_{m_{D}}\right)$ whose copula density function $c_{m}\left(u_{1}, \cdots, u_{D}, \boldsymbol{\Theta}_{m}\right)$ is known. Then, $\hat{f}(\mathbf{x} \mid \hat{\boldsymbol{\Theta}})$ is the estimate of the joint PDF using the copula density function $c_{m}(\cdot)$ associated with another model $f_{m}\left(\mathbf{x}_{m} \mid \boldsymbol{\Theta}_{m}\right)$, which shares the same characteristics of dependence:

$$
\begin{gather*}
f(\mathbf{x} / \boldsymbol{\Theta}) \sim \hat{f}(x \mid \hat{\boldsymbol{\Theta}})=\left(\prod_{i=1}^{D} f_{i}\left(\mathbf{x}_{i} ; \boldsymbol{\varphi}_{i}\right)\right) \cdot c\left(F_{1}\left(x_{1} \mid \boldsymbol{\varphi}_{i}\right), F_{2}\left(x_{2} \mid \boldsymbol{\varphi}_{2}\right), \cdots, F_{D}\left(x_{D} \mid \boldsymbol{\varphi}_{D}\right) \mid \hat{\boldsymbol{\Lambda}}\right),  \tag{2.17}\\
\hat{\boldsymbol{\Theta}}=\left\{\boldsymbol{\varphi}, \hat{\boldsymbol{\Lambda}}=\left\{\boldsymbol{\varphi}_{m}, \boldsymbol{\Lambda}_{m}\right\}\right\}
\end{gather*}
$$

Figure 2.3 shows an example of a multivariate data with two dependent random variables whose marginals are known and different, but whose joint PDF is unknown. If we consider only the marginal contribution (i.e., consider that the variables are independent), the obtained PDF does not fit the real PDF. By using a bivariate normal, we can obtain the copula density function that models the linear dependence between the variables.

The parameters of the multivariate copula function are usually estimated using maximum likelihood methods, assuming that regularity conditions of asymptotic distribution of maximum likelihood estimation are accomplished (both for copula and marginal densities). Examples of those methods are inference functions for margins (IFM) and canonical maximum likelihood [31]. The selection of a suitable copula density function for an application is not straightforward since the dependence properties of the random variables are a priori unknown. Thus, a selection from a set of different copula function should be done. Minimum description length (MDL) is a framework very employed to select the optimum copula model. The following selection criteria


Figure 2.3. Example of PDF modeling of two random variables using copulas.
can be applied in MDL: Akaike information criterion (AIC), Bayesian information criterion (BIC), stochastic information complexity (SIC), and normalized maximum likelihood (NML). These criteria try to calculate a relative index that takes into account the tradeoff between model performance and increase of complexity.

The copula function itself can be derived from known PDFs such as multivariate Gaussian, multivariate $t$-Student, and mixtures of Gaussians. These copulas are called elliptic because the contour curves of the random variables form ellipses representing symmetric dependence relations [260]. Another family of copula functions are the so-called "Archimedean" that allow the dependency in high variable dimension to be modeled using only one parameter. Examples of this family are Clayton, Frank, and Gumbel copulas [172]. All of these methods model specific dependency structures, expect GMM, which is able to model many structures of arbitrary dependency. A more general method consists of using a hierarchical procedure where the dependency is calculated for every pair of variables forming a copula tree that decomposes the multivariate PDF [18].

### 2.3.2. Latent variable modeling

Latent variable modeling (LVM) assumes that in each group of the data the underlying discrete distribution depends of some covariates that can be modeled through a set of latent variables. These variables are random variables whose measured values are hidden. The properties of these unrecorded variables can be extracted from the observed variables by means of a statistical LVM that relates both kinds of variables. LVM has been increasingly studied and currently is a booming field of research both in theoretical developments and in applications. Examples of LVM in recent literature, to quote a few, include the following: covariate measurement error in nonlinear models [42]; spatial statistics [208]; learning harmonium models with infinite latent features using graphical undirected LVM [52]; tensor decomposition for LVM [11]; semiparametric and parametric LVM in the presence of measurable outcomes of mixed type (continuous and ordinal) in medicine [248]; error and bias estimation in sources and components using Monte Carlo estimators [271]; selection of latent variables for multiple mixed-outcome models [289]; hierarchical Bayesian models using LVM for network data [194]; fast algorithms for computing deviance information criterion (DIC) of high-dimensional LVM [46]; and extending the factor analysis from individual to groups of variables [137].

In this section, the main foundations of LVM are reviewed, but comprehensive literature can be found in $[27,246,243,28]$ and the references within. In general, LVM can be defined as a generalized regression function that can be written as $f(E(\mathbf{X}))=g(\mathbf{S})$, where $f$ is a link function, $E$ is the expectation operator, $\mathbf{x}$ denotes a matrix of observed variables, $\mathbf{s}$ is a latent structure, and $g$ is some function that relates the latent structure to the observed variables. If, upon a suitable choice of $f$, the function $g$ is linear, then the resulting family of models is covered by generalized linear regression theory [181].

When unrecorded variables are believed to influence only one recorded variable directly, they are commonly modeled as noise. However, when they influence two or more measured variables directly, the objective is to identify them and their influences, i.e., the causal relations of (often unknown) unrecorded variables that influence multiple recorded variables. Frequently, it is assumed that recorded variables do not influence unrecorded variables, although in some cases recorded variables may influence one another. This is specified as conditional independence of the observed variables given the latent variables, and thus $p\left(\mathbf{x}_{j} \mid \mathrm{s}_{j}\right)=\prod_{i=1}^{N} p\left(x_{i j} \mid \mathrm{s}_{j}\right)$, where $N$ is the total number of observed variables and $j$ represents a unit of analysis of a latent variable. This is also called "local independence."

The association between LVM and FMM can be defined by relating the data (observations) with the variables of the generative probabilistic data model (latent structure). Let us consider the following generative probabilistic process for GMM: (i) draw mixture proportions $\theta \sim \operatorname{Dirichlet}(\alpha)$; (ii) for each mixture component $k$, draw $\mu_{k} \sim N\left(0, \sigma_{0}{ }^{2}\right)$; (iii) for each data point $n$, draw mixture assignment $z_{n} \mid \theta \sim \operatorname{Discrete}(\theta)$ and draw data point $x_{n} \mid z_{n}, \mu \sim N\left(\mu_{z_{n}}, 1\right)$. Given a dataset, the posterior distribution can be considered to reverse this process and to estimate the distribution of the hidden structure that probably generated them. The model can be represented with the factored joint distribution of its hidden and observed variables. For GMM, this joint distribution is

$$
\begin{equation*}
p\left(\theta, \mu, z, x \mid{\sigma_{0}}^{2}, \alpha\right)=p(\theta \mid \alpha) \prod_{k=1}^{K} p\left(\mu_{k} \mid \sigma_{0}^{2}\right) \prod_{i=1}^{N} p\left(z_{i} \mid \theta\right) p\left(x_{i} \mid z_{i}, \mu\right) \tag{2.18}
\end{equation*}
$$

where $p(\theta \mid \alpha)$ is the Dirichlet density, $p\left(\mu \mid \sigma_{0}{ }^{2}\right)$ is the Gaussian density, $p\left(z_{i} \mid \theta\right)=\theta_{z_{i}}$ is a discrete distribution, and $p\left(x_{i} \mid z_{i}, \mu\right)$ is a Gaussian density centred at the $z_{i}$-th mean. Note that local variables have terms inside the product over $N$ data points, whereas global variables have terms outside of this product. Thus, the posterior of the GMM can be estimated from its joint distribution as

$$
\begin{equation*}
p\left(\theta, \mu, z, x \left\lvert\,{\left.\sigma_{0}^{2}, \alpha\right)=\frac{p\left(\theta, \mu, z, x \mid \sigma_{0}^{2}, \alpha\right)}{p\left(x \mid \sigma_{0}^{2}, \alpha\right)}}_{\text {2 }}\right.\right. \tag{2.19}
\end{equation*}
$$

This posterior can be used to examine the particular hidden structure that is manifest in the observed data.

On the other hand, LVM can be represented as a probabilistic graphical model (PGM) where the dependencies between the variables of the observed and latent variables are encoded. The graphical model shows the structure of the factorized joint distribution and the flow of the generative process. In this graph, nodes represent random variables and edges denote dependence between them (Figure 2.4 shows an example of probabilistic graphical model for a mixture of two Gaussians). PGM is related with signal processing on graphs, which is a field of increasing research interest in applications of big data $[66,67]$.

There are several kinds of LVMs, which are often categorized in terms of the type of observed and latent variables, (i.e., continuous or categorical variables). Table 2.1 shows a classification of classical LVMs.

|  |  | Latent variables |  |
| :---: | :---: | :---: | :---: |
|  |  | Continuous | Categorical |
| Observed variables | Continuous | Common factor model <br> Structural equation model <br> Linear mixed model <br> Covariate measurement error model | Latent profile model |
|  | Categorical | Latent trail model (item-response theory (IRT) model) | Latent class model |

Table 2.1. Types of latent variable models.


Figure 2.4. Example of probabilistic graphical models for a mixture of two Gaussians (dashed-line nodes are observed variables, continuous-line nodes are latent (hidden) variables, and double-line nodes are fixed hyperparameters).

In latent class models, a latent categorical variable is measured with error by a set of categorical variables $x_{i j}, i=1, \ldots, n$, considering $j=1, \ldots, N$ independent units. The categories of the latent variable represent labels for $C$ subpopulations or latent classes, $c=1, \ldots, C$, with class membership probabilities $\pi_{c}$. Considering binary variables, the conditional probability for measure $i$ given latent class membership $c$ is specified as $p\left(x_{i j}=1 \mid c\right)=\pi_{\| \mid c}$, where $\pi_{\| \mid c}$ are free parameters, thus, $x_{i j}$ and $x_{i, j}$ are conditionally independent given class membership. The marginal likelihood can be expressed as a function of the parameters $\pi$,

$$
\begin{equation*}
L^{\mu}(\boldsymbol{\pi})=\prod_{j=1}^{N} p\left(\mathbf{x}_{j} ; \boldsymbol{\pi}\right)=\prod_{j=1}^{N} \sum_{c=1}^{c} \pi_{c} \prod_{i=1}^{n} \pi_{i \mid c}^{x_{j c}}\left(1-\pi_{i \mid c}\right)^{1-x_{j}} \tag{2.20}
\end{equation*}
$$

It is evident that this latent class model is a multivariate finite mixture model with $C$ components. An important application of latent class models is in medical diagnosis where both latent classes (disease versus no disease) and the sets of measurements (diagnostic test results) are dichotomous (e.g., [264]). A latent profile model for continuous variables has the same structure as latent class model, but a different conditional distribution, $x_{i j} \mid c \sim N\left(\mu_{i \mid c}, \sigma_{i}^{2}\right)$.

Item-response theory (IRT) models consider the case where a latent continuous variable or "latent trait" $\tau_{j}$ is measured with error by a set of categorical variables usually called "items." The classical example is from education testing, where the items are exam questions, $x_{i j}$ is equal to 1 if examinee $j$ answered item $i$ correctly and 0 otherwise, and $\tau_{j}$ represents the ability (latent variable) of the examinee. In the simplest IRT model, the one-parameter logistic (1-PL) model, the conditional response probability for item $i$ given "ability" $\tau_{j}$, is specified as $p\left(x_{i j}=1 \mid \tau_{j}\right)=\frac{\exp \left(\tau_{j}-b_{i}\right)}{1+\exp \left(\tau_{j}-b_{i}\right)}$. This is called a "one-parameter" model because there is one
parameter, "item difficulty" $b_{i}$, for each item. Assuming Gaussianity in distribution of the random variable ability, a marginal likelihood can be easily estimated.

1-PL can be extended to a more general model that is more realistic. Thus, a two-parameter logistic (2-PL) model can be specified, incorporating the 1-PL as a special case: $p\left(x_{i j}=1 \mid \tau_{j}\right)=\frac{\exp \left[a_{i}\left(\tau_{j}-b_{i}\right)\right]}{1+\exp \left[a_{i}\left(\tau_{j}-b_{i}\right)\right]}$. There are two parameters for each item, a discrimination parameter $a_{i}$ and an item difficulty parameter $b_{i}$. More complex IRT models accommodate more parameters: guessing, rating scale, grade response, and so on. IRT models are extensively applied in fields such as in sociology, social psychology, neuropsychology, and epidemiology [261]. Some uncertainty arises from the kinds of variables involved in those applications since they cannot be considered as strictly observable or at least measurable. The distinction between observed and latent variables is of suggested epistemological character, i.e., accessible or not epistemically accessible. For instance, intelligence quotient (IQ) scores are recorded, but general intelligence is not; hence general intelligence is a latent variable and IQ and observed variable. In addition, dealing with categorical variables is not easy and some bias is introduced by assigning ranges of numerical values to the categories as observations of those variables [28].

In common factor analsys (CFA), it is assumed that each manifest variable is a function of $f$ common factors (i.e., latent variables that influence more than one manifest variable) and one unique factor (i.e., a latent variable that influences only one manifest variable). This can be described as [70]

$$
\begin{equation*}
\mathbf{X}=\mathbf{Y} \mathbf{L}_{F}{ }^{T}+\mathbf{Z}+\mathbf{e} \tag{2.21}
\end{equation*}
$$

where $\mathbf{X}$ is an $[N \times p]$ matrix of standardize scores on $p$ manifest variables, $\mathbf{Y}$ is an $[N \times f]$ matrix of standardized common factor scores; $\mathbf{L}_{F}$ is a $[p \times f]$ matrix of least square multiple regression weights (the common factor pattern) for predicting the scores of $\mathbf{X}$ from those in $\mathbf{Y}$; and $\mathbf{Z}$ is a $[N \times p]$ matrix of unique factors. The common and unique factors are uncorrelated $\left(\mathbf{Y}^{T} \mathbf{Z}=0\right)$ and the unique factors for different manifest variables are uncorrelated as well, i.e, $\frac{\mathbf{Z}^{T} \mathbf{Z}}{N}=\mathbf{U}^{2}$ is a $[p \times p]$ diagonal matrix of unique factor variances. Because the unique factors are uncorrelated with each other and with the common factors, it is possible to interpret $\mathbf{Y}$ as containing common factors that account for correlations between manifest variables. Let us assume an orthogonal common factor model, meaning that the $f$ factors in $\mathbf{Y}$ are uncorrelated with each other. Because of sampling error and model error (e.g., nonlinear relationships between manifest variables and common factors, or minor factors), the common factor model will almost never hold exactly, and therefore e ( $[N \times p]$ ) is included as a residual matrix. Thus, (2.21) may be written as $\mathbf{S}=\frac{\mathbf{X}^{T} \mathbf{X}}{N}=\mathbf{L}_{F} \mathbf{L}_{F}{ }^{T}+\mathbf{U}^{2}+\mathbf{E}$, where $\mathbf{S}$ is a $[p \times p]$ sample correlation matrix and $\mathbf{E}$ is a $[p \times p]$ matrix of residual correlations. Factor analysis procedures attempt to keep $\mathbf{E}$ as small as possible by optimally choosing $\mathbf{L}_{F}$ and $\mathbf{U}^{2}$. Estimation in CFA typically employs an iterative procedure, where $\mathbf{L}_{F}$ is calculated at each $\mathbf{U}^{2}$ found by the algorithm. The iterative principal axis factoring procedure is a popular method that provides a result which is asymptotically equivalent to the unweighted least square discrepancy function. The squared multiple correlations can be used as initial communalities. Factor scores are then calculated by decomposing the reduced correlation matrix as

$$
\begin{equation*}
\mathbf{S}=\mathbf{V} \mathbf{K} \mathbf{V}^{T}+\mathbf{U}^{2} \tag{2.22}
\end{equation*}
$$

where $\mathbf{V}$ is a $[p \times p]$ marix of eigenvectors normalized to unit norm and $\mathbf{K}$ is a $[p \times p]$ diagonal matrix containing the corresponding eigenvalues of the reduced correlation matrix $\left(\mathbf{S}-\mathbf{U}^{2}\right)$.

A relevant example of CFA is the "independent clusters model," where $\mathbf{L}_{F}$ has many elements set to zero such that each variable measures one and only one factor. Figure 2.5 shows a path diagram of an independent cluster factor model example of two factors with correlation $s_{21}$.

Considering the similarities in the different approaches for latent modeling, a general framework called GLLAMM (Generalized Linar Latent and Mixed Models) has been proposed [246].

Principal Component Analysis (PCA) is a technique that searches for a matrix that relates to the co-variations of the original variables with a set of latent variables, as in CFA. PCA replaces the $p$ original variables (manifest) with $f$ linear combinations of them $(f \leq p)$, chosen so that they are ordered by decreasing amount of variance. These combinations (the latent variables) are the "principal components." PCA finds a linear rotated orthogonal system such that the elements of the original vectors in the new coordinates become uncorrelated, so the redundancy induced by correlation is removed. The components are obtained as eigenvectors of the sample correlation or covariance matrix.

The principal difference as compared to CFA is that each manifest variable is a linear function of principal components with no separate representation of unique variables:

$$
\begin{equation*}
\mathbf{x}=\mathbf{Y}_{c} \mathbf{L}_{c}{ }^{T} \tag{2.23}
\end{equation*}
$$

where $\mathbf{Y}_{C}$ is an $[N \times p]$ matrix of standardized component scores and $\mathbf{L}_{c}$ is a $[p \times p]$ matrix of component loadings. The correlation matrix $S$ can be decomposed as follows:

$$
\begin{equation*}
\mathbf{S}=\mathbf{W} \mathbf{M} \mathbf{W}^{T} \tag{2.24}
\end{equation*}
$$

where $\mathbf{W}$ is a $[p \times p]$ matrix of eigenvectors and $\mathbf{M}$ is a $[p \times p]$ diagonal matrix of eigenvalues of $\mathbf{S}$. The component scores $\mathbf{Y}_{c}$ are $\mathbf{Y}_{c}=\mathbf{x} \mathbf{w ~}_{\mathbf{m}^{-1 / 2}}$ and the $[p \times p]$ matrix of component loadings is calculated as $\mathbf{L}_{c}=\mathbf{W} \mathbf{M}^{1 / 2}$. Usually, only the first $f$ components are retained. The retained components accounts for less than $100 \%$ of the variance in the data. In PCA, the component scores are uniquely determined by the data in $\mathbf{x}$.


Figure 2.5. Example of an independent cluster factor model.

From equations (2.22) and (2.24), we can conclude that the main difference between CFA and PCA is that CFA involves a reduction of the diagonal elements of the correlation matrix whereas PCA does not. CFA explains the off-diagonal elements of $\mathbf{S}$ according to a discrepancy function. In contrast, the retained components in PCA optimally account for the 1s of the diagonal of $\mathbf{S}$; i.e., for $r$ retained components, $\mathbf{L}_{c_{r}} \mathbf{L}_{c_{r}}{ }^{T}$ maximizes $\operatorname{tr}(\mathbf{S})$ among all possible orthogonal linear transformations of $\mathbf{X}$. Thus, the principal objective of PCA is to optimally estimate the maximum amount of variance with the minimum number of components. In addition, it can be demonstrated that the difference between CFA and PCA loadings will be small when the unique variances in $\mathbf{U}^{2}$ are small.

The analysis of the differences between PCA and CFA has covered aspects such as factors and component loadings depending on the number of variables (similarity increases as the number of variables increases since the diagonal elements increase arithmetically but the off-diagonal elements increase geometrically); data sphericity condition; and generalizability of results, i.e., consistency of factors and components for different subsets of variables (see for instance [70,263,187]).

A natural evolution of statistical signal processing, in connection with the progressive increase in computational power, has been the extension of PCA (based on second order statistics and correlation) to ICA (based on independence) for exploiting higher-order information. In the next section, we approach ICA, which is a multivariate statistical method that is particularly suitable for uncovering latent source signals from high-dimensional complex data.

### 2.3.3. Independent component analysis (ICA)

Independent component analysis was introduced by C. Jutten in [132,129,130,131], although its first thorough mathematical formulation was performed by P. Comon [60]. Since then, many different algorithms have been proposed for estimating the ICA parameters (see for example $[111,55,150,56,59])$. The large number of applied problems where ICA has been considered as a practical solution is also remarkable.

ICA is formulated as a linear model of the observed data vector $\mathbf{x}=\left[x_{1}(n), \ldots, x_{M}(n)\right]^{T}$ which is assumed to be a linear transformation of a vector $\mathbf{s}=\left[s_{1}(n), \ldots, s_{M}(n)\right]^{T}$ in the form (we assume for simplicity the square model, where $\mathbf{A}$ is a square $[M \times M$ ] matrix):

$$
\begin{equation*}
\mathbf{x}=\mathbf{A} \mathbf{s} \tag{2.25}
\end{equation*}
$$

The elements of $s$ are assumed to be statistically independent components [111], while dependence is allowed among the elements of $\mathbf{x}$ : every component of $\mathbf{x}$ is generated from a linear combination of the same independent variables $s_{1}, \ldots, s_{M}$. This simple model can be seen from different perspectives. The most obvious is that of modeling multivariate probability density functions in presence of statistical dependence. If $\mathbf{A}$ is square and invertible, we may express the joint probability density $p_{x}(\mathbf{x})$ in terms of $p_{s}(\mathbf{s})=p\left(s_{1}\right) \cdot \ldots \cdot p\left(s_{M}\right)$ in the form

$$
\begin{equation*}
p_{x}(\mathbf{x})=\frac{1}{|\operatorname{det} \mathbf{A}|} p_{s}\left(\mathbf{A}^{-1} \mathbf{x}\right) \tag{2.26}
\end{equation*}
$$

Thus, the joint probability modeling is decomposed into two parts: modeling of the marginal densities $p\left(s_{1}\right) \cdot \ldots p\left(s_{M}\right)$ (which implies $M$ univariate models) and estimating the mixing matrix $\mathbf{A}$, which is the responsible for the statistical dependence among the elements of $\mathbf{x}$. As long as the marginal are non-Gaussian, $p_{x}(\mathbf{x})$ will be multivariate non-Gaussian. Notice the
wide range of multivariate non-Gaussian probability densities which can be modeled by modifying the marginal distribution and the mixing matrix.

From a different perspective, if the elements of $\mathbf{x}$ and $\mathbf{s}$ are time (or any other domain) indexed, we may define a problem of instantaneous signal separation in the form

$$
\begin{equation*}
\left[s_{1}(n), \ldots, s_{M}(n)\right]^{T}=\mathbf{A}^{-1}\left[x_{1}(n), \ldots, x_{M}(n)\right]^{T} \tag{2.27}
\end{equation*}
$$

The elements of vector $\mathbf{s}$ are usually termed "sources", hence the problem is to "separate" these sources $s_{1}(n), \ldots, s_{M}(n)$ in a blind or semi-blind manner, depending on the presence or not of some kind of prior knowledge about the mixing matrix $\mathbf{A}$ or about the sources $\mathbf{s}[108,80,73]$. Figure 2.6 shows a schema that illustrates the instantaneous mixing and unmixing model for blind source separation (BSS) based on ICA.

Finally, ICA can be also understood as a classical decomposition model that expresses the observed vector in terms of some base vectors, namely

$$
\begin{equation*}
\mathbf{x}=\sum_{i=1}^{M} s_{i} \mathbf{a}_{i} \tag{2.28}
\end{equation*}
$$

where $\mathbf{a}_{i}, i=1, \ldots, M$, are the columns of $\mathbf{A}$. This is a generalization of principal component analysis, which assumes incorrelation between the weights $s_{1}, \ldots, s_{M}$. In ICA, uncorrelation is generalized to independence, which are not equivalent concepts when Gaussianity is not assumed. Thus, the $\mathbf{a}_{i}$ can be used as essential descriptors of underlying phenomena that, randomly combined, explain the observed vector $\mathbf{x}$. This also has application in pattern recognition or classification methods where the elements of $\mathbf{A}$ are used as input features.

Usually, the elements of A are estimated by optimization of a properly-defined contrast or cost function. In general, optimization criteria are based on forcing independence between the source elements. Some methods approximate the distributions of the sources within a specified class of


Figure 2.6. Independent component analysis model with two sources and two recorded variables $(M=2)$. The color of the arrows denotes the weight of the corresponding component/source: dark colors are higher than light colors.
distributions, and then mutual information, likelihood function, or similar [60,114,9,8,113,200] are used to define the contrast function. Other methods optimize different contrast functions without explicitly approximating the source distributions. These functions can be, for instance, non-Gaussianity (using negentropy or kurtosis), and nonlinear correlation among estimated sources [129,110,285]. The optimization techniques applied to the contrast function are mainly based on gradient descent (natural, steepest...) and approximate Newton methods. There are also some direct estimation procedures that exploit specific algebraic structures of the involved matrices (see Section VII of [40] and references therein, [282,273]).

### 2.4. Mixtures of independent component analyzers

### 2.4.1. Definition

As explained, ICA may serve the purpose of modeling multivariate non-Gaussian PDFs. Although a wide range of multivariate probability densities can modeled by ICA, larger versatility can be achieved by mixtures of ICAs. This leads to a natural extension of the classical Gaussian mixture model ( [54]). GMM is limited in two main aspects: (i) the size $\left(M^{2}\right)$ of each covariance matrix becomes extremely large when the dimension ( $M$ ) of the problem increases; and (ii) each component is Gaussian, which is a condition that is rarely found in real data sets.

Antecedents of ICAMM can be found in [262] with the so-called probabilistic principal component analysis (PPCA) where, staring from a GMM, each component of the mixture was replaced with a PPCA, allowing the covariance matrix dimension to be reduced. A further modification of this method was presented in [93] using variational Bayesian inference to infer the optimum number of analysers, obtaining the so-called mixture of factor analysers (MoFA). Afterwards, a robust approach for PPCA that exploits the adaptive distribution tails of the Student $-t$ was proposed $[12,257]$. The latter allows the performance of the method to remain unaffected in the presence of non-Gaussian noise (e.g., outliers).

Notice that a mixture model emanates in a natural manner in the framework of classification/segmentation methods. If the data can be categorized into several mutually exclusive classes, where each class is characterized by a given multivariate probability density, the whole data multivariate probability density can be considered a mixture of the classconditioned probability densities. Thus it is not strange that ICAMM was proposed in the framework of pattern recognition. It was introduced in [153] considering a source model switching between Laplacian and bimodal densities. Afterward, the model was extended using generalized exponential sources [204], variational Bayesian inference [54] and $\beta$-divergence [176]. Related aspects like estimation of the number of ICA mixtures have been considered in [48,195] using variational Bayesian learning and in [157] by adaptive estimation of the clusters comparing log-likelihood of the data.

The general expression of ICAMM requires some bias vectors to separate the components of the mixture, i.e.,

$$
\begin{equation*}
\mathbf{x}_{k}=\mathbf{A}_{k} \mathbf{s}_{k}+\mathbf{b}_{k}, k=1, \ldots, K \tag{2.29}
\end{equation*}
$$

where $k$ is the class, denoted by $C_{k} ; \mathbf{A}_{k}$ and $\mathbf{s}_{k}$ are respectively the mixing matrix and the source vector of the ICA model of class $k$; and $\mathbf{b}_{k}$ is the corresponding bias vector. Essentially, $\mathbf{b}_{k}$ determines the location of the cluster and $\mathbf{A}_{k} \mathbf{s}_{k}$ its shape. The classes in ICAMM are assumed to be exclusive, and thus, the ICA mixture model is a switching model between the $\kappa$ estimated ICA, as shown in Figure 2.7.

Figure 2.8 compares the behavior of ICA and ICAMM for a toy example where two data channels were generated from a mixture of two sources using two different classes (mixing matrices; both classes had the same sources and bias vectors). The results of ICAMM for source separation are show in Figure 2.8.a, where it can be seen the sources were perfectly recovered by the method. ICA, however, was not flexible enough to compensate for the two classes and the separated sources were still mixed, as shown in Figure 2.8.b.

Figure 2.9 and Figure 2.10 illustrate an application of ICA for image segmentation. First, in Figure 2.9, we can see how every small square subimage of the whole image is modeled with a specific ICA mixing matrix and centroid. Notably differences can be appreciate among the different model parameters, especially when comparing subimages corresponding to different classes of the original whole image. Then, in Figure 2.10, the ICA model is used to segment the images so that and automatic classifier could easily separate the two classes of images (text and picture).


Figure 2.7. Outline of the ICA mixture model as a switching model of $K$ separate ICA models.


Figure 2.8. Comparison of ICA versus ICAMM for a source separation task: a) two sources are mixed with two classes to obtain two recorded variables, which are then separated by a two-class ICAMM; b) result of ICA for the same source separation task. The colors of the mixing/de-mixing matrices denote the weight of the corresponding element: dark colors are higher than light colors.


Figure 2.9. Estimation of an ICA mixture model with two classes (frog and text). Each class produces a different ICA, as shown by their different mixing matrices and centroids.


Figure 2.10. Segmentation of an image using ICAMM.

## ICAMM estimation

In a supervised scenario, the problem of estimating all the parameters involved in an ICAMM can be decomposed in many simpler problems of estimating the ICA model corresponding to each component of the mixture, plus the estimation of the centroids or bias $\mathbf{b}_{k}$. However unsupervised or semi-supervised scenarios require simultaneous estimation of all the parameters. Four main approaches have considered until now: maximum-likelihood [153], $\beta$ divergence [176], variational Bayesian [54] and non-parametric semi-supervised learning in ICAMM [231]. We describe these methods in the following.

### 2.4.2. Maximum likelihood

An unsupervised maximum-likelihood classification algorithm for ICAMM estimation was proposed in [153]. Given a set of independent observations $\mathbf{x}_{n}, n=1, \ldots, N$ that emanates from an ICAMM composed by $K$ ICA components and characterized by a set of parameters $\boldsymbol{\Theta}=\left[\boldsymbol{\theta}_{1}, \ldots, \boldsymbol{\theta}_{K}\right]$, the likelihood of the data is given by the joint density $p(\mathbf{X} \mid \boldsymbol{\Theta})=\prod_{n=1}^{N} p\left(\mathbf{x}_{n} \mid \boldsymbol{\Theta}\right)$, where $\mathbf{x}=\left[\mathbf{x}_{1}, \ldots, \mathbf{x}_{N}\right]$. We assume that the observation multivariate probability density function is a mixture of the form $p\left(\mathbf{x}_{n} \mid \boldsymbol{\Theta}\right)=\sum_{k=1}^{K} p\left(\mathbf{x}_{n} \mid C_{k}, \boldsymbol{\theta}_{k}\right) \cdot P\left(C_{k}\right)$, where $P\left(C_{k}\right)$ measures the importance of component $k$ in the mixture (in terms of classification, $P\left(C_{k}\right)$ is the a priori probability of class $k$ ). Iterative algorithms are required to obtain the ICAMM parameters that maximize the log likelihood. Thus, in [153], the Extended InfoMax algorithm ( [151]) is used for adapting the mixture matrices

$$
\begin{equation*}
\Delta \mathbf{A}_{k} \propto-P\left(C_{k} \mid \mathbf{x}_{n}, \boldsymbol{\Theta}\right) \cdot \mathbf{A}_{k} \cdot\left[\mathbf{I}-\mathbf{K} \cdot \tanh \left(\mathbf{s}_{k}\right) \cdot \mathbf{s}_{k}^{T}-\mathbf{s}_{k} \cdot \mathbf{s}_{k}^{T}\right] \tag{2.30}
\end{equation*}
$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{K}$ is a diagonal matrix with values 1 (super-Gaussian regime) or -1 sub-Gaussian regimen) of the corresponding source component extracted at the current iteration. On the other hand we can estimate $P\left(C_{k} \mid \mathbf{x}_{n}, \boldsymbol{\Theta}\right)=\frac{p\left(\mathbf{x}_{n} \mid \boldsymbol{\theta}_{k}, C_{k}\right) \cdot P\left(C_{k}\right)}{K}$ using the

$$
\sum_{l=1}^{n} p\left(\mathbf{x}_{n} \mid \boldsymbol{\theta}_{l}, C_{l}\right) \cdot P\left(C_{l}\right)
$$

current parameters of ICAMM, and we can estimate also the centroids at every iteration as

$$
\begin{equation*}
\mathbf{b}_{k}=\frac{\sum_{n=1}^{N} \mathbf{x}_{n} \cdot p\left(C_{k} \mid \mathbf{x}_{n}, \boldsymbol{\Theta}\right)}{\sum_{n=1}^{N} p\left(C_{k} \mid \mathbf{x}_{n}, \boldsymbol{\Theta}\right)} \tag{2.31}
\end{equation*}
$$

An extension was made in [48] where the number of clusters and the intrinsic dimension of each cluster were determined by a variational Bayesian method similar to the method proposed in [204]. An on-line version for partitioning the input-output space for fuzzy neural networks was proposed in [157].

### 2.4.3. Beta-divergence

Notice that ICA model can be expressed in terms of the recovered sources $\mathbf{s}=\mathbf{A}^{-1} \cdot \mathbf{x}-\mathbf{A}^{-1} \cdot \mathbf{b}=\mathbf{W} \cdot \mathbf{x}-\boldsymbol{\mu}$, where $\mathbf{W}$ is the de-mixing matrix and $\boldsymbol{\mu}$ a recovery bias. In the $\beta$-divergence method, the hidden mixture components are sequentially extracted in the following manner. The estimation method starts by defining an initial $\mu_{1}$. Then, an initial demixing matrix $\mathbf{W}_{1}$ is estimated by minimizing the $\beta$-divergence between the empirical distribution of the whole data set of observations $\mathbf{x}$ and the distribution derived from the assumed initial ICA model,

$$
\begin{equation*}
p_{X}(\mathbf{x})=\left|\operatorname{det} \mathbf{W}_{1}\right| p_{S}\left(\mathbf{W}_{1} \mathbf{x}-\boldsymbol{\mu}_{1}\right)=\left|\operatorname{det} \mathbf{W}_{1}\right| \prod_{m=1}^{M} p_{S_{m}}\left(\mathbf{w}_{1 m}^{T} \mathbf{x}-\mu_{1 m}\right) \tag{2.32}
\end{equation*}
$$

where specific forms are used for the source marginal probability densities $p_{s_{s}}(\cdot), m=1, \ldots, M$ : $p(z)=c_{2} / \cosh (z)$ for super-gaussian signals and $p(z)=c_{1} \cdot \exp \left(-c_{2} \cdot z^{4}\right)$ for sub-gaussians.
$\beta$-divergence $[12,176]$ is a measure of the distance between two probability density functions $p(\mathbf{x})$ and $q(\mathbf{x})$, defined as

$$
\begin{equation*}
D_{\beta}(p, q)=\int\left[\frac{1}{\beta}\left(p^{\beta}(\mathbf{x})-q^{\beta}(\mathbf{x})\right) p(\mathbf{x})-\frac{1}{\beta+1}\left(p^{\beta+1}(\mathbf{x})-q^{\beta+1}(\mathbf{x})\right)\right] \cdot d \mathbf{x}, \beta>0 \tag{2.33}
\end{equation*}
$$

which is non-negative and equal to zero if and only if $p(\mathbf{x})=q(\mathbf{x}) \cdot \beta$-divergence reduces to Kullback-Leibler divergence when $\beta \rightarrow 0$.

The next step is to calculate a new bias $\mu_{2}$ by using only those observations that can qualified as outliers of the initial ICA (i.e., those having a low probability in the initial ICA model as computed from $\left.\left|\operatorname{det} \mathbf{W}_{1}\right| \prod_{m=1}^{M} p_{S_{m}}\left(\mathbf{w}_{1 m}^{T} \mathbf{x}-\mu_{1 m}\right)\right)$, and then a new recovering matrix $\mathbf{W}_{2}$ is obtained as before. The procedure is repeated $K$ times until all the $K$ hidden classes are estimated.

### 2.4.4. Variational Bayesian

This method was proposed in [54]. This is a complex method which consists in considering that the observations $\mathbf{x}$ are obtained from a generative model that can be described by a Bayesian network. Hence, variational Bayesian methods can be used for the computation of all the required parameters. In essence, it is a maximum likelihood method where a Gaussian mixture is assumed for every single source probability density and where a "noise" term is added to the ICA model. A detailed description of the method is given in [54]. We omit it here as this method has not been under consideration throughout the rest of the thesis.

### 2.4.5. Non-Parametric

This method [231] is a generalization of the maximum likelihood method previously presented. A non-parametric estimation of the sources is proposed, thus obtaining large generality as no special constraints are required for the sources distributions. Other significant generalization is the possibility of using semi-supervised learning. This method has been applied across the thesis, so we include here a schematic description of it.

Let us consider that the set of observed feature vectors is formed by $\mathbf{x}_{n}, n=1, \ldots, N$. We divide this set into two subsets. The first subset is formed by $\mathbf{x}_{n}, n=1, \ldots, N_{1}, N_{1} \leq N$, where we may assign some probability of belonging to class $C_{k}$, namely $P^{(0)}\left(C_{k} \mid \mathbf{x}_{n}\right)$ for $k=1, \ldots, K$. The second subset is formed by $N_{2}=N-N_{1}$ vectors where no knowledge exists about the possible class they belong to. The learning algorithms proceeds in the manner shown in Table 2.2.

```
Initialization
For \(k=1 \ldots K\), compute:
    \(\mathbf{b}_{k}^{(0)}=\sum_{n=1}^{N_{1}} \mathbf{x}_{n} \cdot P^{(0)}\left(C_{k} \mid \mathbf{x}_{n}\right) \quad\) (if \(M_{1}=0\), select the initial centroids randomly);
    \(\mathbf{W}_{k}{ }^{(0)}\) (randomly initialized) ;
    \(\mathbf{s}_{k n}{ }^{(0)}=\mathbf{W}_{k}{ }^{(0)} \cdot\left(\mathbf{x}_{n}-\mathbf{b}_{k}{ }^{(0)}\right) \mathbf{s}_{k m}^{(0)}=\mathbf{W}_{k}^{(0)}\left(\mathbf{x}_{m}-\mathbf{b}_{k}^{(0)}\right)\)
    \(p^{(0)}\left(s_{k}\right)\) (a non-parametric estimator is used)
```


## Updating

For $i=1 \ldots \mathrm{I}$ and for $k=1 \ldots K$, compute:
For the probabilistically labeled vectors

$$
P^{(i)}\left(C_{k} \mid \mathbf{x}_{n}\right)=P^{(0)}\left(C_{k} \mid \mathbf{x}_{n}\right), n=1, \ldots, N_{1}
$$

For the unlabeled vectors,

$$
\begin{aligned}
& P^{(i)}\left(C_{k} \mid \mathbf{x}_{n}\right)=p^{(i)}\left(\mathbf{x}_{n} \mid C_{k}\right) \cdot P\left(C_{k}\right) / p\left(\mathbf{x}_{n}\right)= \\
& =\left|\operatorname{det} \mathbf{W}_{k}^{(i-1)}\right| \cdot p^{(i-1)}\left(\mathbf{s}_{k n}^{(i-1)}\right) \cdot P\left(C_{k}\right) / \sum_{k^{\prime}=1}^{K}\left|\operatorname{det} \mathbf{W}_{k^{\prime}}^{(i-1)}\right| \cdot p^{(i-1)}\left(\mathbf{s}_{k^{\prime} \cdot m}^{(i-1)}\right) \cdot P\left(C_{k^{\prime}}\right) \quad n=N_{1}+1, \ldots, N \\
& \mathbf{b}_{k}^{(i)}=\sum_{n=1}^{N} \mathbf{x}_{n} \cdot P^{(i)}\left(C_{k} \mid \mathbf{x}_{n}\right) ; \\
& \mathbf{W}_{k}{ }^{(i)}=\mathbf{W}_{k}^{(i-1)}+\Delta \mathbf{W}_{k}{ }^{(i-1)}, \Delta \mathbf{W}_{k}^{(i-1)}=\sum_{n=1}^{N} \Delta \mathbf{W}_{k n(I C A)}^{(i-1)} \cdot P^{(i-1)}\left(C_{k} \mid \mathbf{x}_{n}\right) ; \text { where } \\
& \Delta \mathbf{W}_{k n(I C A)}^{(i-1)} \text { is the update due to sample } \mathbf{x}_{n} \text { in the selected embedded ICA algorithm; } \\
& \mathbf{s}_{k n}^{(i)}=\mathbf{W}_{k}^{(i)} \cdot\left(\mathbf{x}_{n}-\mathbf{b}_{k}^{(i)}\right) \\
& p^{(i)}\left(\mathbf{s}_{k n}^{(i)}\right) \text { (a non-parametric estimate is used, e.g., by the kernel method). }
\end{aligned}
$$

Table 2.2. Non-parametric learning algorithm.

### 2.5. Conclusions

The main objective of this chapter has been to situate ICAMM in the context of non-Gaussian mixture models of the underlying probability density of a set of observations. Non-Gaussian mixtures are the natural extension of Gaussian mixtures. However, there is significantly less literature on non-Gaussian mixtures than in Gaussian mixtures, due to the lack of general methods for optimum estimation of the mixture parameters. Thus, non-Gaussian mixtures pose attractive challenges for further work.

We have started by considering the univariate case. The techniques presented in this chapter assume the same type of probability for all the mixture components, thus easing the problem of estimating the corresponding parameters at the price of some loss of adaptation to specific scenarios. Different non-Gaussian densities have been considered: Exponential, Poisson, binomial and multinomial. They are illustrative of both continuous and discrete random variables, although many other types of distributions could be devised.

The extension of univariate mixtures to the multivariate case is immediate if it can be assumed that the components of the multivariate random variable are statistically independent, so that the multivariate probability density can be expressed as the product of the marginals. Then, every marginal can be modeled as a mixture of univariate densities. In presence of statistical dependence, however, the extension is not so easy. Firstly, the extension of typical univariate densities to their corresponding multivariate is not trivial or even possible in most cases. A
notable exception is the multivariate Gaussian case, where dependence is parameterized by a covariance matrix. Hence we have considered in this chapter three methods for multivariate modeling of a non-Gaussian and non-independent probability density: copulas, latent variables and ICA. The latter may be considered a special case of the latent variables method. Regarding the copulas, it is outside the scope of this thesis a detailed comparison with ICA. In fact, mixtures of copulas have not been considered until now, while some methods exist for computing mixtures of ICAs. We have presented four of these methods: maximum likelihood, $\beta$-divergence, variational Bayes and non-parametric. Due to its generality, the latter will be mostly used across the thesis for estimating the ICAMM parameters in the two main problems considered: prediction based on ICAMM and extension of ICAMM to dynamic non-stationary scenarios.

# Building non-linear prediction structures from independent component analysis 

## Chapter 3 - Building non-linear prediction structures from independent component analysis

This chapter presents two novel non-linear prediction methods that are based on independent component analysis mixture modeling. The first method is based on the maximization of the log-likelihood of the data with respect to the ICAMM parameters. We have called this method PREDICAMM (Prediction using ICAMM). The second method is an approximation of the optimal predictor with respect to the mean squared error of the prediction: the conditional expectation of missing data with respect to known data and the ICAMM parameters. This second method we have named E-ICAMM (Expectation assuming ICAMM). Unlike preexisting methods, these algorithms do not use ICA mixture models as a pre-processing step, but as the base of the prediction itself, since they use of both known data and the ICAMM to predict missing data.

PREDICAMM performs the maximization of the log-likelihood of the data with a gradient. Therefore, we performed a sensitivity analysis in order to determine the effect of the initial value and the number of classes in the results of this prediction algorithm.

The performance of the proposed predictors was assessed by prediction missing values in synthetic data modeled with two, three and four classes. In order to test the sensitivity of PREDICAMM and E-ICAMM when the base assumptions are not completely fulfilled, the performance was also tested on several sets of nonlinearly-corrupted data. In all cases, the proposed predictor was compared with four other classical and state-of-the-art methods: matrix completion (a non-linear method that makes use of the structure of a matrix); splines (a commonly-used interpolation method); Wiener structures (a combination of a linear predictor and a non-linear correction); and Kriging (a classical linear predictor that is commonly used in geostatistical applications). The comparison shows that the proposed ICAMM-based methods can be competitive for data prediction even if the basic conditions of ICAMM are not satisfied. In addition, the proposed methods usually performed better than Wiener structures, matrix completion, splines and Kriging. Finally, we performed a last experiment to test the performance of the proposed methods with respect to an increasing number of missing values in each observation. Some of the simulations in this chapter have been reported in [219,224], and results for real-data applications are included in Chapter 5.

We refer to the proposed methods as "predictors," which might imply that the method is used to predict future data from past values of the same signal. However, both PREDICAMM and EICAMM have been designed as general-purpose methods that can be applied to prediction, interpolation and regression. The proposed methods reconstruct missing data from an observation using only the ICAMM parameters and known data from the same observation. Therefore, there is no dependence on time in the algorithm, and thus the reconstruction yielded by PREDICAMM and E-ICAMM is independent from the order in which the observations are reconstructed; the method only considers dependencies within the current sample. ICA and ICA mixture models have been used on data with no time dependence, such as natural images and single frames of brain imaging [114]. The flexibility of the method allows it to reconstruct very different information depending on the sampling scheme considered, as shown in Figure 3.1. Here, by "sampling scheme" we mean how the different values in the signal are mapped to observations to work with the proposed methods. The most typical scheme performs interpolation by considering each time sample as an observation (see Figure 3.1.a); in this case, PREDICAMM and E-ICAMM can interpolate missing data from one spatial location by considering known information from other locations in the same sample and the ICA mixture model. This sampling scheme was considered in the simulations in Section 3.4 and applied on real data in Section 5.4. However, one could also consider the time values of a given spatial location (variable) as the input to the reconstruction method (see Figure 3.1.b). This scheme would perform regression or prediction, since PREDICAMM and E-ICAMM would use the information from one variable at several time samples to interpolate the value of the same variable in other samples. Another sampling scheme consists in dividing the signal into square windows or "patches" and taking each window as a separate observation (see Figure 3.1.c); such is the case when ICA is used for feature extraction in natural images [114,112]. In this instance, the methods are used to reconstruct missing values within a patch using other values from the same patch. Thus, the proposed ICAMM-based methods would allow us to take advantage of the 2-D spatial dependencies for the reconstruction of data, both for predicting data (e.g., predict data outside the borders of an image) and for interpolation (e.g., reconstructing missing or noisy values of a picture), depending on the location of the patch within the image. This sampling scheme was considered for the reconstruction of real data in Sections 5.1, 5.2 and 5.3. Finally, some unconventional sampling could be used in order to exploit known dependencies in a data set, such as the diagonal sampling shown in Figure 3.1.d. The schemes in Figure 3.1.b and


Figure 3.1. Sampling schemes for use in PREDICAMM and E-ICAMM: a) time; b) space; c) windows or patches; d) diagonal. The empty green rectangles represent all the data, areas shadowed in green denote the current observation, areas enclosed in dotted lines represent other observations, and black areas denote missing values. Dotted arrows show some possible sweeping trajectories to reconstruct all missing data.


Figure 3.2. General definition of the prediction process using PREDICAMM and E-ICAMM. Note that there are several method configurations that we can use, which will be explained in Section 3.4.3.b. The asterisks denote the original contributions in this work.

Figure 3.1.d were not considered in this thesis, and they remain open for future work. The general definition of the prediction process with the proposed methods, including the sampling scheme, is shown in Figure 3.2.

### 3.1. Prediction based on maximum likelihood: PREDICAMM

Let us consider an observation vector $\mathbf{x}(n)$ of size $[M \times 1]$. The meaning of the elements of $\mathbf{x}(n)$ is not constrained in any sense. They may represent a segment of a temporal or spatial sequence; they may correspond to a 1D alignment of 2D data (see Figure 3.1), and so on. Assuming that $M_{u n k}$ values from this vector are unknown, the vector values can be grouped into two smaller dimension vectors: $\mathbf{y}(n)$ (known values) and $\mathbf{z}(n)$ (unknown values). That is,

$$
\mathbf{x}(n)=\left[\begin{array}{l}
\mathbf{y}(n)  \tag{3.1}\\
\mathbf{z}(n)
\end{array}\right\rfloor
$$

In the following we will omit the $(n)$ to simplify the notation. The goal of the algorithm is to optimally estimate or predict $\mathbf{z}$ from $\mathbf{y}$. Estimation theory [266] gives us well-known optimization criteria and their corresponding solutions. Basically, two general criteria have been considered in practice: maximum likelihood and least mean squares error, which leads to two alternative solutions, namely

$$
\begin{align*}
& \mathbf{z}_{M L}=\max _{\mathrm{z}} p(\mathbf{z} \mid \mathbf{y}) \\
& \mathbf{z}_{\text {LMSE }}=E[\mathbf{z} \mid \mathbf{y}]=\int \mathbf{z} \cdot p(\mathbf{z} \mid \mathbf{y}) \cdot d \mathbf{z} \tag{3.2}
\end{align*}
$$

PREDICAMM performs this prediction by the ML criterion, that is, selecting the $z$ that maximizes the conditional posterior probability $p(\mathbf{z} \mid \mathbf{y})$. This maximization is performed by assuming that the data are modeled by a non-Gaussian mixture. In particular, we will assume that $\mathbf{x}$ is generated from a mixture of independent component analyzers ( [114]). ICAMM is a versatile model that encompasses almost every statistical description of the data. In particular, it generalizes the extensively used Gaussian mixture model (see, for instance, [26]). We thus obtained a very general ML solution.

Unfortunately, $p(\mathbf{z} \mid \mathbf{y})$ is complicated to calculate even if the underlying ICA mixture model is known. Using Bayes' rule, however, it can be seen that $p(\mathbf{z} \mid \mathbf{y})=p(\mathbf{y}, \mathbf{z}) / p(\mathbf{y})$. The maximization of $p(\mathbf{z} \mid \mathbf{y})$ is equivalent to the maximization of $p(\mathbf{y}, \mathbf{z})$, since known data (and thus $p(\mathbf{y})$ ) are fixed during maximization. Given the ICA mixture model, the calculation of the joint probability density $p(\mathbf{y}, \mathbf{z})$ (and its derivatives) is much easier than the calculation of the conditional probability density, since $p(\mathbf{y}, \mathbf{z}) \equiv p(\mathbf{x})$. Thus, we will seek the maximization of $p(\mathbf{y}, \mathbf{z})$ in the following.

Let us assume that data $\mathbf{x}$ can be modeled using an ICA mixture model with $K$ classes, where the parameters of the model are known: the de-mixing matrices, $\mathbf{w}_{k}$; the probability density function of the sources, $p\left(\mathbf{s}_{k}\right)$; and the centroids, $\mathbf{b}_{k}$; where $k=1, \ldots, K$ is the class. Then, $p(\mathbf{x})$ can be expressed as

$$
\begin{equation*}
p(\mathbf{x})=\sum_{k=1}^{K} p\left(\mathbf{x} \mid C_{k}\right) \cdot P\left(C_{k}\right)=\sum_{k=1}^{\kappa}\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot p\left(\mathbf{s}_{k}(n)\right) \cdot P\left(C_{k}\right) \tag{3.3}
\end{equation*}
$$

where the sources are calculated from the data using the ICAMM parameters, i.e., $\mathbf{s}_{k}(n)=\mathbf{W}_{k} \cdot\left(\mathbf{x}(n)-\mathbf{b}_{k}\right)$; and $C_{k}$ denotes class $k$. It is possible to develop this equation a bit further in order to separate the contribution to the sources of known data from the contribution of unknown data. Each de-mixing matrix $\mathbf{W}_{k}$ can be treated as a block matrix such that $\mathbf{W}_{k}=\left[\begin{array}{ll}\mathbf{w}_{y, k} & \mathbf{W}_{z, k}\end{array}\right]$, where $\mathbf{w}_{y, k}$ is composed of the first $M-M_{u n k}$ columns of matrix $\mathbf{W}_{k}$ and $\mathbf{w}_{z, k}$ is composed of the last $M_{u n k}$ columns of matrix $\mathbf{W}_{k}$. Then, the sources can be calculated as

$$
\left.\mathbf{s}_{k}=\left[\begin{array}{ll}
\mathbf{w}_{y, k} & \mathbf{w}_{\mathbf{z}, k}
\end{array}\right] \cdot\left(\begin{array}{l}
\mathbf{y}  \tag{3.4}\\
\mathbf{z}
\end{array}\right]^{-\mathbf{b}_{k}}\right)=\mathbf{w}_{\mathbf{y}, k} \cdot \mathbf{y}+\mathbf{w}_{\mathbf{z}, k} \cdot \mathbf{z}-\mathbf{w}_{k} \cdot \mathbf{b}_{k}
$$

$\mathbf{w}_{z, k} \cdot \mathbf{z}$ is the only term in (3.4) that changes during the maximization process, since the ICAMM parameters and the known data remain constant.

Equation (3.3) is maximized by using a gradient algorithm, with the joint probability density as the cost function $J(\mathbf{z})$. We obtain the derivative of the cost function with respect to the unknowns z :

$$
\begin{gather*}
\frac{\delta J(\mathbf{z})}{\delta \mathbf{z}}=\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}=\sum_{k=1}^{K}\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot \frac{\delta p\left(\mathbf{s}_{k}\right)}{\delta \mathbf{z}} \cdot P\left(C_{k}\right)  \tag{3.5}\\
\frac{\delta p\left(\mathbf{s}_{k}\right)}{\delta \mathbf{z}}=\sum_{m=1}^{m} \frac{\delta p\left(\mathbf{s}_{k}\right)}{\delta s_{k, m}} \frac{\delta s_{k, m}}{\delta \mathbf{z}} \tag{3.6}
\end{gather*}
$$

where $s_{k, m}$ is the $m$-th component of the sources from the class $k$. The calculation of the derivative of $p\left(\mathbf{s}_{k}\right)$ in (3.6) is very complex for most data distributions, since it is the derivative of a multi-dimensional probability density. However, each class from the ICAMM is modeled by a separate ICA, so we can make use of the independence of the sources (a basic property of the ICA model) to ease our calculations:

$$
\begin{equation*}
\frac{\delta p\left(\mathbf{s}_{k}\right)}{\delta s_{k, m}}=\frac{\delta}{\delta s_{k, m}} \prod_{l=1}^{M} p\left(s_{k, l}\right)=\frac{\delta p\left(s_{k, m}\right)}{\delta s_{k, m}} \cdot \prod_{l \neq m} p\left(s_{k, l}\right)=c_{k, m} \tag{3.7}
\end{equation*}
$$

The derivative of $p\left(s_{k, m}\right)$ can be calculated explicitly for many common probability density functions. This requires prior knowledge of the sources, however, which could limit the applicability of the algorithm. To circumvent this requirement, the probability density of each source was estimated using a nonparametric estimator [231] with a Gaussian kernel. Thus, the probability density function of each source and its derivatives are calculated as follows:

$$
\begin{gather*}
p\left(s_{k, m}\right)=a_{0} \cdot \sum_{l=1}^{N_{T}} e^{-\frac{1}{2 h^{2}}\left(s_{k, m}-s_{k, m}^{(l)}\right)^{2}}  \tag{3.8}\\
\frac{\delta p\left(s_{k, m}\right)}{\delta s_{k, m}}=-a_{0} \cdot \frac{1}{h} \sum_{l=1}^{N_{T}}\left(\frac{s_{k, m}-s_{k, m}^{(l)}}{h}\right) e^{-\frac{1}{2 h^{2}}\left(s_{k, m}-s_{k, m}^{(l)}\right)^{2}} \tag{3.9}
\end{gather*}
$$

where $s_{k, m}^{(l)}$ is the value of the $l$-th available sample of $s_{k, m}$ for estimating the source probabilities, being $N_{T}$ the number of such available samples; $h$ is the bandwidth of the nonparametric estimator; and $a_{0}$ is a scaling constant calculated so that $\int_{-\infty}^{\infty} p\left(s_{k, m}\right) \cdot \mathrm{d} s=1$. For Gaussian kernels, this scaling constant is $a_{0}=1 /\left(\sqrt{2 \pi h} \cdot\left(N_{T}-1\right)\right)$.

Returning to (3.6), the derivative of the sources with respect to unknown data can be calculated from (3.4),

$$
\begin{gather*}
s_{k, m}=\mathbf{w}_{\mathbf{y}, k, m}{ }^{T} \cdot \mathbf{y}+\mathbf{w}_{\mathbf{z}, k, m}{ }^{T} \cdot \mathbf{z}-\mathbf{w}_{k, m}{ }^{T} \cdot \mathbf{b}_{k}  \tag{3.10}\\
\frac{\delta s_{k, m}}{\delta \mathbf{z}}=\mathbf{w}_{\mathbf{z}, k, m} \tag{3.11}
\end{gather*}
$$

where $\mathbf{w}_{y, k, m}{ }^{T}$ is the $m$-th row of $\mathbf{w}_{y, k}, \mathbf{w}_{z, k, m}{ }^{T}$ is the $m$-th row of $\mathbf{W}_{z, k}$, and $\mathbf{w}_{k, m}{ }^{T}$ is the $m$-th row of the de-mixing matrix $\mathbf{W}_{k}$. Thus,

$$
\begin{equation*}
\frac{\delta p\left(\mathbf{s}_{k}\right)}{\delta \mathbf{z}}=\sum_{m=1}^{M} \mathbf{w}_{\mathbf{z}, k, m}{ }^{T} \cdot c_{k, m}=\mathbf{W}_{\mathbf{z}, k}{ }^{T} \cdot \mathbf{c}_{k} \tag{3.12}
\end{equation*}
$$

where $\mathbf{c}_{k}=\left[c_{k, 1}, c_{k, 2}, \ldots, c_{k, M}\right]^{T}$. Finally, the derivative of the cost function can be calculated as

$$
\begin{equation*}
\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}=\sum_{k=1}^{K}\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot P\left(C_{k}\right) \cdot \mathbf{W}_{\mathbf{z}, k}{ }^{T} \cdot \mathbf{c}_{k} \tag{3.13}
\end{equation*}
$$

### 3.1.1. Optimization procedure

The optimization of the cost function can be performed using a gradient ascent method [24]:

$$
\begin{equation*}
\mathbf{z}_{(i+1)}=\mathbf{z}_{(i)}+\left.\alpha \cdot \frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}\right|_{(i)} \tag{3.14}
\end{equation*}
$$

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where (i) denotes the current iteration and $\alpha$ is the learning rate. Both the initial value, $\mathbf{z}_{(0)}$, and the learning rate are important to the algorithm, and they will be analyzed in detail in Section 3.4.3.

The gradient algorithm in (3.14) is a classical algorithm, but it has some disadvantages, primarily related with convergence speed, as shown in [24]. Thus, two alternative versions of the gradient were considered to improve its convergence speed.

The first alternative is normalizing the derivative of the cost function (discarding its modulus) and setting a constant learning rate:

$$
\begin{equation*}
\mathbf{z}_{(i+1)}=\mathbf{z}_{(i)}+\left.\alpha \cdot \frac{\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}}{\left\|\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}\right\|}\right|_{(i)} \tag{3.15}
\end{equation*}
$$

This change achieves a convergence speed that is dependent on the learning rate, $\alpha$, and not on the modulus of the derivative. This can speed up convergence, particularly at points far from the true maximum, which could result in small derivatives. This is not necessarily always the case, however, since we could be far from the true maximum and still have strong derivatives, whereas the derivative would typically become small as we approach a stationary point. On the other hand, the normalization could also make the algorithm oscillate around a maximum if the learning rate is set too high. This effect can be alleviated by adding an "annealing" procedure, that is, taking random steps to check the convergence of the algorithm by avoiding local minima and oscillations [136].

The second alternative is similar, but includes a variable learning rate $\alpha=\alpha_{(i)}$. This variable rate will follow Armijo's rule. That is, $\alpha$ will decrease every time the algorithm detects the solution is oscillating [24],

$$
\begin{equation*}
\mathbf{z}_{(i+1)}=\mathbf{z}_{(i)}+\left.\alpha_{(i)} \cdot \frac{\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}}{\left\|\frac{\delta p(\mathbf{y}, \mathbf{z})}{\delta \mathbf{z}}\right\|}\right|_{(i)} \tag{3.16}
\end{equation*}
$$

We have named the algorithm explained above, with its corresponding maximization procedure, as PREDICAMM (Prediction using ICAMM) [219].

### 3.2. Prediction based on least mean squared error: E-ICAMM

As stated in Section 3.1, the two most commonly used criteria to estimate missing data, $\mathbf{z}$, from known data, $\mathbf{y}$, are the ML criterion and the LMSE criterion, as shown in (3.2). The LMSE criterion seeks a nonlinear function that can reasonably approximate the conditional expectation $E[\mathbf{z} \mid \mathbf{y}]$. This can be done in several ways. The simplest form is to assume that a linear approximation is sufficient, thus reaching the solution of the linear LMSE criterion. The advantage of this criterion is that the linear operator can be obtained by simply solving a linear equation system (the Wiener-Hopf equations [236]). Moreover, only second-order statistics are necessary to define this system.

In this work, we propose a novel LMSE method that implements $E[\mathbf{z} \mid \mathbf{y}]$ by assuming an ICA mixture model with $K$ classes for the data $\mathbf{x}$, as shown in (3.3). The conditional probability $p(\mathbf{z} \mid \mathbf{y})$ can be expressed as

$$
\begin{gather*}
p(\mathbf{y}, \mathbf{z})=p(\mathbf{z} \mid \mathbf{y}) p(\mathbf{y})=\sum_{k=1}^{K} p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) p\left(\mathbf{y} \mid C_{k}\right) P\left(C_{k}\right)=\sum_{k=1}^{K} p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) P\left(C_{k} \mid \mathbf{y}\right) p(\mathbf{y})  \tag{3.17.a}\\
p(\mathbf{z} \mid \mathbf{y})=\sum_{k=1}^{\kappa} p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) p\left(C_{k} \mid \mathbf{y}\right) \tag{3.17.b}
\end{gather*}
$$

Hence, the conditional expectation will be

$$
\begin{align*}
E[\mathbf{z} \mid \mathbf{y}] & =\int \mathbf{z} \cdot p(\mathbf{z} \mid \mathbf{y}) \cdot d \mathbf{z}=\int \mathbf{z} \cdot\left(\sum_{k=1}^{K} p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) \cdot P\left(C_{k} \mid \mathbf{y}\right)\right) \cdot d \mathbf{z}=  \tag{3.18}\\
& =\sum_{k=1}^{K}\left(\int \mathbf{z} \cdot p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) \cdot d \mathbf{z}\right) \cdot P\left(C_{k} \mid \mathbf{y}\right)=\sum_{k=1}^{\kappa} E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot P\left(C_{k} \mid \mathbf{y}\right)
\end{align*}
$$

where $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$ is the conditional expectation for class $k$, and it could be regarded as the solution assuming that the current observation belongs to class $k$. In the ICA mixture model, each class is modeled by a separate ICA model. Thus, $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$ can be computed from the ICA model for $k$. From (3.4),

$$
\begin{equation*}
\mathbf{w}_{z, k} \cdot \mathbf{z}=\mathbf{s}_{k}+\mathbf{w}_{k} \cdot \mathbf{b}_{k}-\mathbf{w}_{y, k} \cdot \mathbf{y} \tag{3.19}
\end{equation*}
$$

Taking expectations on both sides of (3.19) results in

$$
\begin{align*}
& E\left[\mathbf{w}_{z, k} \cdot \mathbf{z} \mid \mathbf{y}, C_{k}\right]=E\left[\mathbf{s}_{k}+\mathbf{w}_{k} \cdot \mathbf{b}_{k}-\mathbf{w}_{y, k} \cdot \mathbf{y} \mid \mathbf{y}, C_{k}\right]  \tag{3.20}\\
& \mathbf{w}_{\mathbf{z}, k} \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]=E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]+\mathbf{w}_{k} \cdot \mathbf{b}_{k}-\mathbf{w}_{y, k} \cdot \mathbf{y}
\end{align*}
$$

Given the known values, $\mathbf{y}$, (3.20) represents an overdetermined linear system of equations, which can be solved in the unknown $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$, for instance, using the pseudoinverse $\mathbf{w}_{\mathbf{z}, k}{ }^{+}$:

$$
\begin{equation*}
E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]=\mathbf{w}_{\mathbf{z}, k}{ }^{+} \cdot\left(E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]+\mathbf{w}_{k} \cdot \mathbf{b}_{k}-\mathbf{w}_{y, k} \cdot \mathbf{y}\right) \tag{3.21}
\end{equation*}
$$

Solving the system requires knowledge of $E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]$. We have considered an iterative algorithm that iteratively computes $E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]$ and $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$, which is shown in Table 3.1.

## Initialization

$$
\operatorname{Set} E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]_{(0)}=\mathbf{0}
$$

## Updating

For $i=1, \ldots, I$, with $I$ being the maximum number of iterations:

$$
\begin{aligned}
& \left.E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]\right|_{(i)}=\mathbf{w}_{z, k}+\cdot\left(\left.E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right|_{(i-1)}+\mathbf{w}_{k} \cdot \mathbf{b}_{k}-\mathbf{w}_{y, k} \cdot \mathbf{y}\right) \\
& \left.\left.E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right|_{(i)}=\mathbf{w}_{z, k} \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]\right]_{(i)}+\mathbf{w}_{y, k} \cdot \mathbf{y}-\mathbf{w}_{k} \cdot \mathbf{b}_{k} \\
& \text { Continue until convergence or the maximum number of iterations is reached }
\end{aligned}
$$

Table 3.1. Iterative algorithm to compute the conditional expectation $E\left[\mathbf{z} \mid \mathbf{y}, \mathrm{C}_{\mathrm{k}}\right]$.

Results in this work correspond to only one iteration ( $I=1$ ) because no significant improvements were observed for more than one iteration. This iterative procedure is repeated for every class to obtain the values $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right], k=1, \ldots, K$ required in (3.18). Note that in the case of models with only one class $(K=1), E[\mathbf{z} \mid \mathbf{y}]=E\left[\mathbf{z} \mid \mathbf{y}, C_{1}\right]$ and the solution only requires solving (3.20). Otherwise, we need to compute $P\left(C_{k} \mid \mathbf{y}\right), k=1, \ldots, K$. Using Bayes' rule:

$$
\begin{equation*}
P\left(C_{k} \mid \mathbf{y}\right)=\frac{p\left(\mathbf{y} \mid C_{k}\right) \cdot P\left(C_{k}\right)}{p(\mathbf{y})}=\frac{p\left(\mathbf{y} \mid C_{k}\right) \cdot P\left(C_{k}\right)}{\sum_{l=1}^{K} p\left(\mathbf{y} \mid C_{l}\right) \cdot P\left(C_{l}\right)} \tag{3.22}
\end{equation*}
$$

where $p\left(\mathbf{y} \mid C_{k}\right), k=1, \ldots, K$, may be obtained using any statistical modeling from training data. In this thesis, we considered two possible options. If there is only one known value ( $M_{u n k}=1$ and therefore, $\mathbf{y}=y$ is scalar), the probabilities $p\left(y \mid C_{k}\right)$ are calculated from training data using non-parametric estimation using a Gaussian kernel, (3.8). If there is more than one known value ( $M_{u n k} \geq 2$ ), a second ICAMM is calculated using training data and only considering the known values $\mathbf{y}$. Then, the probabilities $p\left(\mathbf{y} \mid C_{k}\right)$ are calculated using (3.3).

We have named the above method E-ICAMM (Expectation using ICAMM). Figure 3.3 shows the behavior of E-ICAMM for two toy examples with one known variable and one unknown variable. As mentioned above, the values $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$ could be understood as several possible reconstructions which are then locally weighed by $P\left(C_{k} \mid \mathbf{y}\right)$.

This is shown clearly in Figure 3.3.a, which considers a case with two well-separated classes. The final reconstruction, $E[\mathbf{z} \mid \mathbf{y}]$, is very similar to $E\left[\mathbf{z} \mid \mathbf{y}, C_{1}\right]$ for values of $\mathbf{y}$ that clearly belong to class 1 and very similar to $E\left[\mathbf{z} \mid \mathbf{y}, C_{2}\right]$ for values that clearly belong to class 2 . At the crossing between the two classes, $E[\mathbf{z} \mid \mathbf{y}]$ is obtained as a weighted sum of $E\left[\mathbf{z} \mid \mathbf{y}, C_{1}\right]$ and $E\left[\mathbf{z} \mid \mathbf{y}, C_{2}\right]$. Figure 3.3.b shows a more complicated example: in this case, scattered data in the shape of a horseshoe were modeled by a five-class ICAMM. The reconstruction is locally weighed by the $P\left(C_{k} \mid \mathbf{y}\right)$ so that it follows the horseshoe shape, even though the $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$, $k=1 \ldots 5$, are straight lines.

a) Known values, $\mathbf{y}$

b) Known values, $\mathbf{y}$

Figure 3.3. E-ICAMM reconstruction for two toy examples: a) data drawn from an ICAMM with two classes; b) horseshoe-shaped unlabeled data modeled using an ICAMM with five classes.

### 3.2.1. Bias and local prediction error of E-ICAMM

Since it is the solution to the LMSE criterion, E-ICAMM is unbiased. This can be proved using (3.18). If we denote the prediction error by $\mathbf{e}=\left(\mathbf{z}-\hat{\mathbf{z}}_{E-I \text { Самм }}\right)=(\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}])$, then the bias is the expected prediction error with respect to known and unknown data,

$$
\begin{equation*}
E[\mathbf{e}]=E_{\mathbf{z}, \mathbf{y}}[\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}]]=E_{\mathbf{z}}[\mathbf{z}]-E_{\mathbf{y}}[\mathbf{z} \mid \mathbf{y}]=E_{\mathbf{z}}[\mathbf{z}]-E_{\mathbf{z}}[\mathbf{z}]=0 \tag{3.23}
\end{equation*}
$$

The mean squared error of the prediction can be obtained as the trace of the error covariance matrix:

$$
\begin{align*}
& E_{\mathbf{z}, \mathbf{y}}\left[\mathbf{e} \cdot \mathbf{e}^{T}\right]=E_{\mathbf{z}, \mathbf{y}}\left[(\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}])(\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}])^{T}\right]= \\
& =E_{\mathbf{z}, \mathbf{y}}\left[\mathbf{z} \cdot \mathbf{z}^{T}\right]-E_{\mathbf{z}, \mathbf{y}}\left[E[\mathbf{z} \mid \mathbf{y}] \cdot \mathbf{z}^{T}\right]-E_{\mathbf{z}, \mathbf{y}}\left[\mathbf{z} \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}\right]+E_{\mathbf{z}, \mathbf{y}}\left[E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}\right]=  \tag{3.24}\\
& =E_{\mathbf{z}}\left[\mathbf{z} \cdot \mathbf{z}^{T}\right]-2 \cdot E[\mathbf{z}] \cdot E[\mathbf{z}]^{T}+E_{y}\left[E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}\right]
\end{align*}
$$

One could also obtain the local mean squared error, i.e., the estimate of the prediction error of E-ICAMM for any given set of observed values $\mathbf{y}$. It is usually defined as the trace of the conditional covariance with respect to known data, $E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right]$. Being an expectation, this estimate is not likely to be a good indicator of the actual error of any one sample. However, this error can be used to estimate the variability of the true values around the prediction yielded by E-ICAMM, obtaining the prediction interval of E-ICAMM. This prediction interval can be used to determine the quality of the prediction and identifying points that are likely to be badly estimated.

Using the mixture model in (3.3), we can express $E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right]$ as a combination of $E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right], k=1 \ldots K:$

$$
\begin{align*}
E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right] & =\int \mathbf{e} \cdot \mathbf{e}^{T} \cdot p(\mathbf{z} \mid \mathbf{y}) \cdot d \mathbf{z}=\int \mathbf{e} \cdot \mathbf{e}^{T} \cdot\left[\sum_{k=1}^{K} p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) \cdot P\left(C_{k} \mid \mathbf{y}\right)\right] \cdot d \mathbf{z}=  \tag{3.25}\\
& =\sum_{k=1}^{K}\left[\int \mathbf{e} \cdot \mathbf{e}^{T} \cdot p\left(\mathbf{z} \mid \mathbf{y}, C_{k}\right) \cdot d \mathbf{z}\right] \cdot P\left(C_{k} \mid \mathbf{y}\right)=\sum_{k=1}^{K} E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right] \cdot P\left(C_{k} \mid \mathbf{y}\right)
\end{align*}
$$

The local error for each class, $E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right]$, can be expressed as

$$
\begin{align*}
& E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right]=E\left[(\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}]) \cdot(\mathbf{z}-E[\mathbf{z} \mid \mathbf{y}])^{T} \mid \mathbf{y}, C_{k}\right]= \\
& =E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]-E\left[\mathbf{z} \cdot E[\mathbf{z} \mid \mathbf{y}]^{T} \mid \mathbf{y}, C_{k}\right]-  \tag{3.26}\\
& -E\left[E[\mathbf{z} \mid \mathbf{y}] \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]+E\left[E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T} \mid \mathbf{y}, C_{k}\right]= \\
& =E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]-E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}-E[\mathbf{z} \mid \mathbf{y}] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}+E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}
\end{align*}
$$

where $E[\mathbf{z} \mid \mathbf{y}]$ is the E-ICAMM prediction and $E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right], k=1, \ldots, K$, are obtained during the process. The calculation of $E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]$ from (3.19) is straightforward, but complicated
and time consuming. Let us consider first the conditional correlation of $\mathbf{z}$ with respect to the known data and class $k, \Sigma_{z \mid y, c_{k}}$ :

$$
\begin{align*}
\Sigma_{z \mid y, C_{k}} & =E\left[\left(\mathbf{z}-E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]\right) \cdot\left(\mathbf{z}-E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]\right)^{T} \mid \mathbf{y}, C_{k}\right]= \\
& =E\left[\mathbf{w}_{\mathbf{z}, k}^{+}\left(\mathbf{s}_{k}-E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right) \cdot\left(\mathbf{s}_{k}-E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right)^{T}\left(\mathbf{w}_{\mathbf{z}, k}^{+}\right)^{T} \mid \mathbf{y}, C_{k}\right]=  \tag{3.27}\\
& =\mathbf{w}_{\mathbf{z}, k}{ }^{+} \cdot E\left[\left(\mathbf{s}_{k}-E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right) \cdot\left(\mathbf{s}_{k}-E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right]\right)^{T} \mid \mathbf{y}, C_{k}\right] \cdot\left(\mathbf{w}_{\mathbf{z}, k}^{+}\right)^{T}= \\
& =\mathbf{W}_{\mathbf{z}, k}{ }^{+} \cdot \Sigma_{\mathbf{s} \mid \mathbf{y}, C_{k}} \cdot\left(\mathbf{w}_{\mathbf{z}, k}{ }^{+}\right)^{T}
\end{align*}
$$

where $\Sigma_{z \mid y, c_{k}}$ is the conditional correlation of the sources with respect to known data and class $k$. Since $\Sigma_{z \mid \mathbf{y}, C_{k}}=E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]-E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}$,

$$
\begin{align*}
E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right] & =\Sigma_{\mathbf{z} \mid, \cdot C_{k}}+E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}=  \tag{3.28}\\
& =\mathbf{w}_{\mathbf{z}, k}^{+} \cdot \Sigma_{s \mid \mathbf{y}, C_{k}} \cdot\left(\mathbf{w}_{z, k}^{+}\right)^{T}+E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}
\end{align*}
$$

Solving the above requires knowledge of $E\left[\mathbf{s}_{k} \mid \mathbf{y}, C_{k}\right], E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]$ and $\Sigma_{s \mid y, c_{k}}$. We have considered a more refined version of the iterative algorithm in Table 3.1, which includes the calculation of these new variables. This iterative algorithm is shown in Table 3.2.

Results in this work correspond to only one iteration $(I=1)$ because no significant improvements were observed for more than one iteration. This iterative procedure is repeated for every class to obtain the values $E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right], k=1, \ldots, K$ required in (3.26). Afterward, the results of (3.28) can be substituted back in (3.26) to obtain:

$$
\begin{align*}
& E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right]=E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]-E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}- \\
& -E[\mathbf{z} \mid \mathbf{y}] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}+E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}=\Sigma_{z \mid \mathbf{y}, k}+E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}-  \tag{3.29}\\
& -E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}-E[\mathbf{z} \mid \mathbf{y}] \cdot E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]^{T}+E[\mathbf{z} \mid \mathbf{y}] \cdot E[\mathbf{z} \mid \mathbf{y}]^{T}= \\
& =\Sigma_{\mathbf{z} \mid \mathbf{y}, k}+\left(E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]-E[\mathbf{z} \mid \mathbf{y}]\right) \cdot\left(E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]-E[\mathbf{z} \mid \mathbf{y}]\right)^{T}
\end{align*}
$$

Finally, substituting (3.29) into (3.25),

$$
\begin{align*}
& E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right]=\sum_{k=1}^{K} E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{k}\right] \cdot P\left(C_{k} \mid \mathbf{y}\right)=  \tag{3.30}\\
& =\sum_{k=1}^{K} \Sigma_{z \mid \mathbf{y}, k} \cdot P\left(C_{k} \mid \mathbf{y}\right)+\sum_{k=1}^{K}\left(E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]-E[\mathbf{z} \mid \mathbf{y}]\right) \cdot\left(E\left[\mathbf{z} \mid \mathbf{y}, C_{k}\right]-E[\mathbf{z} \mid \mathbf{y}]\right)^{T} \cdot P\left(C_{k} \mid \mathbf{y}\right)
\end{align*}
$$

The conditional class probabilities $P\left(C_{k} \mid \mathbf{y}\right)$ are calculated as indicated for E-ICAMM (see (3.22)) and then used in (3.25). Finally, the local MSE can be found as $M S E_{\text {local }}=\operatorname{tr}\left\{E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right]\right\}$. Note that in the case of models with only one class $(K=1)$, $E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}\right]=E\left[\mathbf{e} \cdot \mathbf{e}^{T} \mid \mathbf{y}, C_{1}\right]$ and the solution only requires taking the trace of (3.26).


Table 3.2. Iterative algorithm to compute the conditional covariance $E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, \mathrm{C}_{\mathrm{k}}\right]$.
Figure 3.4 shows the estimated local prediction error for the two examples in Figure 3.3. The prediction error has been presented as a prediction interval: the area shadowed in light blue shows the prediction interval of the solution taking the average of the $E\left[\mathbf{z} \cdot \mathbf{z}^{T} \mid \mathbf{y}, C_{k}\right]$, and the area shadowed in gray represents the prediction interval of the solution of E-ICAMM, $E[\mathbf{z} \mid \mathbf{y}]$. These intervals were calculated as the solution, plus or minus twice the square root of the mean square error. The prediction intervals show the difference between the confidence in the results of the average and E-ICAMM, since E-ICAMM obtained a much smaller prediction interval across all values of the known variable. In both cases, the prediction interval covered almost all of the true data, confirming the interpretation of the local mean square error as the prediction interval.

The local prediction error was also an indicator of the average prediction error in the area. In fact, the difference between the actual MSE over the whole datasets and the average of the estimated local prediction errors was very small. The results of E-ICAMM shown in Figure 3.4.a have a true MSE equal to 0.0310 , and the average of the estimated MSE is 0.039 . Conversely, the values in Figure 3.4.b have a true MSE equal to 0.0233 and an estimated MSE of 0.0600 .


Figure 3.4. Estimated local prediction error for E-ICAMM for the two toy examples in Figure 3.3.

### 3.3. Other methods

In this work, the proposed prediction methods are compared with several types of predictors. These methods were selected due to their similarities to E-ICAMM or PREDICAMM, or due to their application to real data (which will be shown in Chapter 5).

The first method selected for comparison was Kriging [116], which is a classical linear predictor that is widely-used in geostatistics and other applications where the topographical distribution of the signal is of importance. It was chosen because of this importance, and it was considered both for simulated data and real data. Kriging is an implementation of the linear LMSE criterion for spatial data, making it similar to E-ICAMM, which optimizes the LMSE criterion.

The second method for comparison was Wiener structures [278], a simple nonlinear prediction method that is composed of a linear predictor followed by a nonlinear correction term. Wiener structures have been used to successfully predict data from NDT applications [211], which is the reason for their choosing. Wiener structures were used on simulated data and on real data.

The third considered method was matrix completion [36], a nonlinear method that estimates missing data from a matrix from a few revealed entries. This method was chosen because of its similarities with E-ICAMM and PREDICAMM, since it is an interpolator that considers existing data and an underlying structure in order to reconstruct missing data. Given the requirements of matrix completion (as explained in Section 3.3.3), it was considered only for simulated data.

The fourth and last method for comparison was splines [69]. In splines, the data are usually modeled using low-order polynomials that represent the lines or surfaces of lower energy. They are a classic interpolation method. Furthermore, spherical splines are the typical interpolator for electroencephalographic data [199], which is the reason why they were chosen for comparison against E-ICAMM and PREDICAMM. Since they assume an underlying spherical structure, spherical splines were only considered for their application on real data from an EEG experiment, in Chapter 5. For non-EEG data, linear splines were used.

There are other methods that could be used for prediction, such as artificial neural networks (ANN). However, previous works show that simpler methods (e.g., Wiener structures) can model the nonlinearities in the data and obtain a good prediction at a lower computational cost than ANN [222].

### 3.3.1. Kriging

Linear prediction is a fundamental tool in many different fields: adaptive filtering, system identification, economics, geophysics, etc. [163]. It flows naturally from scenarios where one can assume an underlying linear system, and it is optimal in those cases where the signals follow Gaussian distributions.

Let us assume that there is a random stationary signal $x(n)$. The goal of linear prediction is to estimate the value of the signal at time $n+l, \hat{x}(n+l)$, from its last $N$ values, $x(n-1), x(n-2), \ldots, x(n-N)$, where $l$ is known as the "lag" in the prediction given by the algorithm. Thus, the linear prediction can be written as

$$
\begin{equation*}
\hat{x}(n+l)=\sum_{i=1}^{N} a_{i} \cdot x(n-i)=\mathbf{a}^{T} \cdot \mathbf{x}(n-1) \tag{3.31}
\end{equation*}
$$

where the vector $\mathbf{x}(n-1)=[x(n-1), x(n-2), \ldots, x(n-N)]^{T}$ comprises known data and the predictor's weights are included in vector $\mathbf{a}=\left[a_{1}, a_{2}, \ldots, a_{N}\right]^{T}$ (super index $T$ indicates matrix transpose). Linear predictors are usually classified by their lag value; depending on $l$, we speak of prediction $(l>0)$, interpolation $(l=0)$ or regression $(l<0)$. The unknown parameters a are usually optimized with respect to the mean squared error (MSE) between real values and predicted values, resulting in the optimal values, $\mathbf{a}_{o p t}$. In this case, the cost function, $J(\mathbf{a})$, is

$$
\begin{equation*}
J(\mathbf{a})=E\left[(x(n+1)-\hat{x}(n+1))^{2}\right]=E\left[e^{2}(n+1)\right] \tag{3.32}
\end{equation*}
$$

where $e(n)$ is the prediction error. The gradient of the cost function can be used to find an optimal set of parameters, $\mathbf{a}_{\text {opt }}$. Assuming stationary Normally-distributed data, this process will result in the Wiener-Hopf equations [236]:

$$
\begin{gather*}
\mathbf{R}_{x} \cdot \mathbf{a}_{o p t}=\mathbf{r}_{x, 0}  \tag{3.33}\\
\mathbf{R}_{x}=\left[\begin{array}{cccc}
r_{x}(0) & r_{x}(1) & \cdots & r_{x}(N-1) \\
r_{x}(1) & r_{x}(0) & \cdots & r_{x}(N-2) \\
\vdots & \vdots & \ddots & \vdots \\
r_{x}(N-1) & r_{x}(N-2) & \cdots & r_{x}(0)
\end{array}\right]  \tag{3.34.a}\\
\mathbf{r}_{x, 0}=\left[\begin{array}{l}
\left.r_{x}(l+1), r_{x}(l+2), \ldots, r_{x}(l+N)\right]^{T}
\end{array}\right] \tag{3.34.b}
\end{gather*}
$$

where $\mathbf{R}_{x}$ is the covariance matrix of signal $x(n), \mathbf{r}_{x, 0}$ is its covariance vector, and $r_{x}(\tau)$ is the covariance function for lag $\tau$. Assuming that the covariance matrix is nonsingular, the optimal linear predictor can be calculated by inverting $\mathbf{R}_{x}$,

$$
\begin{equation*}
\mathbf{a}_{o p t}=\mathbf{R}_{x}^{-1} \cdot \mathbf{r}_{x, 0} \tag{3.35}
\end{equation*}
$$

Since $\mathbf{R}_{x}$ is a Toeplitz matrix (each descending diagonal from left to right is constant), the system of equations (3.33) can be solved efficiently by using the classical Levinson-Durbin algorithm [155].

Geostatistics is a field where linear predictors show a large presence. One of the most important algorithms in this area is Kriging, a linear interpolator that calculates $\mathbf{a}_{\text {opr }}$ using the spatial covariance of data [116]. The original algorithm, Simple Kriging, is similar to a 2-D linear predictor. Thus, equation (3.31) becomes

$$
\begin{equation*}
x\left(\mathbf{p}_{0}\right)=\sum_{i=1}^{N} a_{i} \cdot x\left(\mathbf{p}_{i}\right)=\mathbf{a}^{T} \cdot \mathbf{x} \tag{3.36}
\end{equation*}
$$

where $\mathbf{p}_{i}$ is the position of the $i$-th data point, $x\left(\mathbf{p}_{i}\right)$, and $\mathbf{x}=\left[x\left(\mathbf{p}_{1}\right), x\left(\mathbf{p}_{2}\right), \ldots, x\left(\mathbf{p}_{N}\right)\right]^{T}$. Typically, only the $N$ nearest positions are chosen for prediction, or $N$ is equal to the number of points within a certain distance of the unknown data point. Equations (3.34.a) and (3.34.b) are modified to include the spatial distribution of $x\left(\mathbf{p}_{0}\right)$ :

$$
\begin{gather*}
\mathbf{R}_{x}=E\left[\mathbf{x} \cdot \mathbf{x}^{T}\right]=\left[\begin{array}{cccc}
r_{x}\left(\mathbf{p}_{1}-\mathbf{p}_{1}\right) & r_{x}\left(\mathbf{p}_{1}-\mathbf{p}_{2}\right) & \cdots & r_{x}\left(\mathbf{p}_{1}-\mathbf{p}_{N}\right) \\
r_{x}\left(\mathbf{p}_{2}-\mathbf{p}_{1}\right) & r_{x}\left(\mathbf{p}_{2}-\mathbf{p}_{2}\right) & \cdots & r_{x}\left(\mathbf{p}_{2}-\mathbf{p}_{N}\right) \\
\vdots & \vdots & \ddots & \vdots \\
r_{x}\left(\mathbf{p}_{N}-\mathbf{p}_{1}\right) & r_{x}\left(\mathbf{p}_{N}-\mathbf{p}_{2}\right) & \cdots & r_{x}\left(\mathbf{p}_{N}-\mathbf{p}_{N}\right)
\end{array}\right]  \tag{3.37.1}\\
\mathbf{r}_{x, 0}=E\left[\mathbf{x} \cdot x\left(\mathbf{p}_{0}\right)\right]=\left[\begin{array}{l}
\left.r_{x}\left(\mathbf{p}_{1}-\mathbf{p}_{0}\right), r_{x}\left(\mathbf{p}_{2}-\mathbf{p}_{0}\right), \ldots, r_{x}\left(\mathbf{p}_{N}-\mathbf{p}_{0}\right)\right]^{T}
\end{array}\right] \tag{3.37.2}
\end{gather*}
$$

Given the properties of the covariance of a real function, $\mathbf{R}_{x}$ is still Toeplitz for the vast majority of applications. Kriging is the best linear unbiased predictor (BLUP) for zero-mean signals. A common extension of the base algorithm, named Ordinary Kriging (OK), achieves the same performance with constant-mean signals. In the case of OK, the system of equations (3.33) becomes

$$
\left[\begin{array}{cc}
\mathbf{R}_{x} & \left.\mathbf{1}_{N, 1}\right\rceil\left\lceil\mathbf{a}_{o p t}\right.  \tag{3.38}\\
\mathbf{1}_{1, N} & 0
\end{array}\right]=\left[\begin{array}{c}
\mathbf{r}_{x, 0} \\
\mu
\end{array}\right]=\left[\begin{array}{c} 
\\
1
\end{array}\right]
$$

where $\mathbf{1}_{M, N}$ is a vector of size $[M \times N]$. Kriging and its variants are very important in geostatistical applications, such as the distribution of ground properties [76], natural properties [209], and reconstruction of missing data traces [45]. Kriging is a classical algorithm, but new variants are still being researched for several applications [103,63,104], some of them including nonlinear stages in order to improve the algorithm [15].

### 3.3.2. Wiener structures

The second method we would like to study is the Wiener-Hammerstein structures. There are three types of structures: Wiener structures, composed of a linear predictor followed by a nonlinear correction stage [278]; Hammerstein structures, composed of a nonlinear function followed by a linear predictor [49]; and Wiener-Hammerstein structures, hybrid structures composed of two nonlinear stages separated by a linear predictor [30]. These three types of structures are shown in Figure 3.5.

The three types of structures are being currently used for the modeling of nonlinear systems [64], as well as active noise control [288]. In many cases, they are considered as an alternative because of their simplicity, since the simple nonlinear model of the system (if not exact) is usually adequate for the application [259,268,211,222]. Wiener structures in particular have been used to model nonlinear systems in many different applications. The GTS has used Wiener structures in several works on infrared applications [268] and seismic data [211,222].

In particular, this work will consider Wiener structures, which comprise a linear stage followed by a nonlinear correction with no memory. The linear stage can implement any linear prediction algorithm; we used Ordinary Kriging ( [116,211]), introduced above.

Let us study the nonlinear stage of the structure. If $x_{p}(n+l)$ is the output of the linear prediction, with $l$ being the lag in the prediction obtained from data samples $x(n-1), \ldots, x(n-N)$. The nonlinear stage of the Wiener structure is defined as

$$
\begin{equation*}
G\left(x_{p}(n+l)\right)=E\left[x(n+l) \mid x_{p}(n+l)\right] \tag{3.39}
\end{equation*}
$$



Figure 3.5. Wiener structure (top), Hammerstein structure (middle), and Wiener-Hammerstein structure (bottom).
Thus, the nonlinearity implemented by the Wiener structure, $G(\cdot)$, is the conditional expectation of real data with respect to the output of the linear predictor. Assuming that $x(n)$ is stationary, $G(\cdot)$ can be estimated from the signal. This estimation can be done in many ways, but we considered two methods: direct sample estimation and polynomial approximation ( [268]).

### 3.3.2.a. Direct sample estimation

The nonlinear function $G(\cdot)$ can be estimated by applying a sliding window on a set of training data:

$$
\begin{equation*}
G\left(\mathbf{x}_{p}(i)\right)=\frac{1}{\Delta} \sum_{i}^{i+\Delta-1} w_{i} \cdot \mathbf{x}_{l}(i) \tag{3.40}
\end{equation*}
$$

where $\mathbf{x}_{p}$ is a vector with the output values of the linear predictor, sorted from lower to higher; $\mathbf{x}_{l}$ is a vector with the real data values that correspond to those same values (and, thus, sorted in the same way as $\mathbf{x}_{p}$ ); and $w_{i}$ is the $i$-th value of the sliding window of length $\Delta$. This estimation will return a finite set of points - the curve $G(\cdot)$ is interpolated from this set.

In this work, all instances of direct sample estimation were done using a rectangular window of length $\Delta=21$. This value was selected rather heuristically using several experiments with simulated data, using the same experiments shown later in this Chapter.

### 3.3.2.b. Polynomial approximation

A one-dimensional approximation of the nonlinear stage of the Wiener structure was presented in [268]. Assuming that $x_{p}(n)$ is a Gaussian sequence with zero mean and normalized variance, and taking $x_{p}(n+l)=x_{p}$ and $x(n+l)=x$ for convenience of notation:

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$$
\begin{equation*}
G\left(x_{p}\right)=\sum_{m=1}^{\infty} \frac{1}{m!} \cdot C_{m}\left(x, x_{p}\right) \cdot H_{m}\left(x_{p}\right) \tag{3.41}
\end{equation*}
$$

where $C_{m}$ is the cross cumulant, defined as $C_{m}(x, y)=$ cumulant $(x, y, \ldots, y)$ and $H_{m}$ is the $m$-th order Hermite polynomial. The assumption of Gaussianity is not as restrictive as it might seem, since $x_{p}(n)$ is the output of a linear predictor - thus, for a large enough $N$, the Central
Limit Theorem ensures the Gaussianity of the data. In previous works, we have found that the series can be truncated at the third term [268]. In that case, the result is:

$$
\begin{equation*}
G_{3}\left(x_{p}\right)=\frac{1}{6}\left(a_{3}-3 a_{1}\right) x_{p}^{3}+\frac{1}{2} a_{2} x_{p}{ }^{2}+\left(\frac{5}{2} a_{1}-\frac{1}{2} a_{3}\right) x_{p}-\frac{1}{2} a_{2} \tag{3.42}
\end{equation*}
$$

where $a_{i}=E\left[x \cdot x_{p}{ }^{i}\right]$ are the cross-moments, estimated from training data.

### 3.3.3. Matrix completion based on smoothed rank function (SRF)

In many practical problems, one would like to recover a matrix from a sampling of its entries; for instance, one could attempt to infer the answers in a partially-answered survey (this is also known as the "Netflix problem"). Matrix completion consist in the reconstruction of these missing entries from known data by assuming that the matrix is structured, i.e., it has low rank [36]. It can be regarded as an extension of compressed sensing, since it shows that many objects or structures, and not only sparse signals and images, can be reconstructed from a limited set of measurements.

Consider a matrix $\mathbf{M}$ of which only a few entries are known. We would like to recover the whole matrix based on these revealed entries; however, it is clear that solving this problem is not possible without any additional information. Now, let us assume that the matrix is of dimension $\left[n_{1} \times n_{2}\right]$ and its rank is $r$; it is straightforward to calculate that the number of degrees of freedom of this matrix is equal to $r\left(n_{1}+n_{2}-r\right)$. So, in order to exactly recover the matrix, it is necessary that the number of revealed entries is larger than this number of degrees of freedom. In fact, recovery of the matrix from a small number of known entries is possible as long as the matrix is low-rank and entries are selected uniformly [36]. In brief, the objetive of matrix completion is to obtain a matrix with minimum rank, given a subset of its entries.

There are many matrix completion algorithms, such as FPCA [97] and SDP [81]. In this work, we considered an algorithm based on a smoothed rank function (SRF) [95], which makes use of a continuous and differentiable approximation of the discontinuous rank function. This function can then be minimized using any classical optimization technique.

Consider an unknown matrix $\mathbf{M}$ of dimension $\left[n_{1} \times n_{2}\right.$ ] and rank $r$ for which only $m$ entries have been revealed. Assume that $m$ is sufficiently large and the locations of the observed entries are sufficiently uniformly distributed; in that case, the matrix completion problem is to find a matrix $\mathbf{X}_{\text {opt }}$ that solves the optimization problem:

$$
\begin{gather*}
\min \operatorname{rank}(\mathbf{X}) \\
\text { s.t. } X_{i j}=M_{i j}, \quad(i, j) \in \Omega \tag{3.43}
\end{gather*}
$$

where $\Omega$ is the set of locations corresponding to the $m$ observed entries. SRF uses a continuous approximation $F(\cdot)$ of the rank function and then applies continuous optimization techniques to minimize it. One such function is the Gaussian function:

$$
\begin{equation*}
F_{\delta}(\mathbf{X})=n-\sum_{k=1}^{n} e^{-\sigma_{k}^{2}(\mathbf{X}) / 2 \delta^{2}} \tag{3.44}
\end{equation*}
$$

where $\delta$ is a parameter, $\sigma_{k}(\mathbf{X})$ is the $k$-th singular value of $\mathbf{X}$, and $n=\min \left(n_{1}, n_{2}\right)$. As $\delta$ approaches zero, $F_{\delta}(\cdot)$ approaches the rank function. Equation (3.44) is minimized using any gradient algorithm while enforcing the condition $X_{i j}=M_{i j},(i, j) \in \Omega$.

### 3.3.4. Splines

Splines are smooth polynomial curves that are piecewise-defined, and are smooth at the connections between pieces [69]. The highest order of the piecewise polynomials is the order of the spline. Splines can obtain good results even with low orders. For instance, the most commonly-used splines are cubic splines, which are of order 3. The smooth curve obtained by splines can be used for many purposes, one of them being data interpolation, since it can be used to evaluate the fitted function at new points. The term "spline" was adopted from the name of a flexible strip of metal commonly used by draftsmen to assist in drawing curved lines. This strip was held in place at several points or "knots," and the strip would adopt the shape of minimum strain energy between knots.

Let us assume that we have a set of measurements $z\left(y_{j}\right)$ at prescribed points $y_{j}, j=1 \ldots N$. Briefly, cubic splines fit a piecewise function of the form

$$
P(y)= \begin{cases}p_{1}(y), & \text { if } y_{1} \leq y \leq y_{2}  \tag{3.45}\\ p_{2}(y), & \text { if } y_{2} \leq y \leq y_{3} \\ \vdots & \vdots \\ p_{N-1}(y), & \text { if } y_{N-1} \leq y \leq y_{N}\end{cases}
$$

to the measurements, where $p_{i}$ is the 3 rd -degree polynomial $p_{i}(y)=a_{i} \cdot y^{3}+b_{i} \cdot y^{2}+c_{i} \cdot y+d_{i}$ for the $i$-th piece, $i=1 \ldots N-1$. The coefficients $a_{i}, b_{i}, c_{i}, d_{i}$ of the piecewise polynomial are calculated such that: a) $P(y)$ and its first two derivatives are continuous in the range $\left[y_{1}, y_{N}\right]$; b) the piecewise function is exactly equal to the observed value at each one of the nodes, that is, $P\left(y_{j}\right)=z\left(y_{j}\right), j=1 \ldots N$.

### 3.3.4.a. Thin-plate splines

Thin-plate splines (TPS) are a generalization of splines to two or more dimensions [74]. TPS can be likened to the bending of a thin sheet of metal; just like the metal has rigidity, the thinplate splines also resist bending by setting a penalty involving the smoothness of the fitted surface.

Let us assume that we have a set of measurements, $\mathbf{z}\left(\mathbf{y}_{i}\right)$, at prescribed coordinates $\mathbf{y}_{j}$, $j=1 \ldots N$. The thin-plate spline $\mathbf{f}(\mathbf{y})$ is obtained by minimizing the cost function $p \cdot E(\mathbf{f})+(1-p) \cdot R(\mathbf{f})$, where $E(\mathbf{f})$ measures the fitting error, $R(\mathbf{f})$ measures the roughness
of the spline, and $p$ is a smoothing parameter. Assuming that $\mathbf{y}$ is two-dimensional, $\mathbf{y}=\left[y_{1}, y_{2}\right]^{T}$, the two terms can be expressed as

$$
\begin{gather*}
E(\mathbf{f})=\sum_{j=1}^{N}\left\|\mathbf{f}\left(\mathbf{y}_{j}\right)-\mathbf{z}\left(\mathbf{y}_{j}\right)\right\|^{2}  \tag{3.46.a}\\
R(\mathbf{f})=\iint_{\mathbb{R}^{2}} \int^{\left(\left\|\frac{\delta^{2} \mathbf{f}(\mathbf{y})}{\delta y_{1}{ }^{2}}\right\|^{2}+2\left\|\frac{\delta^{2} \mathbf{f}(\mathbf{y})}{\delta y_{1} \cdot \delta y_{2}}\right\|^{2}+\left\|\frac{\delta^{2} \mathbf{f}(\mathbf{y})}{\delta y_{2}{ }^{2}}\right\|^{2}\right) \cdot d y_{1} \cdot d y_{2}} \tag{3.46.b}
\end{gather*}
$$

and the thin-plate spline is obtained by minimizing the cost function. In practice, the TPS is defined as a warp of a flat surface. The parameters of this warp are computed by solving a linear system of equations.

### 3.3.4.b. Spherical splines

Spherical splines are another extension of splines to multiple dimensions. However, whereas thin-plate splines fit an infinite thin plane to a finite number of points, spherical splines fit a thin sphere instead [199]. The advantage is that the mathematical derivations and calculations are easier when the data to fit are spherically distributed. A particularly important case of this is electroencephalographic data and scalp current densities. The topographic patterns of these magnitudes are commonly used to investigate sensory, cognitive and motor activity in the human brain. However, actual studies capture data at a limited number of locations and these topographic images are constructed with the help of interpolation methods. There are many methods, although the most common of them are splines-based methods, the most common being spherical splines. Spherical splines are used because they are easier to implement and because they seem consistent with the widely-used spherical head models. However, these splines do not involve the physics of electric fields in the head. Thus, the application of spherical splines to EEG data is justified only by numerical simulations of dipole sources in the brain. For real EEG data, splines are fit to the potential at the electrodes, which imperfectly sample the superior surface of the head and completely neglect the inferior head surface. However, they are widely used in common applications of EEG, even today [83,84].

The interpolation method is as follows. Let $z(\mathbf{y})$ be the potential at some position $\mathbf{y}$ on the surface of a sphere of radius $r$, and let $\mathbf{y}_{j}$ be the location of the $j$-th measurement electrode, $j=1 \ldots N$. Spherical splines assume that the potential at any point $\mathbf{y}$ on the surface of the sphere can be approximated by:

$$
\begin{gather*}
z(\mathbf{y})=a_{0}+\sum_{j=1}^{N} a_{j} \cdot g_{m}\left(\mathbf{y}^{T} \mathbf{y}_{j}\right)  \tag{3.47.a}\\
g_{m}(x)=\frac{1}{4 \pi} \sum_{n=1}^{\infty} \frac{2 n+1}{(n(n+1))^{m}} P_{n}(x) \tag{3.47.b}
\end{gather*}
$$

where $P_{n}(x)$ is the ordinary Legendre polynomial of order $n$. In practice, the sum is truncated at some finite number of terms $n_{\max }$, depending upon the value of the parameter $m$. The best results are achieved when $m$ equals 3 or 4 [86], and these values have been used in most studies. The coefficients $a_{j}, j=0,1, \ldots, N$ are determined by satisfying two conditions. First, the interpolation function must return the data when evaluated at the original data points. Second, the coefficients must add up to zero. These conditions can be combined into a single linear system of equations.

### 3.4. Simulations

The proposed methods were tested using several simulations before their application on real data (which will be studied in Chapter 5). Figure 3.6 summarizes the different methods and combinations considered in this Chapter: E-ICAMM, PREDICAMM, and the proposed state-of-the-art methods.


Figure 3.6. Different method configurations considered during the simulations in this chapter. The shaded boxes represent the original contributions of this thesis.

### 3.4.1. Problem description

### 3.4.1.a. Probability density functions used for simulated data

Four different probability density functions were chosen to test the proposed methods: uniform within the interval $[-1,1]$, Laplacian density with zero mean and unit variance; and two different K-distributions ( $[120,119]$ ) with shape parameters $v=1$ (K1) y $v=10$ (K10) (both with zero mean). All four distributions considered, and their statistics, are shown in Table 3.3. The selection of these distributions was based on several reasons. The uniform distribution was chosen because of its simplicity and because it is the most typical platykurtic (sub-Gaussian) distribution. The Laplacian distribution was chosen since it is the most typical leptokurtic (super-Gaussian) distribution. Finally, both K-distributions were chosen because they best model common noise in many non-destructive testing applications, especially radar (including GPR) [202].

The probability density functions were used to generate several different datasets, each one with a different combination of number of classes ( $K$ ), number of variables ( $M$ ), number of unknowns ( $M_{u_{n k},}, M_{u_{n k k}}<M$ ), and sources. Details for each one of these datasets are shown in Table 3.4. The number of unknown variables is indicated only for prediction purposes. In practice, data were generated completely known, and missing values were removed just before prediction.

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| Probability density <br> function | Skewness | Kurtosis | Plot |
| :---: | :---: | :---: | :---: |
| Uniform | 0 | -1.2 (platykurtic) |  |
| Laplacian | 0 | 3 (leptokurtic) |  |
| K1 | 1.7 | 5.3 (leptokurtic) |  |
| K10 | 0.8 |  |  |

Table 3.3. Data distributions used for simulation.

| Dataset |  | $\begin{gathered} \# \text { of } \\ \text { classes, } K \end{gathered}$ | $\begin{gathered} \# \text { of } \\ \text { variables, } \\ M \end{gathered}$ | \# of unknown variables, $M_{u n k}$ | Probability density functions of the sources, $p\left(s_{k}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Single-class datasets | 1 | 1 | 2 | 1 | Uniform, Laplacian |
|  | 2 | 1 | 3 | 1 | Uniform, Laplacian, K1 |
|  | 3 | 1 | 4 | 2 | Uniform, Laplacian, K1, K10 |
|  | 4 | 1 | 4 | 2 | Uniform |
|  | 5 | 1 | 4 | 2 | Laplacian |
| Multipleclass datasets | 6 | 2 | 3 | 1 | Uniform, Laplacian |
|  | 7 | 2 | 4 | 2 | Uniform, Laplacian |
|  | 8 | 2 | 4 | 2 | Laplacian, K1 |
|  | 9 | 2 | 4 | 2 | K1, K10 |
|  | 10 | 3 | 3 | 1 | Uniform, Laplacian, K1 |
|  | 11 | 3 | 4 | 2 | Uniform, Laplacian, K1 |
|  | 12 | 3 | 3 | 1 | Uniform, Laplacian, K1, K10 |
|  | 13 | 3 | 4 | 2 | Uniform, Laplacian, K1, K10 |

Table 3.4. Details of all datasets used in the simulated experiment.

### 3.4.1.b. Parameter estimation

During each iteration of the experiments, the generated data were split 50/50 into training and test, as shown in Figure 3.7. The training data were used to estimate the parameters of each of the proposed methods using supervised training.

E-ICAMM and PREDICAMM require the estimation of the ICAMM parameters, $\mathbf{W}_{k}, p\left(\mathbf{s}_{k}\right), \mathbf{b}_{k}, \quad k=1 \ldots K$. These parameters were estimated using supervised training with the MIXCA procedure [231] with JADE as the embedded ICA method. Prediction was performed using the sampling scheme shown in Figure 3.1.a. As mentioned in Section 3.1.1, the selection of the initial value for PREDICAMM is very important, as is the selection of the gradient algorithm. These values were set experimentally, and the results are shown in Section 3.4.3.

For Kriging, the data were treated as if the description in Figure 3.7 was a two-dimensional problem, and the $m$-th value of the $n$-th observation was denoted as $x(\mathbf{p}), \mathbf{p}=[m, n]^{T}$. The covariance matrix and the covariance vector ( $\mathbf{R}_{x}$ and $\mathbf{r}_{x, 0}$ respectively) were estimated using the sample spatial covariance calculated from training data, and each unknown position was reconstructed using all the known positions within a distance of $M_{K_{r i g}}$ samples. This value was chosen empirically.


Figure 3.7. Graphical description of the prediction problem. The hatched area indicates missing data.
The linear stage of the Wiener structure was implemented using Kriging. The nonlinear correction was obtained using the second half of the training data as validation data. To this effect, the last $M_{u n k}$ variables were predicted as if they were missing, and the prediction was compared against the true values in order to estimate the nonlinear correction using direct sample estimation (as shown in Section 3.3.2.a).

The splines prediction was performed using thin-plate splines. The splines' parameters were fit using the training data, considering the first $M-M_{u n k}$ variables as the coordinates, $\mathbf{y}$, and the latter $M_{u n k}$ variables as the values to fit, $\mathbf{z}$. The smoothing value for the fit estimation, $p$, was set empirically to 1 .

SRF requires no previous training. For prediction, all the data were passed to the algorithm as a single $[M \times N]$ matrix with missing values as indicated in Figure 3.7. The iteration parameters of the algorithm were set empirically, and they are the same as in [95].

### 3.4.2. Error indicators

Table 3.5 shows the four error indicators that were selected to evaluate the performance of all method: signal-to-interference ratio, Kullback-Leibler divergence, correlation at lag zero, and mean structural similarity.

### 3.4.2.a. Signal-to-interference ratio

The first indicator chosen was the Signal-to-Interference Ratio (SIR), a measure of the average squared error in the data, and a commonly-used error indicator [269]. It is defined as:

$$
\begin{equation*}
S I R=\frac{\sum_{n=1}^{N}\|\mathbf{z}(n)\|^{2}}{\sum_{n=1}^{N}\|\mathbf{z}(n)-\hat{\mathbf{z}}(n)\|^{2}} \tag{3.48}
\end{equation*}
$$

where $\hat{\mathbf{z}}(n)$ is the estimate of the true data, $\mathbf{z}(n), N$ is the number of data samples to estimate, and $\|\cdot\|^{2}$ is the Euclidean norm of a vector. Notice that SIR is the inverse of the normalized square error of the estimate.

| Error indicator | Acronym | Measured quality |
| :---: | :---: | :---: |
| Signal-to-Interference Ratio <br> $[\mathbf{2 6 9 ]}$ | SIR | Squared prediction error |
| Kullback-Leibler divergence <br> $[146]$ | KLD | Divergences between probability density |
| functions |  |  |

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Table 3.5. Summary of the prediction error indicators considered in this work.
3.4.2.b. Kullback-Leibler divergence

The second error indicator was the Kullback-Leibler divergence (KLD), a classical indicator of distance between two probability distribution functions [146]. In this case, we will compute the distance between the probability density of the predicted data $\left(p_{\hat{\mathbf{z}}}(\mathbf{v})\right)$ and that of the real data $\left(p_{\mathbf{z}}(\mathbf{v})\right)$. A symmetrized version of the indicator was used:

$$
\begin{equation*}
K L D=\int_{-\infty}^{\infty} p_{\hat{\mathbf{z}}}(\mathbf{v}) \cdot \log \left(\frac{p_{\hat{\mathbf{z}}}(\mathbf{v})}{p_{\mathbf{z}}(\mathbf{v})}\right) \cdot \mathrm{d} \mathbf{v}+\int_{-\infty}^{\infty} p_{\mathbf{z}}(\mathbf{v}) \cdot \log \left(\frac{p_{\mathbf{z}}(\mathbf{v})}{p_{\hat{\mathbf{z}}}(\mathbf{v})}\right) \cdot \mathrm{d} \mathbf{v} \tag{3.49}
\end{equation*}
$$

### 3.4.2.c. Cross-correlation

The value of both the previously-mentioned indicators does not depend on the positioning of each error. This is especially true for KLD, since densities are compared without considering their position within the data. Because of this, the third error indicator chosen was the crosscorrelation between true data and predicted data (CORR), which measures the temporal similarity between those data [192]. It is a classical measure of similarity between two sequences of numbers. It can be defined in a different, related form. In our case, we have defined it as

$$
\begin{equation*}
\operatorname{COR} R=\frac{\sum_{n=1}^{N} \mathbf{z}(n)^{T} \hat{\mathbf{z}}(n)}{\max \left(\sum_{n=1}^{N}\|\mathbf{z}(n)\|^{2}, \sum_{n=1}^{N}\|\hat{\mathbf{z}}(n)\|^{2}\right)} \tag{3.50}
\end{equation*}
$$

With this definition, we assure that the CORR value is inside the range $[-1,1]$.

### 3.4.2.d. Structural similarity index

The fourth and last error indicator was the structural similarity index (SSIM), an indicator of the likeness of the structures in two images [275]. This comparison is performed first at a local level, by comparing the differences in "luminance," "contrast" and "structures" corresponding to each couple $z_{m}(n), \hat{z}_{m}(n), m=1, \ldots, M_{u n k}$, as defined by the following equations:

$$
\begin{align*}
& \text { luminance comparison: } l\left(z_{m}(n), \hat{z}_{m}(n)\right)=\frac{2 \mu_{z}(n) \cdot \mu_{\hat{z}}(n)+C_{1}}{\mu_{z}^{2}(n)+\mu_{\hat{z}}^{2}(n)+C_{1}} \\
& \text { contrast comparison: } c\left(z_{m}(n), \hat{z}_{m}(n)\right)=\frac{2 \sigma_{z}(n) \cdot \sigma_{\hat{z}}(n)+C_{2}}{\sigma_{\hat{z}}^{2}(n)+\sigma_{\hat{z}}^{2}(n)+C_{2}}  \tag{3.51}\\
& \text { structure comparison: } s\left(z_{m}(n), \hat{z}_{m}(n)\right)=\frac{\sigma_{z \hat{z}}(n)+C_{3}}{\sigma_{z}(n) \cdot \sigma_{\hat{z}}(n)+C_{3}}
\end{align*}
$$

where $n$ denotes the $n$-th estimated sample, $n=1, \ldots, N ; \mu_{z}(n), \mu_{i}(n)$ are the local estimates of the means of the true and the predicted values, respectively; $\sigma_{z}(n), \sigma_{\hat{z}}(n)$ are the corresponding local estimates of the standard deviation; $\sigma_{z z}(n)$ is the local estimate of the cross-correlation coefficient; and $C_{1}, C_{2}, C_{3}$ are small positive values that give stability to the indicator. The local SSIM is calculated using these values:

$$
\begin{equation*}
\operatorname{SSIM}\left(z_{m}(n), \hat{z}_{m}(n)\right)=\left[l\left(z_{m}(n), \hat{z}_{m}(n)\right)\right]^{\alpha} \cdot\left[c\left(z_{m}(n), \hat{z}_{m}(n)\right)\right]^{\beta} \cdot\left[s\left(z_{m}(n), \hat{z}_{m}(n)\right)\right]^{\gamma} \tag{3.52}
\end{equation*}
$$

where $\alpha, \beta, \gamma$ are parameters that set the relative importance of each term. In this work, we consider $\alpha=\beta=\gamma=1, C_{1}=R / 100, C_{2}=R * 3 / 10$ and $C_{3}=C_{2} / 2$ (where $R$ is the dynamic range of the true values). The mean SSIM (or MSSIM) between two images is the average of all the local SSIM

$$
\begin{equation*}
M \operatorname{SSIM}=\frac{1}{N} \cdot \frac{1}{M_{u n k}} \sum_{m=1}^{M_{m n k}} \sum_{n=1}^{N} \operatorname{SSIM}\left(z_{m}(n), \hat{z}_{m}(n)\right) \tag{3.53}
\end{equation*}
$$

### 3.4.2.e. Relative importance

The relative importance of these error indicators depends on the application. SIR would be the most common, given that most algorithms attempt to minimize the mean squared error, which is equivalent to maximizing the SIR. It is a good general indicator of the prediction performance, perhaps the most important in applications where a low error is needed. It is quite popular in blind-source separation applications, in order to estimate the goodness of the recovered sources [276,35].

KLD would be more important in applications where the resulting density of predicted data is a factor, e.g., a predictor that was a pre-processing step to an algorithm that depends on the probability density function of the data. It is also quite popular in pattern recognition applications, and even more so in speech processing [242] and image processing [96]. The best possible value for the KLD is zero (it being a distance), unlike the other considered error indicators.

CORR is important in applications where the spatial or temporal structure of predicted data must be preserved. It is a robust measure of the temporal synchronicity between two signals and it can be reliably estimated from sample data. CORR is a popular method for the determination of the distance between two sets of neuron spike trains [238,193].

MSSIM is a common error indicator in the field of image processing. Unlike other error evaluation methods, MSSIM is based on a model of the human visual system (HVS), a fact that allows it to better estimate the perceived quality of processed images [275,274]. It has been used for evaluating image processing results in several applications, such as image watermarking [5] and radar imaging [21].

### 3.4.3. Parameter setting for PREDICAMM

### 3.4.3.a. Convergence analysis

The study of the convergence of PREDICAMM was conducted in an empirical fashion, using exhaustive search with Monte Carlo experiments. The data for each iteration of the experiment were simulated using an ICAMM whose sources followed one or more of the considered datasets shown in Table 3.4; class parameters $\mathbf{W}_{k}, p\left(\mathbf{s}_{k}\right)$ and $\mathbf{b}_{k}$ were randomly set for each class, and all classes were assumed to be equiprobable. This model was used to generate 1,000 observations. As explained in Section 3.4.1, the first half of these observations was used to estimate the ICAMM parameters using supervised training. The second half of the observations was used to test the prediction performance of PREDICAMM. The Monte Carlo experiment comprised 100 iterations, with the end result being the average of all partial results. This process is shown in Figure 3.8.


Figure 3.8. Diagram showing each iteration of the Monte Carlo experiment for the simulation. This process is repeated a number of times during each Monte Carlo experiment.

First, we tested the stability of the prediction with respect to the input values in a simple case, dataset \#1 from Table 3.4; a case with one known variable and one unknown variable (i.e., $M=2$ and $M_{u n k}=1$ ), uniform and Laplacian sources, and one class. For each experiment, we added uniform noise to the true value (i.e., the intended target for the algorithm) and used that as the input to PREDICAMM, checking for any difference in the output, both in the end value $z_{\text {end }}$ and in the number of iterations until convergence. To better compare the results between experiments, the values in both axes were centered around the true value. Furthermore, the Gaussian noise had zero mean and unit variance. Thus, a perfect predictor would always return a horizontal line at $z_{(e n d)}=0$.

The results are shown in Figure 3.9. There are three distinct regions in the Figure. The first region, named No Convergence (NC), is the region where the algorithm does not converge at all, since the input is equal to the output. This is because of the gradient algorithm, since values too far away from the solution can have a probability exactly equal to zero, and thus a null gradient. The second region was named Failed Convergence (FC), since the algorithm converges to a wrong value, either because it exceeds the maximum number of iterations (thus not reaching the correct value) or because it converges to a local maximum. Finally, the third region was named Convergence ( C ) because values within it do converge to the correct result. The values within region C not only converge, but they do so in a lower amount of iterations than values in other regions. Region C spans from -2 to +2 around the true value, which means that the size of this region is approximately four times the standard deviation of $\mathbf{x}$.

To check the effect of a more complex case, we considered dataset \#6 from Table 3.4, a case with two different classes. The experiment was performed in the same way as the one shown in Figure 3.9, and the results are shown in Figure 3.10. These results are very similar to the case with only one class, including the size of region C. However, the method seems to reach the maximum number of iterations faster than it did for the previous case. This means that convergence is slow for any value outside of region C .

Finally, we considered a case with two unknown variables, case \#5 from Table 3.4. The results for this case are shown in Figure 3.11. It can be seen that the results are still similar, even though the number of unknown variables has increased. In this case, regions FC and C are more difficult to separate from each other, but they are clearly different from region NC. The radius of region C is slightly lower than it was in the one-unknown-variable case, but it is still greater than the standard deviation of $\mathbf{x}$.


Figure 3.9. Stability of the prediction in a case with one unknown variable and one class. a) output variable, normalized with respect to the true result; b) number of iterations taken. For reference, a perfect solution would mean that the output variable is always equal to 0 , and the number of iterations would always be close to 0 .


Figure 3.10. Stability of the prediction for the case with one unknown variable and two classes. a) output variable, normalized with respect to the true result; b) number of iterations taken. For reference, a perfect solution would mean that the output variable is always equal to 0 , and the number of iterations would always be close to 0 .

Considering the above results, it seems adequate to choose the average of the data as the initial value, $\mathbf{z}_{0}$. By using that value, and assuming stationarity, most data to predict should fall within region C. In that case, the algorithm would achieve a good performance. Of course, one could also use the results of another prediction algorithm as the initial value. These options are compared in another simulation in Section 3.4.3.b to test their relative performances.

To test the speed of convergence of the algorithm, the cost function $(p(\mathbf{y}, \mathbf{z}))$ was calculated for all iterations of the algorithm. The evolution of the cost function for each one of the previous experiments is shown in Figure 3.12. The cost function is maximized gradually, with no "valley" or negative peak in its progression. The probability density values are much lower in amplitude than the components of $\mathbf{x}$, which implies that the gradient should be normalized in order to improve convergence.

Of course, this convergence is also dependent on the gradient algorithm. The same kind of Monte Carlo experiment was used to compare the performance of the three proposed versions of the steepest ascent method (3.14)-(3.16), with the average results shown in Table 3.6. The column with the average number of iterations taken allows us to quantify the speed of convergence of each variant. The second variant achieved the best results for KLD, CORR and MSSIM, while the first variant had the lowest number of iterations and SIR. At any rate, it is worth noting that the results of both variants are very similar. Since the speed of convergence was important, we used the first variant of steepest ascent, (3.15), to maximize the joint probability density.

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Figure 3.11. Stability of the prediction for the case with two unknown variables and two classes. a) number of iterations taken; b) normalized value of the first output variable after convergence; c) normalized value of the second output variable after convergence. For reference, a perfect solution would mean that the output variable is always equal to 0 and the number of iterations would always be close to 0 ; in the above, it would correspond to dark blue areas in all three sub-Figures.


Figure 3.12. Joint probability densities with respect to the number of iterations, depending on the number of classes in the model (single, two or three classes).

| Method | Number of <br> iterations | SIR (dB) | KLD | CORR | MSSIM |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Classical method, (3.14) | 389.53 | -0.8746 | 7.2733 | 0.2180 | 0.2967 |
| First variant, (3.15) | 88.02 | 0.6920 | 7.2635 | 0.2305 | 0.3097 |
| Second variant, (3.16) | 97.49 | 0.6880 | 6.9751 | 0.2677 | 0.3258 |

Table 3.6. Comparative study between the three considered variants of the steepest ascent method.

### 3.4.3.b. Selection of the starting value

Besides the gradient procedure, the selection of the initial value $\mathbf{z}_{(0)}$ is very important for convergence. This choice is a classical challenge in optimization, since a good initial value speeds up convergence and reduces the possibility of converging to local maxima, while a bad initial value may impede convergence [24]. The initial value can be determined in a number of ways. The easiest one would be to take a vector of zeroes, $\mathbf{z}_{(0)}=\mathbf{0}$, or the expected values for each unknown variable, $\mathbf{z}_{(0)}=E[\mathbf{z}(n)]$. A more refined option is to take the result from a previous prediction step, e.g., with a linear predictor, and use that result as the initial value for the gradient. A good instance of previous predictor would be E-ICAMM. Since both methods can use the same ICA mixture model, this initial value would suppose no additional restrictions or assumptions on the underlying data model. However, any value could potentially be used as the initial value for PREDICAMM.

As shown in Figure 3.6, the following options were considered for the starting value for PREDICAMM: PREDICAMM initialized with zeroes (PREDICAMM+0); PREDICAMM initialized with the result of Kriging (PREDICAMM+Krig); PREDICAMM initialized with the result for Wiener structures (PREDICAMM+Wiener); PREDICAMM initialized with the result for SRF (PREDICAMM+SRF); PREDICAMM initialized with the result for thin-plate splines (PREDICAMM+Splines); and PREDICAMM initialized with the result yielded by E-ICAMM (PREDICAMM+E-ICAMM). The performance of PREDICAMM initialized with each of the possible methods was tested using a Monte Carlo experiment like the one shown in Figure 3.8, with 100 iterations. This experiment was repeated for each of the datasets shown in Table 3.4.

The results are shown in Figure 3.13. PREDICAMM+E-ICAMM achieved the best performance in all four error indicators. PREDICAMM+Splines achieved the second best performance, and obtained the lowest KLD (see Figure 3.13.b), while PREDICAMM+SRF performed at a similar level for single-class cases (datasets \#1 to \#5 from Table 3.4). The other proposed initial values performed worse than E-ICAMM and SRF: PREDICAMM+0 yielded the worst result; PREDICAMM+Krig performed a bit better than the former; and PREDICAMM+Wiener achieved a better result than PREDICAMM+Krig for datasets with multiple classes (datasets \#6 to \#13 from Table 3.4). In light of these results, only PREDICAMM+E-ICAMM was considered in the following.


Figure 3.13. Error indicators for the proposed initial values for PREDICAMM.

### 3.4.4. Simulation on data from ICA mixture models

Once the parameters for PREDICAMM were set, the performance of the proposed methods was tested through several Monte Carlo experiments similar to the one described in Section 3.4.3 (see Figure 3.8). In this case, each Monte Carlo experiment comprising 500 repetitions for increased robustness of the result. The experiment was repeated for each one of the datasets in Table 3.4, resulting in a total of 6,500 iterations.

The results of the prediction using PREDICAMM and E-ICAMM were compared with those of a classical linear predictor, Ordinary Kriging, Wiener structures, SRF and splines. These methods were introduced respectively in Sections 3.3.1, 3.3.2, 3.3.3 and 3.3.4. With respect to splines, the spherical splines method is not used in this experiment because it is tailored to the interpolation of electroencephalographic data. Therefore, only thin-plate splines were considered. Furthermore, only the best possible initial value for PREDICAMM was considered (PREDICAMM+E-ICAMM, as seen in Section 3.4.3.b). In total, six methods were tested.

Preliminary results showed that the behavior of the proposed methods was slightly different for single-class cases (datasets \#1 to \#5 from Table 3.4) and for multiple-class cases (datasets \#6 to \#13 from Table 3.4), particularly for Wiener structures and Kriging. Because of this, the performance analyses are split into two sub-sections.

### 3.4.4.a. Single-class cases

Figure 3.14 presents a typical prediction test of dataset \#3; datasets \#1 to \#5 display similar results. It can be seen that the reconstructed values yielded by E-ICAMM, PREDICAMM and SRF (Figure 3.14.c) closely resembled the true values (Figure 3.14.a). Conversely, Splines obtained a result not as good, while Kriging and Wiener obtained the worst results (see Figure 3.14.b).

The results of the considered prediction methods for the five datasets with one class are shown in Figure 3.15. For the most part, the shown values are in concordance with Figure 3.14. The best result was obtained by PREDICAMM, E-ICAMM and SRF. All three methods yielded


Figure 3.14. Typical prediction result for dataset \#3: a) true data; b) predictions obtained by the methods with worst performance; c) predictions obtained by the methods with best performance.


Figure 3.15. Error indicators for the single-class datasets.
similar values, although SRF performed slightly worse on average than the ICAMM-based methods. Kriging and Wiener structures obtained the worst results, while Splines obtained an intermediate result, except for dataset \#1 (in which Splines obtained a result comparable to EICAMM and PREDICAMM). When comparing the two proposed methods, PREDICAMM yielded better values of KLD and CORR, yet lower values of SIR and MSSIM. This is in concordance with the criterion followed by each algorithm, as explained in Sections 3.1 and 3.2: PREDICAMM maximizes the log-likelihood of the data, while E-ICAMM minimizes the square error. This behavior was common during the simulations, as we will see.

Figure 3.15 also shows that the results were overall better for cases with one missing variable (datasets \#1 and 2) than for cases with more than one missing variable (datasets \#3, 4 and 5). This is due to the lower amount of missing data in those cases, which. This improvement is higher when considering SIR (Figure 3.15.a) and CORR (Figure 3.15.c).

### 3.4.4.b. Multiple-class cases

Figure 3.16 shows the results of one of the variables from a single prediction of dataset \#13; the other datasets with multiple classes achieved similar performance. Kriging, Splines and Wiener structures behaved similarly as they did for the single-class case (compare with Figure 3.14); however, Wiener structures performed slightly better, given the presence of nonlinearities in the data due to multiple classes. SRF performed worse than for the single-class case, and obtained a similar result to Splines. Finally, the best reconstructions were obtained by E-ICAMM and PREDICAMM, whose values followed closely the true values to reconstruct (compare Figure 3.14.a and .c with Figure 3.16.a and .c). At any rate, the predicted values are less precise than those for the case with a single class.

This behavior is in concordance with the performance of the proposed methods, as shown in Figure 3.17. In general, the performance of the methods was worse for cases with multiple classes, particularly in the SIR (as seen in the difference between Figure 3.15.a and Figure 3.17.a). This owed to the increase in complexity of the underlying model, with multiple classes

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Figure 3.16. Typical prediction result for one of the variables of dataset \#13.


Figure 3.17. Error indicators for the multiple-class datasets.
that introduce nonlinearities. Furthermore, the performances of the methods were more spread for multiple classes than they were for one class. E-ICAMM and PREDICAMM yielded the best reconstructions, with the best values for all the considered indicators. Splines obtained the third best result, and the SIR was similar to that of the ICAMM-based methods. SRF obtained a worse result than it did for the cases with a single class, and its performance is similar to those Wiener structures. Wiener structures improved its performance with respect to the single-class case due to the nonlinearities in the model. Kriging obtained the worst result. When comparing the two proposed methods, E-ICAMM obtained a slightly higher SIR than PREDICAMM, while the latter obtained better KLD and MSSIM than the latter.

Parallel to what happened with single-class cases, performance was higher for datasets with only one missing variable (in this case, datasets \#6, \#10 and \#12). These are easily noticed in Figure 3.17, since they show up as local maxima.

### 3.4.5. Simulation on data from ICA mixture models with random nonlinearities

The results shown in Section 3.4.4 were calculated for several datasets generated from ICA mixture models, which is the ideal scenario for PREDICAMM and E-ICAMM. To test the robustness of the methods with respect to alterations of the base model, the data were corrupted with a nonlinear element and then the Monte Carlo experiment was repeated; the new process is shown in Figure 3.18. This nonlinearity was implemented with a feed-forward neural network (one hidden layer with 30 neurons) with random weights for each neuron. To quantify the nonlinearity caused by the neural network, only a certain amount of data was corrupted in this way, with the amount of corrupted data being called the "distortion rate." Thus, a distortion rate of 0.5 means that half the data were corrupted using the neural network and the other half were not. The distortion rate was changed from 0 to 1 in steps of 0.1 , and a separate Monte Carlo experiment with 500 iterations was performed for each value of the distortion rate.

Given the large number of experiments, this Section only shows results for datasets \#4, \#9 and \#13 from Table 3.4 (datasets with one, two and three classes, respectively). The results of these simulations are shown in Figure 3.19 for dataset \#4, Figure 3.20 for dataset \#9, and Figure 3.21 for dataset \#13.

As a general rule, results from Section 3.4.4 do hold true: PREDICAMM and E-ICAMM obtained the overall best performance; SRF obtained the third best performance for the singleclass case, but dropped for cases with multiple classes; Kriging and Wiener structures obtained the worst results; and Splines obtained an intermediate result. PREDICAMM obtained better KLD and CORR, yet lower SIR and MSSIM than E-ICAMM. Finally, the further we increase the number of classes in the models, the lower the performance becomes for all of the proposed methods (besides the effect caused by distortion).

In general, performance worsened with increasing distortion. This effect seemed more noticeable for the case with a single class, in which the methods showed a steep drop in performance. As the number of classes in the model increased, the effect of the distortion was less important. The decrease in performance was more marked for the ICAMM-based methods, due to the deformation of the underlying model. It was also important for SRF in the single-


Figure 3.18. Diagram showing the process of each iteration of the Monte Carlo experiment with nonlinear data. This process is repeated several times during each Monte Carlo experiment. Note that the third step, where data are corrupted with a nonlinearity, is what separates it from the Monte Carlo experiment in Section 3.4.4.
class case (see Figure 3.19). Conversely, Kriging and Wiener structures are not very affected by the distortion.

There was an unexpected behavior on the part of SRF and the ICAMM-based methods. At first, their performance decreased with increasing distortion rate, as one would expect. Once distortion became high, however, their performance stopped worsening, or even improved. This effect is more noticeable in Figure 3.19, but is also present in Figure 3.20 and Figure 3.21. It is unlikely to be produced by the gradient in PREDICAMM since both E-ICAMM and SRF (a completely different method) do follow the same pattern.

This unexpected behavior could be due to the nature of the mixture model. One could consider that distorted data from one class are actually data from a new class, i.e., distorted and nondistorted data from a given class could be split into two separate classes. This effect means that the underlying model becomes more complex, since the original model with $K$ equiprobable classes becomes a model with $2 K$ classes with different prior probabilities; the larger the distortion rate, the more probable these new classes become.

The prior probabilities of these "new" (distorted) classes are directly related to the distortion rate. As the latter rises, the new classes become more probable until the distortion rate is equal to 0.5 , when the new classes are as probable as the original (undistorted) classes. At this point, we could consider that the model is composed of $2 K$ equiprobable classes and that it is maximally different from the original model. Once the distortion rate increases over 0.5 , the new classes become more probable than the original classes and the model becomes gradually closer to the original one until finally, for unit distortion rate, the original classes have been completely replaced by the distorted classes. Thus, the model is again composed of only $K$ classes, the same as the undistorted model. This variable complexity explains the behavior of the proposed methods, and the simulations in this work (particularly those of Section 3.4.4) show that there was indeed a decrease in performance as the number of classes increased.


Figure 3.19. Error indicators for the proposed methods with respect to the distortion rate of a single-class ICA (mixture) model, dataset \#4.


Figure 3.20. Error indicators for the proposed methods with respect to the distortion rate of a two-class ICAMM, dataset \#9.


Figure 3.21. Error indicators for the proposed methods with respect to the distortion rate of a three-class ICAMM, dataset \#13.

There is a second cause of error, which is caused by the fact that distorted data do not satisfy the ICA assumption due to the nonlinearities caused by the neural network. This kind of error seems more dominant in the single-class case, since the performance of PREDICAMM and EICAMM increased only for distortion rate rises over 0.8 (see Figure 3.19). However, as shown by the progression from Figure 3.19 to Figure 3.21, this second type of error is less important for the cases with multiple classes. The performance for very high distortion rates is generally lower than that for very low distortion rates.

### 3.4.5.a. Convergence of the gradient algorithm

One might wonder whether these changes in the data will affect the convergence of the gradient algorithm in PREDICAMM. To test whether this is the case, the convergence experiment shown in section 1.4.3 was repeated, but considering nonlinearly-corrupted data with a distortion rate equal to 0.5 . The results are shown in Figure 3.22, where the base models are called "linear ICAMM" and the corrupted models are called "nonlinear ICAMM." Values shown in the Figure were normalized with respect to the maximum probability density, which corresponds to the single-class case linear ICAMM. All curves converge rapidly and nonlinear cases achieve lower values of the target joint probability density. This lower result is due to the corruption of the model, which causes the ICA mixture model to lose likelihood (since data are less likely to come from the hypothesized ICAMM, not being generated by a linear mixture of independent sources).


Figure 3.22. Joint probability densities for linear cases (regular line) and nonlinear cases (dotted line). The nonlinear cases were obtained for a distortion rate of 0.5.

### 3.4.6. Simulation with an increasing number of missing traces

The experiments in Sections 3.4.4 and 3.4.5 have shown that the performance of the proposed methods decreases with increasing number of classes. In order to test the performance of the algorithm with respect to the number of missing traces, a further simulation was performed using a Monte Carlo experiment such as the ones with non-distorted data (see Figure 3.8). The data for each iteration of the experiment were generated following a model similar to the dataset \#9 from Table 3.4, but with $M=16$ sources instead of just four, and an increasing number of missing traces, $M_{u n k}$. This increase was so the number of missing traces could change further than 1 to 3 . The missing traces were consecutive and as centered as possible. This does not affect PREDICAMM or E-ICAMM, but it can affect the other methods. This process was repeated 500 times for a number of missing traces ranging from $M_{u n k}=1$ to $M_{u n k}=15$, for a total of 7,500 iterations.

The average results of the experiment are shown in Figure 3.23. Performance was usually better than for the cases in Section 3.4.4, owing to the higher amount of information available (16 variables, as opposed to 3 or 4). PREDICAMM and E-ICAMM yielded the best results, far exceeding those of the other considered methods. Wiener structures and SRF obtained the second best result, and Kriging and Splines yielded the worst results. PREDICAMM and EICAMM achieved an almost equivalent performance, although E-ICAMM yielded slightly higher values of SIR (in concordance with the LMSE criterion). The performance of all methods degraded progressively as the number of missing traces increased. The proposed methods, however, decreased their performance at a slower rate, or experienced a slight increase in performance for some cases. In fact, the results for the correlation and MSSIM indicators were almost constant until more than 10 variables were missing.


Figure 3.23. Error indicators for the proposed methods with respect to the number of missing variables.

### 3.4.6.a. Simulation with dimensionality reduction

One of the known disadvantages of ICA is its relatively high computational cost. Because of this, many applications utilize a pre-processing stage that performs dimensionality reduction, e.g., using PCA. Let us assume a set of data whose dimensionality has been reduced from $M$ to $M^{\prime}, M^{\prime}<M$, using a PCA with coefficient matrix $\mathbf{P}$ of size $\left[M^{\prime} \times M\right]$. The reduced data, $\mathbf{x}^{\prime}$, can be obtained as $\mathbf{x}^{\prime}=\mathbf{P} \cdot(\mathbf{x}-E[\mathbf{x}])$. Let us also assume that these reduced data were used to fit an ICA mixture model with $M^{\prime}$ sources (i.e., with square de-mixing matrices) and $K$ classes.

In principle, there are two possible options to work with this ICA (mixture) model: a) work on reduced data by first applying the same PCA with matrix $\mathbf{P}$ and then consider the ICAMM; and b) work directly on the unreduced data using an ICAMM that combines the effect of PCA and ICAMM. However, a) is simply not possible with missing data, as some of the data are unknown and therefore the components cannot be obtained. Thus, only option b) remains. The ICA (mixture) model can be converted by considering the sources for class $k$ as a function of the original data, $\mathbf{x}$ :

$$
\begin{align*}
& \mathbf{s}_{k}=\mathbf{W}_{k} \cdot\left(\mathbf{x}^{\prime}-\mathbf{b}_{k}\right)=\mathbf{W}_{k} \cdot {\left[\mathbf{P} \cdot(\mathbf{x}-E[\mathbf{x}])-\mathbf{b}_{k}\right]=\mathbf{W}_{k} \cdot\left(\mathbf{x}-\mathbf{b}_{k}{ }^{\prime}\right) }  \tag{3.54.a}\\
& \mathbf{W}_{k}^{\prime}=\mathbf{W}_{k} \cdot \mathbf{P}  \tag{3.54.b}\\
& \mathbf{b}_{k}^{\prime}=E[\mathbf{x}]+\mathbf{P}^{+} \cdot \mathbf{b}_{k} \tag{3.54.c}
\end{align*}
$$

where $\mathbf{W}_{k}{ }^{\prime}, \mathbf{s}_{k}, \mathbf{b}_{k}{ }^{\prime}, k=1, \ldots, K$ are the ICAMM parameters of the converted model. Note that $\mathbf{w}_{k}{ }^{\prime}$ is now no longer square, but rectangular of size $\left[M^{\prime} \times M\right.$ ]. Unfortunately, PREDICAMM cannot work with non-square matrices because, as far as we know, the transformation of probability densities shown in (3.3) is only defined for square matrices. Thus, PREDICAMM cannot be used if there is dimensionality reduction in the data. E-ICAMM, however, can still be used with rectangular de-mixing matrices. Thus, the question arises: how does this dimensionality reduction method affect the performance of E-ICAMM?

In order to answer this question, a further Monte Carlo experiment was performed. This experiment was similar to that in Section 3.4.6, and it is shown in Figure 3.24. The data for each iteration of the experiment were generated following a model similar to the dataset \#9 from Table 3.4, but with $M=16$ sources instead of just four, and an increasing number of missing traces, $M_{u n k}$. The number of missing traces ranged from 1 to 15 , and missing traces were consecutive and as centered as possible. After the data were generated, PCA was applied to reduce their dimensionality from $M$ to $M^{\prime}$ variables, $M^{\prime} \leq M$. An ICAMM was fitted to these reduced data and its parameters were then corrected to include the PCA using (3.54.b) and (3.54.c). Finally, this model was used by E-ICAMM to predict the randomly-selected missing traces from the data, and the goodness of the prediction was estimated. This process was repeated with a decreasing number of components $M^{\prime}$ from $M$ to 2 for each iteration of the experiment. The Monte Carlo experiment was repeated 100 iterations and results were averaged.

The results of the experiment are shown in Figure 3.25. Only the values for E-ICAMM are shown, since other methods are not affected by the PCA. Their values, however, can be found in Figure 3.23 for comparison. Results were in concordance with those of E-ICAMM in Figure 3.23 , with a gradual decrease in performance as the number of missing variables increased. It can be seen that there is also a decrease in performance every time that we decrease the number of remaining components in the reduced data, $M^{\prime}$. This decrease was experienced in two ways: a) a general reduction of performance for all values; and b) a degradation of the curve, which lost performance at an increasing rate. Thus, it was as if the curve was displaced to the lower left corner of the Figures (upper left in the case of KLD). This loss is present even if the amount of retained variance in the data is very close to $100 \%$.

Therefore, it can be seen that any amount of dimensionality reduction will cause a slight decrease in prediction performance. This fact introduces a trade-off parameter to the dimensionality reduction step. Depending on the application, this reduction in performance will be compensated by the reduced computational time of E-ICAMM (particularly, the estimation of the ICA mixture model and). In this thesis, however, there are no particularly time-restrictive applications and thus we opted for the optimal solution in terms of performance (no dimensionality reduction) for the applications to real data in Chapter 5.


Next iteration, start again with $M^{\prime}=M$
Figure 3.24. Diagram showing the process of each iteration of the Monte Carlo experiment with dimensionality reduction. This process is repeated several times during each Monte Carlo experiment.


Figure 3.25. Error indicators for E-ICAMM with respect to the number of missing variables and to the reduced dimensionality, $M^{\prime} \leq M, M=6$. Each line is numbered by its corresponding value of $M^{\prime}$. The amount of explained variance by each line ranged from $92.5 \%\left(M^{\prime}=2\right)$ to $100 \%\left(M^{\prime} \geq 15\right)$.

### 3.5. Conclusions

This chapter has introduced two novel prediction methods based on ICA mixture models, called E-ICAMM and PREDICAMM. Both methods interpolate missing data using known data and the ICA mixture model. PREDICAMM maximizes the log-likelihood of the data given the model, that is, seeks the maximum likelihood criterion. E-ICAMM minimizes the mean square error, that is, seeks the LMSE criterion. Both methods require a previous training step in order to calculate the model, but other than that, they are general-purpose and can be used in many signal processing fields, such as time series forecast, image reconstruction, etc.

Since PREDICAMM uses a gradient algorithm for optimization, its convergence depends heavily on the gradient algorithm itself and the starting value. Several experiments were performed to select the optimal combination for this work. In the end, the selected parameters were a normalized gradient descent algorithm and the output of E-ICAMM as the initial value. Since E-ICAMM and PREDICAMM use the same model, this step does not require further training.

The performance of the proposed methods was tested using Monte Carlo experiments on several sets of simulated data generated from an underlying ICA mixture model. E-ICAMM and PREDICAMM were compared with the following predictors: a classical linear predictor, Ordinary Kriging; a nonlinear predictor, Wiener structures; a matrix completion algorithm based of SRF; and thin-plate splines. In all cases, the performance of the proposed methods exceeded that of the methods selected for comparison. SRF obtained similar results to E-ICAMM and PREDICAMM, but only for cases with a single class ( $K=1$ ), and its performance dropped in cases with multiple classes. It was confirmed that performance decreased with increasing number of classes for all methods. The proposed methods, however, experienced a smaller decrease in performance than the methods selected for comparison. When comparing the two
proposed methods with one another, PREDICAMM obtained better values of CORR and KLD, while E-ICAMM obtained better values of SIR and MSSIM. Their performances, however, were similar.

A second set of Monte Carlo experiments was run to test the behavior of the proposed methods with respect to alterations of the underlying model. To this effect, the performance was run with data generated from an ICAMM and then corrupted by a nonlinear element. This nonlinearity was implemented by a randomly-initialized neural network. Results for this second series of tests were similar to those for the first series, and E-ICAMM and PREDICAMM obtained the best performance even though the base model was not completely valid. All considered methods decreased their performance as the number of distorted data grew larger. The proposed ICAMM-based methods and SRF were the most affected by this effect, while Kriging, Wiener structures and Splines were the least affected. It was shown that this decrease in performance owed to the increase in complexity in the underlying model (i.e., the distorted data were treated as new "classes" of data), rather than to the distortion of the validity of the ICA mixture model.

Another Monte Carlo experiment was run to test the performance of E-ICAMM and PREDICAMM with respect to the number of missing data, $M_{u n k}$. The results of this experiment were consistent with those of the previous experiments, and the proposed methods obtained the best performance. Both proposed methods yielded very similar results, although E-ICAMM obtained slightly better SIR values. All methods decreased in performance as the number of missing data increased, and this decrease was much slower for the proposed methods. PREDICAMM and E-ICAMM achieved a good performance until the number of missing traces was high ( $M_{u n k}>10$ out of 16 variables). This demonstrates the robustness of E-ICAMM and PREDICAMM with respect to the number of missing data.

A final Monte Carlo experiment tested the performance of the proposed methods when dimensionality reduction is performed before estimating the underlying ICAMM. Since PREDICAMM cannot function in this case, only E-ICAMM was considered for this final test. The experiments confirm the loss in performance with increasing number of missing values. Furthermore, the dimensionality reduction method did cause a further decrease in performance. This loss is present even if the amount of retained variance in the data is very close to $100 \%$. Therefore, the dimensionality reduction method introduces a trade-off between performance and computational time.

# A general dynamic modeling approach based on synchronized ICA mixture models: G- and UG-SICAMM 

## Chapter 4-A general dynamic modeling approach based on synchronized ICA mixture models: G- and UG-SICAMM

This chapter presents two new procedures for dynamic modeling which are based on synchronized ICA mixture models. The starting point of this work is a method that incorporates a hidden Markov model to extend the ICA mixture models to the case of having sequential dependence in the feature observation records. This method can be used to model the dynamic changes of a process in time; we called it sequential ICAMM (SICAMM) [230]. The proposed methods in this chapter extend the one Markov chain employed featured in SICAMM to a general framework to characterize the joint behavior of a number of synchronized dynamic models or "chains." We have called these methods Generalized Sequential ICAMM (GSICAMM) and UG-SICAMM (Unsupervised G-SICAMM). This latter maximizes the loglikelihood of the model with respect to all of the available training data and the parameters of the model. It could be named SG-SICAMM because it also considers the semi-supervised case.

The procedures can be used for classification using maximum a posteriori estimation and the forward-backward procedures as in Baum-Welch and Viterbi algorithms [17,270]. Thus, we have tested the classification accuracy and goodness of fit of G-SICAMM and UG-SICAMM using several sets of synthetic data with two chains and two, three and four classes per chain. Furthermore, the behavior of the proposed methods with respect to dynamically-changing sources is studied. G-SICAMM is compared with dynamic Bayesian networks (DBN), a state-of-the-art method for dynamic modeling. The comparison shows that the proposed method performs better than DBN, even if the sources change dynamically, and thus, the adaptive capabilities of the method to non-stationary process are demonstrated. In addition, we found that the G-SICAMM parameters can be studied to gain further understanding of the modeled data, whereas the DBN parameters cannot be examined in this way.

Let us consider this latter point for a moment. Most of the applications of the proposed method revolve around classification of data in several categories, i.e., the result is a discrete value. In addition, most of the classification methods (e.g., discriminant analysis, DA [169], and Naïve Bayes, [175]) only perform classification and their parameters are difficult to interpret or shed no further light on the classified data. However, there are methods which obtain not only a classification of the data, but also a structured result which is, by itself, a way to interpret the data. Two instances of this kind of methods are decision tree learning [206] and hierarchical

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ICAMM [225], methods in which the data are grouped into hierarchical classes which can let us find dependences and relationships between classes at several levels. For instance, two classes which branch from a common "parent" class will be more closely related between them than related with classes from other parents. Therefore, methods of this second kind return both a classification result and a set of parameters from which we can interpret and deduce further information from the examined data.

Besides the classification results, the proposed method G-SICAMM returns a structured outcome with two main points of interest: i) the G-SICAMM parameters define a subspace structure where the ICA parameters for each subspace (or class) can be separately interpreted, this extends the classic analysis based on only one ICA (see for instance the electroencephalographic signal application [190,127], Figure 4.1); ii) the sequential parameters in G-SICAMM show the existence or absence of time dependences among the chains and classes. For instance, we not only could attempt to locate the EEG sources on the scanned brain surface using the ICA parameters (see Figure 4.1.b to Figure 4.1.d), but we could also search for sequential dependences between groups of sources that describe dynamic interactions between neural centers in the brain.


Figure 4.1. Example of the ICA parameters that can be extracted from one set of EEG data: a) EEG data; b) scalp map for an eye artifact; c) scalp map for the alpha waves; d) scalp map for the beta waves. The distribution of the scalp maps shows that the alpha and beta waves concentrated on the occipital area.

## 4.I. Sequential ICA mixture model: SICAMM

In many cases, ICA and ICA mixture models are estimated under the assumption that the data are time independent, particularly for methods that maximize the log-likelihood to find the model $[59,154]$. This assumption simplifies the calculation of the probabilities involved in the process. However, there are many practical cases where the observations do not behave in a totally independent manner and they show some degree of dependence in the feature observation record; in these cases, the previous assumption no longer holds true. In order to capture such dependences within the framework of ICA mixture models, the calculation of posterior probability densities should consider not only the current observation, $\mathbf{x}(n)$, but also all previous observations, $\mathbf{x}(n-1), \mathbf{x}(n-2), \mathbf{x}(n-3), \ldots, \mathbf{x}(0)$.

The time dependences among observations are considered in sequential ICA mixture models (SICAMM), a method developed by the GTS where the calculation of posterior probability
densities includes information from the current observation and all of the available past samples [230,223]. SICAMM is the basis for the formulation of the proposed methods. In this section, we review it in order to make this chapter self-contained.

SICAMM maximizes $\quad p\left(C_{k}(n) \mid \mathbf{X}(n)\right) \quad$ instead of $\quad p\left(C_{k}(n) \mid \mathbf{x}(n)\right)$, where $\mathbf{X}(n)=[\mathbf{x}(0), \mathbf{x}(1), \ldots, \mathbf{x}(n)], n$ is the current time (with the first observation set at $n=0$ ) and $k=1, \ldots, K$ is the class. This posterior probability can be expressed as a function of the conditional observation densities by using the Bayes rule:

$$
\begin{equation*}
P\left(C_{k}(n) \mid \mathbf{X}(n)\right)=\frac{p\left(\mathbf{X}(n) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)}{p(\mathbf{X}(n))}=\frac{p\left(\mathbf{X}(n) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)}{\sum_{l=1}^{K} p\left(\mathbf{X}(n) \mid C_{l}(n)\right) \cdot P\left(C_{l}(n)\right)} \tag{4.1}
\end{equation*}
$$

where the mixture model is explicit in the denominator of (4.1). The posterior probabilities calculated by SICAMM can be used for classification by maximum a posteriori estimation; that is, each unlabeled observation is assigned to the class for which it has maximum posterior probability.

SICAMM assumes that time dependences can be limited to class selection, and furthermore, that they can be adequately modeled by a Hidden Markov Model [39]. In essence, an HMM is a finite-state machine that switches between different probability density functions to model the observations or "emissions" during that state. The state change is a Markov process, i.e., the state at time $n$ depends only on the state at a previous time $n-\tau$; we will consider a first-order Markov process, hence $\tau=1$. In SICAMM, each state of the HMM corresponds to one of the classes in an underlying ICA mixture model, and the ICA parameters for each class model the observations during the corresponding state. Given the use of the HMM, the Markov assumption is implicit; therefore, each observation is conditionally independent from other observations given its class. Thus, $P\left(\mathbf{X}(n) \mid C_{k}(n)\right)$ can be written as a function of the current observation, $\mathbf{x}(n)$, and past observations:

$$
\begin{equation*}
p\left(\mathbf{X}(n) \mid C_{k}(n)\right)=p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot p\left(\mathbf{X}(n-1) \mid C_{k}(n)\right) \tag{4.2}
\end{equation*}
$$

where $p\left(\mathbf{x}(n) \mid C_{k}(n)\right)=\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot p\left(\mathbf{s}_{k}(n)\right)$ is the probability of the current observation and, thus, it is calculated without considering time dependences. By replacing (4.2) into (4.1) and applying the Bayes rule several times, we arrive at the following:

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$$
\begin{align*}
P\left(C_{k}(n) \mid \mathbf{X}(n)\right) & =\frac{p\left(\mathbf{X}(n) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)}{\sum_{l=1}^{K} p\left(\mathbf{x}(n) \mid C_{l}(n)\right) \cdot P\left(C_{l}(n)\right)}= \\
& =\frac{p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot p\left(\mathbf{x}(n-1) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)}{\sum_{l=1}^{K} p\left(\mathbf{x}(n) \mid C_{l}(n)\right) \cdot p\left(\mathbf{X}(n-1) \mid C_{l}(n)\right) \cdot P\left(C_{l}(n)\right)}=  \tag{4.3}\\
& =\frac{p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{x}(n-1))}{\sum_{l=1}^{K} p\left(\mathbf{x}(n) \mid C_{l}(n)\right) \cdot P\left(C_{l}(n) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{X}(n-1))}= \\
& =\frac{\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot p\left(\mathbf{s}_{k}(n)\right) \cdot P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)}{\sum_{l=1}^{K}\left|\operatorname{det} \mathbf{W}_{l}\right| \cdot p\left(\mathbf{s}_{l}(n)\right) \cdot P\left(C_{l}(n) \mid \mathbf{X}(n-1)\right)}
\end{align*}
$$

The posterior probability of the ICA mixture model (see Table 2.2) is similar to (4.3); the only change is that $P\left(C_{k}(n)\right)$ has been replaced in (4.3) by $P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)$. The prior probabilities (which are constant with respect to time) have been replaced by the conditional probability of each class during the current time instant with respect to previous time instants (which change for each time instant), which introduces time dependences in the model.

Given the Hidden Markov model, the conditional probability $P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)$ can be calculated from the posterior probabilities of the previous time instant as

$$
\begin{equation*}
P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)=\sum_{l=1}^{K} \pi_{k l} \cdot P\left(C_{l}(n-1) \mid \mathbf{X}(n-1)\right) \tag{4.4}
\end{equation*}
$$

where $\pi_{k l}=P\left(C_{k}(n) \mid C_{l}(n-1)\right)$ are the transition probabilities, and they are assumed to be constant with respect to time (that is, equal for all values of $n$ ). If there were no dependences in the feature observation record, $\quad P\left(C_{k}(n) \mid C_{l}(n-1)\right)=P\left(C_{k}(n)\right)$ and thus $P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)=P\left(C_{k}(n)\right)$; in that case, (4.3) would become equal to the regular ICAMM posterior probability.

Thus, the necessary parameters for it are the same parameters required for ICAMM, that is, the ICA model for each class, $\mathbf{w}_{k}, \mathbf{b}_{k}, p\left(\mathbf{s}_{k}\right), k=1, \ldots, K$; and the class transition probabilities, $\pi_{k l}$, for all combinations of classes $l$ and $k$. The SICAMM algorithm is described in Table 4.1, where it is assumed that all of these parameters are known.

## Initialization

Select initial observation, $\mathbf{x}(0)=\mathbf{x}(0)$
Calculate sources for each class, $\mathbf{s}_{k}(0)=\mathbf{W}_{k} \cdot\left(\mathbf{x}(0)-\mathbf{b}_{k}\right), k=1, \ldots, K$
Calculate posteriors, $P\left(C_{k}(0) \mid \mathbf{x}(0)\right)$, using the algorithm in Table 2.2:

$$
P\left(C_{k}(0) \mid \mathbf{x}(0)\right)=\frac{\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot p\left(\mathbf{s}_{k}(0)\right) \cdot P\left(C_{k}(n)\right)}{\sum_{l=1}^{K}\left|\operatorname{det} \mathbf{W}_{l}\right| \cdot p\left(\mathbf{s}_{l}(0)\right) \cdot P\left(C_{l}(n)\right)}
$$

Initial observation is assigned to the class with maximum posterior probability

## Updating

For $n=1, \ldots, N$, with $N+1$ being the number of observations:
Select current observation, $\mathbf{X}(n)=[\mathbf{x}(0), \mathbf{x}(1), \ldots, \mathbf{x}(n)]$
Calculate sources for each class, $\mathbf{s}_{k}(n)=\mathbf{W}_{k} \cdot\left(\mathbf{x}(n)-\mathbf{b}_{k}\right), k=1, \ldots, K$
Calculate conditional class probabilities using (4.4):

$$
P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)=\sum_{l=1}^{K} \pi_{k l} \cdot P\left(C_{l}(n-1) \mid \mathbf{X}(n-1)\right)
$$

Calculate posterior probabilities using (4.3):

$$
P\left(C_{k}(n) \mid \mathbf{X}(n)\right)=\frac{\left|\operatorname{det} \mathbf{W}_{k}\right| \cdot p\left(\mathbf{s}_{k}(n)\right) \cdot P\left(C_{k}(n) \mid \mathbf{X}(n-1)\right)}{\sum_{l=1}^{K}\left|\operatorname{det} \mathbf{W}_{l}\right| \cdot p\left(\mathbf{s}_{l}(n)\right) \cdot P\left(C_{l}(n) \mid \mathbf{X}(n-1)\right)}
$$

Current observation is assigned to the class with maximum $P\left(C_{k}(n) \mid \mathbf{X}(n)\right)$
Table 4.1. The SICAMM algorithm.

### 4.1.1. Training algorithm

In the previous section, the SICAMM parameters are assumed to be estimated during a training stage. The estimation process of these parameters depends on the kind of training. For semisupervised or unsupervised training (i.e., part or all of the training data are unlabeled), all parameters should be estimated simultaneously. An algorithm for unsupervised or semisupervised training is proposed in Section 4.3.

For supervised training, the estimation of the ICA parameters for each class can be performed separately from the estimation of class transition probabilities. The ICA models can be estimated using any of the previously mentioned ICAMM methods (for instance, [231,153]), while the class transition probabilities are estimated by simple counting:

$$
\begin{equation*}
\pi_{k l}=\frac{\# \operatorname{transitions} \text { from class } l \text { to class } k}{\# \text { observations in class } l} \tag{4.5}
\end{equation*}
$$

### 4.1.2. SICAMM variants

As shown in Table 4.1, classification with SICAMM is usually performed using MAP estimation, assigning each observation to the class for which it has maximum posterior probability. We propose here two algorithm variants that make use of the similarities between SICAMM and HMM to improve classification: the Baum-Welch and Viterbi procedures.

### 4.1.2.a. Baum-Welch algorithm

The first proposed extension to SICAMM is the Baum-Welch algorithm [17], which can be used by making use of the correspondences between the classes in SICAMM and the hidden states of the HMM. It is usually used to find the unknown parameters of a HMM, but it can also be used for classification purposes. In that case, the classification of the $n$-th observation is performed by maximizing the conditional probability of the current class given all of the observed data, $P\left(C_{k}(n) \mid \mathbf{X}(N)\right)$; where $n=0, \ldots, N$ and $N+1$ is the number of available observations. However, this probability is complex to calculate explicitly. Instead, the Baum-Welch algorithm calculates the joint probability in two steps: a forward step, where the dependence of each observation with respect to previous observations is considered; and a backward step, where the dependence of each observation with respect to future observations is considered.

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The forward step calculates the "forward" variable $\alpha_{k}(n)=p\left(\mathbf{X}(n), C_{k}(n)\right)$, the joint probability of class $k$ and of all observations up to time $n$. Although it can be calculated explicitly from (4.2), $\alpha_{k}(n)$ is usually calculated iteratively to improve the speed of the algorithm. If we take the Bayes rule several times, and considering the Markov assumption, then

$$
\begin{align*}
\alpha_{k}(n) & =p\left(\mathbf{X}(n) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)= \\
& =p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot p\left(\mathbf{X}(n-1) \mid C_{k}(n)\right) \cdot P\left(C_{k}(n)\right)= \\
& =p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot p\left(C_{k}(n) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{X}(n-1))= \\
& =p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot \sum_{l=1}^{K} \pi_{k l} \cdot p\left(C_{l}(n-1) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{X}(n-1))=  \tag{4.6}\\
& =p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot \sum_{l=1}^{K} \pi_{k l} \cdot p\left(\mathbf{X}(n-1), C_{l}(n-1)\right)= \\
& =p\left(\mathbf{x}(n) \mid C_{k}(n)\right) \cdot \sum_{l=1}^{K} \pi_{k l} \cdot \alpha_{l}(n-1)
\end{align*}
$$

where the initial value is $\alpha_{k}(0)=p\left(\mathbf{x}(0), C_{k}(0)\right)=p\left(\mathbf{x}(0) \mid C_{k}(0)\right) \cdot p\left(C_{k}(0)\right)$. The forward step calculates all possible values of the forward variable for every time instant, $\alpha_{k}(n), k=1, \ldots, K, n=1, \ldots, N$.

After the forward step is complete, the algorithm performs a backward step. This step calculates the "backward" variable $\beta_{k}(n)=p\left(\mathbf{x}(n+1), \mathbf{x}(n+2), \ldots, \mathbf{x}(N) \mid C_{k}(n)\right)$, that is, the joint probability of all future observations conditioned with respect to the current class. Once again, the Baum-Welch algorithm calculates this variable iteratively; from the definition and applying the HMM and the Markov assumption:

$$
\begin{align*}
\beta_{l}(n) & =p\left(\mathbf{x}(n+1), \mathbf{x}(n+2), \ldots, \mathbf{x}(N) \mid C_{l}(n)\right)= \\
& =\sum_{k=1}^{K} \pi_{k l} \cdot p\left(\mathbf{x}(n+1), \mathbf{x}(n+2), \ldots, \mathbf{x}(N) \mid C_{k}(n+1)\right)= \\
& =\sum_{k=1}^{K} \pi_{k l} \cdot p\left(\mathbf{x}(n+1) \mid C_{k}(n+1)\right) \cdot p\left(\mathbf{x}(n+2), \ldots, \mathbf{x}(N) \mid C_{k}(n+1)\right)=  \tag{4.7}\\
& =\sum_{k=1}^{K} \pi_{k l} \cdot p\left(\mathbf{x}(n+1) \mid C_{k}(n+1)\right) \cdot \beta_{k}(n+1)
\end{align*}
$$

where the initial value is $\beta_{l}(N)=1 \forall l=1, \ldots, K$. As the name of the step suggests, this calculation begins at the last observation and moves backwards until all the $\beta_{l}(n)$ values are calculated. Thus, the desired conditional expectation can be found as

$$
\begin{equation*}
\gamma_{k}(n)=p\left(C_{k}(n) \mid \mathbf{X}(N)\right)=\frac{\alpha_{k}(n) \cdot \beta_{k}(n)}{\sum_{l=1}^{N} \alpha_{l}(n) \cdot \beta_{l}(n)} \tag{4.8}
\end{equation*}
$$

As explained above, the classification is performed by choosing the class with maximum $\gamma_{k}(n)$ for each observation.

### 4.1.2.b. Viterbi algorithm

Another classification algorithm is the Viterbi algorithm, a dynamic programming algorithm which searches the most likely sequence of hidden states (classes, in this case) for all $N$ observations, also known as the Viterbi path [270]. This sequence is, in general, different from the sequence obtained by considering the most likely state at each time in isolation.

The search for the Viterbi path is not performed by an exhaustive search, as this would be too computationally expensive for most applications. Instead, the algorithm moves forward; for any state $k$ at time $n$, only the most likely sequence of states ("path") that ends in that state is considered, and all other paths that end in that state are discarded. This process greatly reduces the number of combinations to consider for maximization with respect to an exhaustive search (from $K^{N}$ to $N \cdot K^{2}$ ), since most sequences are discarded during computation, and it keeps similar properties. Figure 4.2 shows the Viterbi algorithm applied during two consecutive time instants; most of the paths are discarded during each time instant and therefore the number of possible paths remains constant across time, instead of increasing as it would do during an exhaustive search, where we have to sample every possible path. For instance, consider time $n-1$ in Figure 4.2; for each state, only one of the incoming paths is accepted, and the rest are discarded.


Figure 4.2. Sample diagram of states (trellis) for three consecutive time instants in a case with four states. Arrows show possible paths; dashed arrows denote discarded paths, and solid arrows denote the most likely path.

To compute the most probable path for each state during a given time instant, the algorithm calculates an auxiliary variable $\delta_{k}(n)$ such that

$$
\begin{equation*}
\delta_{k}(n)=\max _{\substack{\text { sequence } \\ k_{1} \cdots k_{n-1}}} p\left(\mathbf{X}(n-1), C_{k_{1}}(1), C_{k_{2}}(2), \ldots, C_{k_{n-1}}(n-1), C_{k}(n)\right) \tag{4.9}
\end{equation*}
$$

where $C_{k_{i}}(n)=k_{i}$ indicates that the $n$-th observation belongs to class $k_{i}$, and the maximum indicates that only the most likely path will be considered. Hence, each value of $\delta_{k}(n)$ carries an associated path, $k_{1}, \ldots, k_{n-1}, k$.

Formally, this auxiliary variable is the maximum joint probability that the current observation belongs to class $k$, given the previous observations and their respective classes. A recursive relation is derived from (4.9) to help with the calculation:

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$$
\begin{equation*}
\delta_{k}(n+1)=p\left(\mathbf{x}(n+1) \mid C_{k}(n+1)\right) \cdot \max \left(\pi_{k l} \cdot \delta_{l}(n)\right) \tag{4.10}
\end{equation*}
$$

with initial value $\delta_{k}(0)=p\left(\mathbf{x}(0), C_{k}(0)\right)=p\left(\mathbf{x}(0) \mid C_{k}(0)\right) \cdot p\left(C_{k}(0)\right)$. Once all the $\delta_{k}(N)$ have been calculated, there are $K$ possible paths, each one ending in a different state $C_{k}(N)$. The algorithm then selects the path with maximum $\delta_{k}(N)$ and returns the associated sequence of states $k_{1}, \ldots, k_{n-1}, k$ (as seen (4.9) and commented above) as the classification of the observations.

### 4.2. Generalized SICAMM: G-SICAMM

There are applications that require more flexible modeling than SICAMM. For instance, it would be interesting to consider the joint behavior of two (or more) sets of data, each one with its associated ICA mixture model and its own time dependences, but with inter-dependences between sets. Thus, we proposed here an extension of SICAMM to multiple HMM chains that we have called G-SICAMM. The degrees of freedom afforded by this method will allow a broad range of real problems involving the dynamic modeling of complex data densities to be dealt with.

### 4.2.1. The model and the definition of the problem

We assume that there are $L$ groups of data or "chains," each modeled by a different SICAMM with $K_{l}, l=1, \ldots, L$ classes. Furthermore, it is assumed that the individual models are not independent between them, but rather that their inter-dependences can be modeled by a coupled hidden Markov model ( [32]) like the one shown in Figure 4.3. The CHMM refers to a group of HMM models in which the state of one model at time $n$ depends on the states of all models (including itself) at time $n-1$. We considered the fully-coupled CHMM; although there are other CHMM architectures, such as event-coupled HMM [143] and factorial HMM [94], their adaptation to G-SICAMM is outside the scope of this work.

Thus, each class from a chain in G-SICAMM corresponds to a hidden state of the same chain in the CHMM. In this case, the CHMM models class dependences (both inter-chain and intrachain dependences) and the ICA parameters for each class model the observations during the corresponding state of that chain.

Before tackling the model itself, we will define several notations which will ease the theoretical development of G-SICAMM. The observations from each one of the $L$ chains are denoted by $\mathbf{x}_{l}(n), l=1, \ldots, L$; likewise, the history of all observations from the $l$-th chain up to time $n$ is


Figure 4.3. G-SICAMM graph with two chains, whose variables are indicated by $\chi$ (chain 1 ) and $\varphi$ (chain 2). The square blocks represent the classes, the round blocks represent the parameters of each class, and the arrows show dependence between blocks.

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represented by $\mathbf{x}_{l}(n)=\left[\mathbf{x}_{l}(0), \mathbf{x}_{l}(1), \ldots, \mathbf{x}_{l}(n)\right]$. Conversely, the set of observations from all the chains for a given time is the column vector $\mathbf{x}(n)=\left[\mathbf{x}_{1}(n)^{T}, \mathbf{x}_{2}(n)^{T}, \ldots, \mathbf{x}_{L}(n)^{T}\right]^{T}$, and the history of all these sets of observations up to time $n$ is $\mathbf{X}(n)=\left[\mathbf{X}_{1}(n), \mathbf{X}_{2}(n), \ldots, \mathbf{X}_{L}(n)\right]$. Finally, we define the class vector $\mathbf{k}=\left[k_{1}, k_{2}, \ldots, k_{L}\right]^{T}$ as a particular combination of classes from each one of the $L$ chains, with $k_{l}=1, \ldots, K_{l}$. The classes from each one of the chains at each time instant is given by $\mathbf{c}_{\mathbf{k}}(n)=\left[C_{k_{1}}(n) \ldots C_{k_{L}}(n)\right]^{T}$.

It is assumed that observations are conditionally independent between chains given their respective classes; hence, $p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)=\prod_{l=1}^{L} p\left(\mathbf{x}_{l}(n) \mid C_{k_{l}}(n)\right)$. Given the ICA mixture model for each chain and using (2.32), we can obtain that

$$
\begin{equation*}
p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)=\prod_{l=1}^{L} p\left(\mathbf{x}_{l}(n) \mid C_{k_{l}}(n)\right)=\prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right) \tag{4.11}
\end{equation*}
$$

Finally, we extend the Markov assumption from each individual chain to the joint sets by defining $p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)=p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right) \cdot p\left(\mathbf{X}(n-1) \mid \mathbf{c}_{\mathbf{k}}(n)\right)$. Thus, $p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)$ is a function of the current set of observations for all chains and the probability density of the previous set of observations, $\mathbf{x}(n)$.

G-SICAMM can perform classification by MAP estimation, i.e., maximizing $P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n)\right)$. This probability can be estimated as in (4.3), but considering the multiple chains in the CHMM as follows:

$$
\begin{align*}
& P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n)\right)=\frac{p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n)\right)}{p(\mathbf{X}(n))}= \\
& =\frac{p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n)\right)}{\sum_{k_{1}{ }^{\prime}=1}^{K_{1}} \sum_{k_{2}{ }^{\prime}=1}^{K_{2}} \ldots \sum_{k_{L}{ }^{\prime}=1}^{K_{L}} p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}} \cdot(n)\right)}= \\
& =\frac{p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{X}(n-1))}{\sum_{k_{1}{ }^{\prime}=1}^{K_{1}} \sum_{k_{2}{ }^{\prime}=1}^{K_{2}} \ldots \sum_{k_{L}{ }^{\prime}=1}^{K_{L}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n) \mid \mathbf{X}(n-1)\right) \cdot p(\mathbf{X}(n-1))}=  \tag{4.12}\\
& P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right) \\
& \sum_{k_{1}=1}^{K_{1}} \sum_{k_{2}=1}^{K_{2}} \ldots \sum_{k_{L}^{\prime}=1}^{K_{L}} P\left(\mathbf{c}_{\mathbf{k}},(n) \mid \mathbf{X}(n-1)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}{ }^{\prime}}\right| \cdot p\left(\mathbf{s}_{k_{l}^{\prime}}(n)\right)
\end{align*}
$$

where $P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right)$ can be estimated from the CHMM in a similar way to (4.4):

$$
\begin{equation*}
P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right)=\sum_{k_{1}=1}^{K_{1}} \sum_{k_{2}^{\prime}=1}^{K_{2}} \cdots \sum_{k_{L}^{\prime}=1}^{K_{L}} \pi_{\mathbf{k k}^{\prime}} \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \mathbf{X}(n-1)\right) \tag{4.13}
\end{equation*}
$$

where $\pi_{\mathbf{k k}^{\prime}}=P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1)\right)$ is the transition probability from the combinations of classes $\mathbf{k}^{\prime}=\left[k_{1}{ }^{\prime}, k_{2}{ }^{\prime}, \ldots, k_{L} '^{\prime}\right]^{T}$ to the combination $\mathbf{k}=\left[k_{1}, k_{2}, \ldots, k_{L}\right]^{T}$. Thus, the CHMM behaves much like a "super-HMM" where each state of the super-HMM corresponds to a combination of states in the CHMM. The initial values for (4.13) can be estimated as the prior probabilities of each combination of states, $P\left(\mathbf{c}_{\mathbf{k}}(0) \mid \mathbf{X}(-1)\right)=P\left(\mathbf{c}_{\mathbf{k}}(0)\right)$; we can write:

$$
\begin{equation*}
P\left(\mathbf{c}_{\mathbf{k}}(n)\right)=\prod_{l=1}^{L} P\left(C_{k_{l}}(n)\right) \tag{4.14}
\end{equation*}
$$

The G-SICAMM algorithm is described in Table 4.2. The parameters of G-SICAMM are the ICA parameters from each class and from each chain (that is, $\mathbf{W}_{k_{l}}, p\left(\mathbf{s}_{k_{l}}\right), \mathbf{b}_{k_{l}}$, $\left.k_{l}=1, \ldots, K_{l}, L=1, \ldots, L\right)$ and the transition probabilities between every pair of combinations of classes, $\pi_{\mathbf{k k}^{\prime}} \forall \mathbf{k}, \mathbf{k}^{\prime}$.

## Initialization

Select initial observations, $\mathbf{X}(0)=\left[\mathbf{X}_{1}(0) \ldots \mathbf{X}_{L}(0)\right], \quad \mathbf{X}_{l}(0)=\mathbf{x}_{l}(0), \quad l=1, \ldots, L$
Calculate sources for each class, $\mathbf{s}_{k_{l}}(0)=\mathbf{W}_{k_{l}} \cdot\left(\mathbf{x}_{l}(0)-\mathbf{b}_{k_{l}}\right), k_{l}=1, \ldots, K_{l}, l=1, \ldots, L$
Initialize conditional class probability for each combination of classes $\mathbf{k}$ using (4.14):

$$
P\left(\mathbf{c}_{\mathbf{k}}(0)\right)=\prod_{l=1}^{L} P\left(C_{k_{l}}(0)\right)
$$

Calculate posterior probability for each combination of classes $\mathbf{k}$ as

$$
P\left(\mathbf{c}_{\mathbf{k}}(0) \mid \mathbf{x}(0)\right)=\frac{P\left(\mathbf{c}_{\mathbf{k}}(0)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{k}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(0)\right)}{\sum_{k_{1}=1}^{K_{1}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L^{\prime}}=1}^{K_{L}} P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(0)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l^{\prime}}}\right| \cdot p\left(\mathbf{s}_{k_{i}}(0)\right)}
$$

Initial observations are assigned to the combination of classes with maximum posterior

## Updating

For $n=1, \ldots, N$, with $N+1$ being the number of observations:
Select current observations, $\mathbf{X}(n)=\left[\mathbf{X}_{1}(n) \ldots \mathbf{X}_{L}(n)\right], \quad \mathbf{X}_{l}(n)=\mathbf{x}_{l}(n), l=1, \ldots, L$
Calculate sources for each class, $\mathbf{s}_{k_{l}}(n)=\mathbf{W}_{k_{l}} \cdot\left(\mathbf{x}_{l}(n)-\mathbf{b}_{k_{l}}\right), k_{l}=1, \ldots, K_{l}, l=1, \ldots, L$
Calculate conditional class probability for each combination of classes $\mathbf{k}$ using (4.13):

$$
P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right)=\sum_{k_{1}^{\prime}=1}^{K_{1}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L^{\prime}}=1}^{K_{L}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \mathbf{X}(n-1)\right)
$$

Calculate posterior probability for each combination of classes $\mathbf{k}$ using (4.12):

$$
P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n)\right)=\frac{P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right)}{\sum_{k_{1}=1}^{K_{1}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L}=1}^{K_{L}} P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n) \mid \mathbf{X}(n-1)\right) \cdot \prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right)}
$$

Current observations are assigned to the combination of classes with maximum posterior
Table 4.2. The G-SICAMM algorithm.

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### 4.2.2. Training algorithm

The G-SICAMM parameters are not known beforehand, and instead they have to be estimated from training data. The estimation algorithm depends on the kind of data available for training. For unsupervised or semi-supervised data (i.e., data whose classes are only partly known), all parameters should be estimated simultaneously. An algorithm for unsupervised or semisupervised training for G-SICAMM is proposed in Section 4.3.

In the case of supervised training (i.e., the class of all training data is known), the estimation of the ICAMM parameters can be performed separately for each chain and separately from the estimation of the transition probabilities. The ICA mixture model for each chain can be calculated using any of the traditional ICAMM estimation algorithms (e.g., [231,153]), while transition probabilities are usually estimated by counting:

$$
\begin{equation*}
\pi_{\mathbf{k} \mathbf{k}^{\prime}}=\frac{\# \operatorname{transitions} \text { from combination } \mathbf{k}^{\prime} \text { to combination } \mathbf{k}}{\# \text { samples in combination } \mathbf{k}^{\prime}} \tag{4.15}
\end{equation*}
$$

### 4.2.3. G-SICAMM variants

The variants suggested for SICAMM can be applied to G-SICAMM (i.e., the application of the Baum-Welch and Viterbi procedures). These procedures were introduced in Sections 4.1.2.a and 4.1.2.b, respectively. We have considered the G-SICAMM as a "super-HMM," where each state of the super-HMM corresponds to a possible combination of classes of the G-SICAMM. Thus, the procedures will work with combinations of classes rather than working with single classes. Equations (4.6), (4.7) and (4.10) are thus replaced by the following:

$$
\begin{align*}
\alpha_{\mathbf{k}}(n+1) & =p\left(\mathbf{x}(n+1) \mid \mathbf{c}_{\mathbf{k}}(n+1)\right) \cdot \sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot \alpha_{\mathbf{k}^{\prime}}(n)  \tag{4.16}\\
\beta_{\mathbf{k}}(n) & =\sum_{\mathbf{k}^{\prime}} p\left(\mathbf{x}(n+1) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n+1)\right) \cdot \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot \beta_{\mathbf{k}^{\prime}}(n+1)  \tag{4.17}\\
\delta_{\mathbf{k}}(n+1) & =p\left(\mathbf{x}(n+1) \mid \mathbf{c}_{\mathbf{k}}(n+1)\right) \cdot \max _{\mathbf{k}}\left(\pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot \delta_{\mathbf{k}^{\prime}}(n)\right) \tag{4.18}
\end{align*}
$$

where $p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)$ is calculated using (4.11). The initial values for the auxiliary variables $\alpha, \delta$ are changed to $\alpha_{\mathbf{k}}(0)=\delta_{\mathrm{k}}(0)=p\left(\mathbf{x}(0) \mid \mathbf{c}_{\mathrm{k}}(0)\right) \cdot P\left(\mathbf{c}_{\mathrm{k}}(0)\right)$, where $P\left(\mathbf{c}_{\mathrm{k}}(0)\right)$ is calculated using (4.14). Taking these changes into account, both procedures can be used with GSICAMM as an alternative to MAP estimation.

The consideration of the CHMM as a super-HMM, however, is computationally expensive and can become intractable as the number of chains or states grow, given that the number of combinations of states grows exponentially. There are several modifications of the classical Baum-Welch and Viterbi algorithms that alleviate this problem, usually by considering only some of the possible combinations of states at a given time [32], by using approximate inference [147], or by approximating the calculations [234,287]. However, the cases presented in this work were tractable enough, and we only considered the classical version of the algorithms for CHMM (equations (4.16) to (4.18)).

### 4.3. Unsupervised Generalized SICAMM: UG-SICAMM

In Sections 4.1.1 and 4.2.2, the estimation of SICAMM and G-SICAMM has been treated using supervised training. This section introduces an algorithm for unsupervised or semi-supervised training of G-SICAMM and SICAMM based on previous works of the GTS [231]. We have named the algorithm Unsupervised Generalized SICAMM (UG-SICAMM). We will assume the same model presented in Section 4.2.1.

### 4.3.1. The log-likelihood cost function

The proposed algorithm maximizes the log-likelihood of the data with respect to the parameters of the model,

$$
\begin{equation*}
L(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})=\log p(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})=\log \left(\prod_{n=1}^{N} \frac{p(\mathbf{X}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}{p(\mathbf{X}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}\right) \tag{4.19}
\end{equation*}
$$

where $\boldsymbol{\Psi}$ is a compact notation for all of the unknown ICAMM parameters, $\mathbf{w}_{k_{i}}, p\left(\mathbf{s}_{k_{i}}\right), \mathbf{b}_{k_{i}}$, $k_{l}=1, \ldots, K_{l}, l=1, \ldots, L$; and $\pi$ is a compact notation for all of the transition probabilities, $\pi_{\mathbf{k k}^{\prime}}=P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1)\right)$, for all combinations $\mathbf{k}, \mathbf{k}^{\prime} ;$ and assuming $p(\mathbf{X}(0))=1$. The probability $p(\mathbf{X}(n) \mid \Psi, \boldsymbol{\pi})$ can be expressed as a function of previous time instants by making use of the time dependences in G-SICAMM (the Markov assumption) and Bayes rule:

$$
\begin{align*}
& p(\mathbf{X}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})=\sum_{\mathbf{k}} p\left(\mathbf{X}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}\right)= \\
& =\sum_{\mathbf{k}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot p\left(\mathbf{X}(n-1) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}\right)=  \tag{4.20}\\
& =\sum_{\mathbf{k}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot p(\mathbf{X}(n-1) \mid \Psi, \boldsymbol{\pi})
\end{align*}
$$

Using equation (4.20), the log-likelihood (4.19) can be re-written as a combination of the probability of every available feature vector:

$$
\begin{align*}
L(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}) & =\log \left(\prod_{n=1}^{N} \frac{p(\mathbf{X}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}{p(\mathbf{X}(n-1) \mid \Psi, \boldsymbol{\pi})}\right)=\sum_{n=1}^{N} \log \left(\frac{p(\mathbf{X}(n) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}{p(\mathbf{X}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}\right)=  \tag{4.21}\\
& =\sum_{n=1}^{N} \log \left[\sum_{\mathbf{k}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1), \boldsymbol{\Psi}, \boldsymbol{\pi}\right)\right]
\end{align*}
$$

In order to simplify the above equation and the maximization process, the following variables are defined:

$$
\begin{align*}
A(n) & =\sum_{\mathbf{k}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \Psi\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1), \Psi \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \\
B_{\mathbf{k}}(n) & =p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \Psi \mathbf{\Psi}\right)  \tag{4.22}\\
D_{\mathbf{k}}(n) & =P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{X}(n-1), \Psi, \boldsymbol{\Psi}\right)=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k k}^{\mathbf{k}}} \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}} \cdot(n-1) \mid \mathbf{X}(n-1), \Psi \boldsymbol{\Psi}, \boldsymbol{\pi}\right)
\end{align*}
$$

Clearly,

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$$
\begin{equation*}
L(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})=\sum_{n=1}^{N} \log A(n)=\sum_{n=1}^{N} \log \left[\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \cdot D_{\mathbf{k}}(n)\right] \tag{4.23}
\end{equation*}
$$

where $A(n)$ is the contribution of time instant $n$ to the log-likelihood, which is to be computed by summing up the product of the contribution of the current observation $\mathbf{x}(n)\left(B_{\mathbf{k}}(n)\right)$ multiplied by the contribution of the history $\mathbf{X}(n-1)\left(D_{\mathbf{k}}(n)\right)$ for every possible value of the class vector $\mathbf{k} . B_{\mathbf{k}}(n)$ can be calculated considering the assumed ICAMM and the independence of the observations conditioned to the classes:

$$
\begin{equation*}
p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right)=\prod_{l=1}^{L} p\left(\mathbf{x}_{l}(n) \mid C_{k_{l}}(n)\right)=\prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right) \tag{4.24}
\end{equation*}
$$

which is equivalent to (4.1) and (4.11). On the other hand, $D_{\mathrm{k}}(n)$ can be calculated in a recursive manner, as we demonstrate in the following. Using the Bayes rule several times, we have that

$$
\begin{align*}
& D_{\mathbf{k}}(n)=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot p\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \mathbf{X}(n-1), \boldsymbol{\Psi}, \boldsymbol{\pi}\right)= \\
& =\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k}^{\mathbf{k}^{\prime}}} \cdot \frac{p\left(\mathbf{X}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}\right)}{p(\mathbf{X}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}= \\
& =\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k}^{\prime} \mathbf{k}^{\prime}} \frac{p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1), \boldsymbol{\Psi}\right) \cdot p\left(\mathbf{X}(n-2) \mid \mathbf{c}_{\mathbf{k}^{\prime} \cdot}(n-1), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime} \cdot}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}\right)}{\sum_{\mathbf{k}^{\prime \prime}} p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime \prime}}(n-1), \Psi\right) \cdot p\left(\mathbf{X}(n-2) \mid \mathbf{c}_{\mathbf{k}^{\prime \prime}}(n-1), \Psi, \boldsymbol{\Psi}\right) \cdot P\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \boldsymbol{\Psi}, \boldsymbol{\pi}\right)}= \\
& =\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \frac{p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime}} \cdot(n-1), \boldsymbol{\Psi}\right) \cdot p\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \mathbf{X}(n-2), \Psi \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot p(\mathbf{X}(n-2) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}{\sum_{\mathbf{k}^{\prime \prime}} p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime \prime}}(n-1), \boldsymbol{\Psi}\right) \cdot p\left(\mathbf{c}_{\mathbf{k}^{\prime \prime}}(n-1) \mid \mathbf{X}(n-2), \boldsymbol{\Psi}, \boldsymbol{\pi}\right) \cdot p(\mathbf{X}(n-2) \mid \Psi, \boldsymbol{\pi})}=  \tag{4.25}\\
& =\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k}^{\mathbf{k}^{\prime}}} \cdot \frac{p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1), \boldsymbol{\Psi}\right) \cdot p\left(\mathbf{c}_{\mathbf{k}^{\prime}}(n-1) \mid \mathbf{X}(n-2), \boldsymbol{\Psi}, \boldsymbol{\pi}\right)}{\sum_{\mathbf{k}^{\prime \prime}} p\left(\mathbf{x}(n-1) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1), \Psi\right) \cdot p\left(\mathbf{c}_{\mathbf{k}^{\prime \prime}}(n-1) \mid \mathbf{X}(n-2), \Psi, \boldsymbol{\pi}\right)}= \\
& =\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot \frac{B_{\mathbf{k}^{\prime}}(n-1) \cdot D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)}
\end{align*}
$$

where $A(n-1)$ can be calculated from past values using (4.22). The initial value, $D_{k}(0)$, will be considered later. Now, let us compute the gradient $L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})$ so that we can implement algorithms to iteratively estimate the parameters that maximize the log-likelihood. From (4.23) we have that

$$
\begin{align*}
& \frac{\delta L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})}{\delta \mathbf{W}_{m_{i}}}=\sum_{n=1}^{N} \frac{1}{A(n)} \frac{\delta A(n)}{\delta \mathbf{W}_{m_{i}}}=\sum_{n=1}^{N} \frac{1}{A(n)}\left(\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{i}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{i}}}\right) \\
& \frac{\delta L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})}{\delta \mathbf{b}_{m_{i}}}=\sum_{n=1}^{N} \frac{1}{A(n)}\left(\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{i}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{i}}}\right)  \tag{4.26}\\
& \frac{\delta L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})}{\delta \pi_{\mathrm{m} \mathbf{~ m}}}=\sum_{n=1}^{N} \frac{1}{A(n)} \sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \pi_{\mathrm{m} \mathbf{m}}}
\end{align*}
$$

Hence, we must now concentrate in the computation of the derivatives of $D_{\mathbf{k}}(n)$ and $B_{\mathbf{k}}(n)$ with respect to the different parameters of the model. The derivatives of $B_{\mathrm{k}}(n)$ can be calculated by making use of the property $\frac{\delta f(x)}{\delta x}=f(x) \cdot \frac{1}{f(x)} \frac{\delta f(x)}{\delta x}=f(x) \frac{\delta \log f(x)}{\delta x}$ :

$$
\begin{align*}
\frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}} & =B_{\mathbf{k}}(n) \cdot \frac{\delta \log \left[\prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right)\right]}{\delta \mathbf{W}_{m_{l}}}= \\
& =B_{\mathbf{k}}(n) \cdot \sum_{l=1}^{L} \frac{\delta\left(\log \left|\operatorname{det} \mathbf{W}_{k_{l}}\right|+\log \left[p\left(\mathbf{s}_{k_{l}}(n)\right)\right]\right)}{\delta \mathbf{W}_{m_{l}}}=  \tag{4.27}\\
& =\left\{\begin{array}{l}
B_{\mathbf{k}}(n) \cdot\left\{\left(\mathbf{W}_{m_{l}}{ }^{T}\right)^{-1}+\frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(n)\right)\right]}{\delta \mathbf{W}_{m_{l}}}\right\}_{\text {if } k_{l}=m_{l}} \\
\frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}}= \begin{cases}B_{\mathbf{k}}(n) \cdot \frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(n)\right)\right]}{\delta \mathbf{b}_{m_{l}}} & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }\end{cases}
\end{array}\right.
\end{align*}
$$

Whereas the derivatives of $D_{\mathrm{k}}(n)$ are calculated from (4.25):

$$
\begin{align*}
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{i}}}=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k k}} \cdot\left\lceil\left[\frac{B_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta D_{\mathbf{k}^{\prime}} \cdot(n-1)}{\delta \mathbf{W}_{m_{l}}}+\frac{D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta B_{\mathbf{k}^{\prime}}(n-1)}{\delta \mathbf{W}_{m_{i}}}-\right.\right.  \tag{4.29}\\
& \left.-\frac{D_{\mathbf{k}} \cdot(n-1) \cdot B_{\mathbf{k}}(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \mathbf{W}_{m_{l}}}\right\rfloor \\
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}}=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot\left[\frac{B_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta D_{\mathbf{k}^{\prime}}(n-1)}{\delta \mathbf{b}_{m_{l}}}+\frac{D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta B_{\mathbf{k}^{\prime}}(n-1)}{\delta \mathbf{b}_{m_{l}}}-\right.  \tag{4.30}\\
& \left.-\frac{D_{\mathbf{k}^{\prime}}(n-1) \cdot B_{\mathbf{k}^{\prime}}(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \mathbf{b}_{m_{i}}}\right] \\
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \pi_{\mathrm{mm}} \cdot}=\left\{\begin{array}{cl}
\frac{\delta D_{\mathrm{m}}(n)}{\delta \pi_{\mathrm{mm}} .} & \text { if } \mathbf{k}=\mathbf{m} \\
\mathbf{0} & \text { otherwise }
\end{array}\right. \\
& \frac{\delta D_{\mathbf{m}}(n)}{\delta \pi_{\mathrm{m} \mathrm{~m}}{ }^{\prime}}=\frac{\delta}{\delta \pi_{\mathrm{m} \mathrm{~m}}{ }^{\prime}}\left\{\sum_{\mathbf{k}^{\prime}} \pi_{\mathrm{m}^{\prime}} \cdot \frac{B_{\mathbf{k}^{\prime}}(n-1) \cdot D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)}\right\}= \\
& =\frac{B_{\mathbf{m}} \cdot(n-1) D_{\mathbf{m}^{\prime}} \cdot(n-1)}{A(n-1)}+\sum_{\mathbf{k}^{\prime}} \pi_{\mathrm{m} \mathbf{k}^{\prime}} \cdot \frac{\delta}{\delta \pi_{\mathrm{m} \mathbf{m}^{\prime}}}\left\{\frac{B_{\mathbf{k}^{\prime}}(n-1) \cdot D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)}\right\}=  \tag{4.31}\\
& =\frac{B_{\mathrm{m}} \cdot(n-1) D_{\mathrm{m}} \cdot(n-1)}{A(n-1)}+\pi_{\mathrm{m} \mathrm{~m}} \cdot \frac{B_{\mathrm{m}}(n-1)}{A(n-1)} \frac{\delta D_{\mathrm{m}}(n-1)}{\delta \pi_{\mathrm{m} \mathrm{~m}} .}- \\
& -\sum_{\mathbf{k}^{\prime}} \pi_{\mathrm{m} \mathbf{k}^{\prime}} \cdot \frac{B_{\mathbf{k}^{\prime}}(n-1) D_{\mathbf{k}^{\prime}}(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \pi_{\mathrm{m} \mathrm{~m}} .}
\end{align*}
$$

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The derivatives of $A(n-1)$ are required in equations (4.29) to (4.31), but they can be obtained from the derivatives of the other two variables:

$$
\begin{align*}
& \frac{\delta A(n)}{\delta \mathbf{W}_{m_{i}}}=\sum_{\mathrm{k}} B_{\mathrm{k}}(n) \frac{\delta D_{\mathrm{k}}(n)}{\delta \mathbf{W}_{m_{l}}}+D_{\mathrm{k}}(n) \frac{\delta B_{\mathrm{k}}(n)}{\delta \mathbf{W}_{m_{i}}} \\
& \frac{\delta A(n)}{\delta \mathbf{b}_{m_{i}}}=\sum_{\mathrm{k}} B_{\mathrm{k}}(n) \frac{\delta D_{\mathrm{k}}(n)}{\delta \mathbf{b}_{m_{i}}}+D_{\mathrm{k}}(n) \frac{\delta B_{\mathrm{k}}(n)}{\delta \mathbf{b}_{m_{i}}}  \tag{4.32}\\
& \frac{\delta A(n)}{\delta \pi_{\mathrm{mm} .}}=B_{\mathrm{m}}(n) \cdot \frac{\delta D_{\mathrm{m}}(n)}{\delta \pi_{\mathrm{mm} .}}
\end{align*}
$$

Therefore, the derivatives at time instant $n$ can be computed recursively from their values in the previous time instant, $n-1$. The recursion starts at $n=1$, hence we require initial values for all the variables and its derivatives.

The initial values of $B_{k}(0)$ and its derivatives can be calculated from the first available observation, $\mathbf{x}(0)$, using (4.22), (4.27) and (4.28):

$$
\left.\begin{array}{rl}
B_{\mathbf{k}}(0) & =p\left(\mathbf{x}(0) \mid \mathbf{c}_{\mathbf{k}}(0), \boldsymbol{\Psi}\right) \\
\frac{\delta B_{\mathbf{k}}(0)}{\delta \mathbf{W}_{m_{l}}}= \begin{cases}\left.B_{\mathbf{k}}(0) \cdot\left(\mathbf{W}_{m_{l}}{ }^{T}\right)^{-1}+\frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(0)\right)\right]}{\delta \mathbf{W}_{m_{l}}}\right) & \text { if } k_{l}=m_{l}\end{cases}  \tag{4.33}\\
\frac{\delta}{\delta \mathbf{b}_{\mathbf{k}}(0)} & \text { otherwise }
\end{array}\right\} \begin{array}{ll}
B_{m_{l}}(0) \cdot \frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(0)\right)\right]}{\delta \mathbf{b}_{m_{l}}} & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }
\end{array}
$$

At $n=0$ there are no previous observations. We may assume that the conditional probabilities for each combination of classes $\mathbf{k}$ can be replaced by their a priori probabilities, hence $D_{k}(0)=P\left(\mathbf{c}_{\mathbf{k}}(0)\right)$. Finally, the initial value $A(0)$ can be calculated from $B_{k}(0)$ and $D_{k}(0)$. This leads to

$$
\begin{align*}
D_{\mathbf{k}}(0) & =p\left(\mathbf{c}_{\mathbf{k}}(0)\right) \\
A(0) & =\sum_{\mathbf{k}} B_{\mathbf{k}}(0) \cdot D_{\mathbf{k}}(0)  \tag{4.34}\\
\frac{\delta D_{\mathbf{k}}(0)}{\delta \mathbf{W}_{m_{i}}} & =\frac{\delta D_{\mathbf{k}}(0)}{\delta \mathbf{b}_{m_{i}}}=\frac{\delta D_{\mathbf{k}}(0)}{\delta \pi_{\mathbf{k} \mathbf{m}_{i}}}=\frac{\delta A(0)}{\delta \mathbf{W}_{m_{i}}}=\frac{\delta A(0)}{\delta \mathbf{b}_{m_{i}}}=\frac{\delta A(0)}{\delta \pi_{\mathbf{k} \mathbf{m}_{i}}}=0
\end{align*}
$$

Equations (4.27)-(4.34) can be used to calculate the derivatives (4.26) from all of the available observations. These derivatives are used in turn to update the parameters for all classes $m_{l}=1 \ldots K_{l}, l=1 \ldots L$ :

$$
\begin{align*}
& \mathbf{W}_{m_{i}}(i+1)=\mathbf{W}_{m_{l}}(i)+\alpha \cdot \frac{\delta L(\mathbf{X} / \Psi, \boldsymbol{\pi})}{\delta \mathbf{W}_{m_{i}}}(i) \\
& \mathbf{b}_{m_{i}}(i+1)=\mathbf{b}_{m_{i}}(i)+\beta \cdot \frac{\delta L(\mathbf{X} / \Psi, \boldsymbol{\pi})}{\delta \mathbf{b}_{m_{i}}}(i)  \tag{4.35}\\
& \pi_{\mathrm{m} \mathbf{m}} \cdot(i+1)=\pi_{\mathrm{mm}} \cdot(i)+v \cdot \frac{\delta L(\mathbf{X} / \Psi, \boldsymbol{\Psi})}{\delta \pi_{\mathrm{m} \mathbf{m}}}(i)
\end{align*}
$$

where $\alpha, \beta, v$ are the learning rates of the different parameters, (i) denotes the current iteration, and $(i+1)$ denotes the next iteration. After updating the parameters, the algorithm starts again from $n=0$ for the next iteration.

### 4.3.2. UG-SICAMM algorithm

The UG-SICAMM procedure is summarized in Table 4.3.

## Initialization

Initialize the G-SICAMM parameters $\mathbf{w}_{m_{l}}(0), \mathbf{b}_{m_{l}}(0), \pi_{\mathrm{mm}}, \quad, m_{l}=1 \ldots K_{l}, l=1 \ldots L$ at random

## Updating

For each iteration $i=1, \ldots$, M AXITER ,
Calculate initial values for the variables in (4.33)-(4.34):

$$
\begin{aligned}
& B_{\mathbf{k}}(0)=\prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(0)\right) \\
& D_{\mathbf{k}}(0)=p\left(\mathbf{c}_{\mathbf{k}}(0)\right) \\
& A(0)=\sum_{\mathbf{k}} B_{\mathbf{k}}(0) \cdot D_{\mathbf{k}}(0) \\
& \frac{\delta B_{\mathbf{k}}(0)}{\delta \mathbf{W}_{m_{l}}}=\left\{\begin{array}{l}
B_{\mathbf{k}}(0) \cdot\left\{\left(\mathbf{W}_{m_{l}}{ }^{T}\right)^{-1}+\frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(0)\right)\right]}{\delta \mathbf{W}_{m_{l}}}\right\} \\
\mathbf{0} \quad \text { if } k_{l}=m_{l} \\
\text { otherwise }
\end{array}\right. \\
& \frac{\delta B_{\mathbf{k}}(0)}{\delta \mathbf{b}_{m_{l}}}=\left\{\begin{array}{cl}
B_{\mathbf{k}}(0) \cdot \frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(0)\right)\right]}{\delta \mathbf{b}_{m_{l}}} & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }
\end{array}\right. \\
& \frac{\delta D_{\mathbf{k}}(0)}{\delta \mathbf{W}_{m_{l}}}=\frac{\delta D_{\mathbf{k}}(0)}{\delta \mathbf{b}_{m_{l}}}=\frac{\delta D_{\mathbf{k}}(0)}{\delta \pi_{\mathbf{k} \mathbf{m}_{l}}}=\frac{\delta A(0)}{\delta \mathbf{W}_{m_{l}}}=\frac{\delta A(0)}{\delta \mathbf{b}_{m_{l}}}=\frac{\delta A(0)}{\delta \pi_{\mathbf{k m}_{l}}}=0
\end{aligned}
$$

For each observation $n=1, \ldots, N$, with $N+1$ being the number of observations:
Calculate $B_{k}(n)$ using (4.11), $B_{k}(n)=\prod_{l=1}^{L}\left|\operatorname{det} \mathbf{W}_{k_{l}}\right| \cdot p\left(\mathbf{s}_{k_{l}}(n)\right)$
Calculate $D_{k}(n)$ using (4.25), $D_{\mathbf{k}}(n)=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k}^{\prime}} \cdot \frac{B_{\mathbf{k}^{\prime}}(n-1) \cdot D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)}$
Calculate $A(n)$ using (4.22), $A(n)=\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \cdot D_{\mathbf{k}}(n)$
Calculate the derivatives of $B_{k}(n)$ using (4.27), (4.28):

$$
\begin{aligned}
& \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}}=\left\{\begin{array}{c}
B_{\mathbf{k}}(n) \cdot\left\{\left(\mathbf{W}_{m_{l}}{ }^{T}\right)^{-1}+\frac{\delta \log \left[p\left(\mathbf{s}_{m_{l}}(n)\right)\right]}{\delta \mathbf{W}_{m_{l}}}\right) \\
\mathbf{0} \quad \text { if } k_{l}=m_{l} \\
\text { otherwise }
\end{array}\right. \\
& \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}}=\left\{\begin{array}{cl}
B_{\mathbf{k}}(n) \cdot \frac{\delta \log \left[p\left(\mathbf{s}_{m_{t}}(n)\right)\right]}{\delta \mathbf{b}_{m_{l}}} & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }
\end{array}\right.
\end{aligned}
$$

Calculate the derivatives of $D_{k}(n)$ using (4.29)-(4.31):

$$
\begin{aligned}
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{t}}}=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k k}} \cdot \cdot\left[\frac{B_{\mathbf{k}^{\prime}} \cdot(n-1)}{A(n-1)} \frac{\delta D_{\mathbf{k}^{\prime}}(n-1)}{\delta \mathbf{W}_{m_{t}}}+\frac{D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta B_{\mathbf{k}^{\prime}} \cdot(n-1)}{\delta \mathbf{W}_{m_{t}}}-\right. \\
& \left.-\frac{D_{\mathbf{k}^{\prime}}(n-1) \cdot B_{\mathbf{k}^{*}} \cdot(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \mathbf{W}_{m_{i}}}\right\rfloor \\
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{I}}}=\sum_{\mathbf{k}^{\prime}} \pi_{\mathbf{k} \mathbf{k}^{\prime}} \cdot\left\lceil\frac{B_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta D_{\mathbf{k}^{\prime}}(n-1)}{\delta \mathbf{b}_{m_{I}}}+\frac{D_{\mathbf{k}^{\prime}}(n-1)}{A(n-1)} \frac{\delta B_{\mathbf{k}^{\prime}} \cdot(n-1)}{\delta \mathbf{b}_{m_{I}}}-\right. \\
& \left.-\frac{D_{\mathbf{k}^{\mathbf{k}}} \cdot(n-1) \cdot B_{\mathbf{k}^{\cdot}} \cdot(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \mathbf{b}_{m_{i}}}\right] \\
& \frac{\delta D_{\mathbf{k}}(n)}{\delta \pi_{\mathrm{m} \mathbf{m}}}=\left\{\begin{array}{cc}
\frac{\delta D_{\mathrm{m}}(n)}{\delta \pi_{\mathrm{m} \mathrm{~m}} .} & \text { if } \mathbf{k}=\mathbf{m} \\
\mathbf{0} & \text { otherwise }
\end{array}\right. \\
& \frac{\delta D_{\mathrm{m}}(n)}{\delta \pi_{\mathrm{m} \mathbf{m}}}=\frac{B_{\mathrm{m}} \cdot(n-1) D_{\mathrm{m}} \cdot(n-1)}{A(n-1)}+\pi_{\mathrm{m} \mathrm{~m}} \cdot \frac{B_{\mathrm{m}}(n-1)}{A(n-1)} \frac{\delta D_{\mathrm{m}}(n-1)}{\delta \pi_{\mathrm{m} \mathbf{m}}}- \\
& -\sum_{\mathbf{k}^{\prime}} \pi_{\mathrm{m} \mathbf{k}^{\prime}} \cdot \frac{B_{\mathbf{k}^{\prime}}(n-1) D_{\mathbf{k}^{\prime}}(n-1)}{A^{2}(n-1)} \frac{\delta A(n-1)}{\delta \pi_{\mathrm{m} \mathrm{~m}} .}
\end{aligned}
$$

Calculate the derivatives of $A(n)$ using (4.32):

$$
\begin{aligned}
& \frac{\delta A(n)}{\delta \mathbf{W}_{m_{l}}}=\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}} \\
& \frac{\delta A(n)}{\delta \mathbf{b}_{m_{l}}}=\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}} \\
& \frac{\delta A(n)}{\delta \pi_{\mathrm{m} \mathbf{m}}}=B_{\mathrm{m}}(n) \cdot \frac{\delta D_{\mathbf{m}}(n)}{\delta \pi_{\mathrm{m} \mathbf{m}}}
\end{aligned}
$$

Calculate the value of the log-likelihood $L(\mathbf{X}(N) \mid \Psi, \pi)$ using (4.23):

$$
L(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})=\sum_{n=1}^{N} \log \left[\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \cdot D_{\mathbf{k}}(n)\right]
$$

Calculate the derivatives of $L(\mathbf{X}(N) \mid \Psi, \pi)$ using (4.26):

$$
\begin{aligned}
& \frac{\delta L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})}{\delta \mathbf{W}_{m_{i}}}=\sum_{n=1}^{N} \frac{1}{A(n)} \frac{\delta A(n)}{\delta \mathbf{W}_{m_{i}}}=\sum_{n=1}^{N} \frac{1}{A(n)}\left(\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{t}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{t}}}\right) \\
& \frac{\delta L(\mathbf{X}(N) \mid \Psi, \boldsymbol{\pi})}{\delta \mathbf{b}_{m_{t}}}=\sum_{n=1}^{N} \frac{1}{A(n)}\left(\sum_{\mathbf{k}} B_{\mathbf{k}}(n) \frac{\delta D_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{t}}}+D_{\mathbf{k}}(n) \frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{t}}}\right)
\end{aligned}
$$

$$
\frac{\delta L(\mathbf{X}(N) \mid \boldsymbol{\Psi}, \boldsymbol{\pi})}{\delta \pi_{\mathrm{m} \mathrm{~m}^{\prime}}}=\sum_{n=1}^{N} \frac{1}{A(n)} \sum_{\mathrm{k}} B_{\mathrm{k}}(n) \frac{\delta D_{\mathrm{k}}(n)}{\delta \pi_{\mathrm{m} \mathrm{~m}^{\prime}}}
$$

Update G-SICAMM parameters using the gradient algorithm (4.35):

$$
\begin{aligned}
& \mathbf{W}_{m_{l}}(i+1)=\mathbf{W}_{m_{l}}(i)+\alpha \cdot \frac{\delta L(\mathbf{X} / \boldsymbol{\Psi}, \boldsymbol{\pi})}{\delta \mathbf{W}_{m_{t}}}(i) \\
& \mathbf{b}_{m_{t}}(i+1)=\mathbf{b}_{m_{t}}(i)+\beta \cdot \frac{\delta L(\mathbf{X} / \boldsymbol{\Psi}, \boldsymbol{\pi})}{\delta \mathbf{b}_{m_{t}}}(i) \\
& \pi_{\mathrm{m} \mathbf{m}}(i+1)=\boldsymbol{\pi}_{\mathrm{m} \mathbf{m}} \cdot(i)+v \cdot \frac{\delta L(\mathbf{X} / \boldsymbol{\Psi}, \boldsymbol{\pi})}{\delta \pi_{\mathrm{m} \mathbf{m}}}(i)
\end{aligned}
$$

Table 4.3. The UG-SICAMM algorithm.

### 4.3.3. Non-parametric estimation of the source densities

In the previous equations, the derivatives with respect to the sources have been formulated. However, the estimation of these derivatives is not straightforward and it requires prior knowledge of the underlying probability densities of the sources. In this work, we propose the probability density of each source be calculated using a non-parametric kernel density estimator such as the one in [231] (this was introduced in Section 1.1.2, and considered again in Section 3.1 for the proposed prediction algorithm PREDICAMM).

The derivative of the logarithm of the source densities with respect to the ICAMM parameters, required for (4.27), is calculated as

$$
\begin{align*}
\frac{\delta \log \left[p\left(\mathbf{s}_{k_{l}}(n)\right)\right]}{\delta \psi_{k_{l}}} & =\frac{\delta \log \left[\prod_{m=1}^{M} p\left(s_{k_{l}, m}(n)\right)\right]}{\delta \psi_{k_{l}}}=\sum_{m=1}^{M} \frac{\delta \log \left[p\left(s_{k_{l}, m}(n)\right)\right]}{\delta \psi_{k_{l}}}= \\
& =\sum_{m=1}^{M} \frac{1}{p\left(s_{k_{l}, m}(n)\right)} \cdot \frac{\delta p\left(s_{k_{l}, m}(n)\right)}{\delta \psi_{k_{l}}}=  \tag{4.36}\\
& =\sum_{m=1}^{M} \frac{1}{p\left(s_{k_{l}, m}(n)\right)} \cdot \frac{\delta p\left(s_{k_{l}, m}(n)\right)}{\delta s_{k_{l}, m}(n)} \cdot \frac{\delta s_{k_{l}, m}(n)}{\delta \psi_{k_{l}}}
\end{align*}
$$

where $\psi_{k_{i}}$ is a shorthand notation for $\mathbf{w}_{k_{i}}$ or $\mathbf{b}_{k_{i}}$, since (4.36) can be used in both cases, and $p\left(s_{k_{l}, m}(n)\right)$ is the $m$-th source from class $k_{l}$ at time instant $n$. The density of each source, $p\left(s_{k_{1}, m}(n)\right)$, and its derivative with respect to the source, $\delta p\left(s_{k_{1, m}, m}\right) / \delta s_{k_{1}, m}$, were calculated in equations (3.8) and (3.9), respectively. Since each source can be calculated as $s_{k_{l}, m}(n)=\mathbf{w}_{k_{l}, m} \cdot\left(\mathbf{x}_{l}(n)-\mathbf{b}_{k_{i}}\right)$, its derivatives with respect to the ICAMM parameters are

$$
\begin{align*}
& \frac{\delta s_{k_{i}, m}(n)}{\delta \mathbf{W}_{k_{i}}}=\mathbf{d}_{m} \cdot\left(\mathbf{x}(n)-\mathbf{b}_{k_{i}}\right)^{T}  \tag{4.37}\\
& \frac{\delta s_{k_{k}, m}(n)}{\delta \mathbf{b}_{k_{i}}}=-\mathbf{w}_{k_{i}}{ }^{T}
\end{align*}
$$

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where $\mathbf{d}_{m}$ is a column vector of zeros with a 1 in its $m$-th position. Thus, finally, the derivatives of the logarithm of the densities of the sources are:

$$
\begin{align*}
\frac{\delta \log \left[p\left(\mathbf{s}_{k_{l}}(n)\right)\right]}{\delta \mathbf{W}_{k_{l}}} & =\sum_{m=1}^{M} \frac{1}{p\left(s_{k_{l}, m}(n)\right)} \cdot \frac{\delta p\left(s_{k_{l}, m}(n)\right)}{\delta s_{k_{l}, m}(n)} \cdot d_{m} \cdot\left(\mathbf{x}(n)-\mathbf{b}_{k_{l}}\right)^{T}= \\
& =f\left(\mathbf{s}_{k_{l}}(n)\right) \cdot\left(\mathbf{x}(n)-\mathbf{b}_{k_{l}}\right)^{T}  \tag{4.38}\\
\frac{\delta \log \left[p\left(\mathbf{s}_{k_{l}}(n)\right)\right]}{\delta \mathbf{b}_{k_{l}}} & =\sum_{m=1}^{M} \frac{1}{p\left(s_{k_{l}, m}(n)\right)} \cdot \frac{\delta p\left(s_{k_{l}, m}(n)\right)}{\delta s_{k_{l}, m}(n)} \cdot(-1) \cdot \mathbf{w}_{k_{l}}{ }^{T}=-\mathbf{W}_{k_{l}}{ }^{T} \cdot f\left(\mathbf{s}_{k_{l}}(n)\right)
\end{align*}
$$

where $f\left(\mathbf{s}_{k_{l}}(n)\right)$ is a column vector whose $m$-th element is equal to $\frac{1}{p\left(s_{k_{l}, m}\right)} \cdot \frac{\delta p\left(s_{k_{l}, m}\right)}{\delta s_{k_{l}, m}}$, $m=1, \ldots, M$. By substituting (4.38) in (4.27) and (4.28), we obtain that

$$
\begin{gather*}
\frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}}=\left\{\begin{array}{cl}
B_{\mathbf{k}}(n) \cdot\left(\left(\mathbf{W}_{m_{l}}{ }^{T}\right)^{-1}+f\left(\mathbf{s}_{m_{l}}(n)\right) \cdot\left(\mathbf{x}(n)-\mathbf{b}_{m_{l}}\right)^{T}\right) & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }
\end{array}\right.  \tag{4.39}\\
\frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{b}_{m_{l}}}=\left\{\begin{array}{cl}
-B_{\mathbf{k}}(n) \cdot \mathbf{W}_{m_{l}}{ }^{T} \cdot f\left(\mathbf{s}_{m_{l}}(n)\right) & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherw ise }
\end{array}\right. \tag{4.40}
\end{gather*}
$$

Equation (4.39) can be replaced by the natural gradient, a variation of the regular gradient which has demonstrated good convergence properties [7]. In that case, the gradient with respect to the de-mixing matrices becomes

$$
\begin{align*}
\frac{\tilde{\delta} B_{\mathbf{k}}(n)}{\tilde{\delta} \mathbf{W}_{m_{l}}} & =\frac{\delta B_{\mathbf{k}}(n)}{\delta \mathbf{W}_{m_{l}}} \cdot \mathbf{W}_{m_{l}}{ }^{T} \cdot \mathbf{W}_{m_{l}}= \\
& =\left\{\begin{array}{cl}
B_{\mathbf{k}}(n) \cdot\left(\mathbf{I}+f\left(\mathbf{s}_{m_{l}}(n)\right) \cdot \mathbf{s}_{m_{l}}(n)^{T}\right) \cdot \mathbf{W}_{m_{l}} & \text { if } k_{l}=m_{l} \\
\mathbf{0} & \text { otherwise }
\end{array}\right. \tag{4.41}
\end{align*}
$$

### 4.3.4. Semi-supervised training

Let us consider a hybrid case with semi-supervised training, in which we could define some prior knowledge about some observations, such as their class. For instance, if $\mathbf{x}_{l}(n)$ is known to belong to class $k_{l}{ }^{\prime}$, then $P\left(\mathbf{c}_{\mathbf{m}}(n) \mid \mathbf{x}(n)\right)=1$ if $k_{l}=k_{l}{ }^{\prime}$, and $P\left(\mathbf{c}_{\mathbf{m}}(n) \mid \mathbf{x}(n)\right)=0$ otherwise. In that case, we can omit the calculation of $B_{\mathrm{m}}(n)$ for all combinations that do not include class $k_{l}{ }^{\prime}$ :

$$
B_{\mathbf{k}}(n)=p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n), \boldsymbol{\Psi}\right)=\left\{\begin{array}{cl}
B_{\mathbf{k}}(n) & \text { if } k_{l}=k_{l}  \tag{4.42}\\
0 & \text { otherwise }
\end{array}\right.
$$

To help with the correct initialization of the classes, it is convenient to select the initial centroids in the form

$$
\begin{equation*}
\mathbf{b}_{m_{l}}=\frac{\sum_{n \in n s} \mathbf{x}_{l}(n) \cdot P\left(c_{m_{l}}(n) \mid \mathbf{x}_{l}(n), \boldsymbol{\Psi}\right)}{\sum_{n \in n s} P\left(c_{m_{l}}(n) \mid \mathbf{x}_{l}(n), \Psi\right)} \tag{4.43}
\end{equation*}
$$

where $n s$ is the set of observations for which there is prior knowledge about the posterior probability of the $l$-th chain. Any classes that are learnt in a totally unsupervised manner can be initialized randomly. Furthermore, the centroids can be estimated using this prior knowledge about the observations, replacing the gradient method in (4.35) for any iteration of the procedure.

### 4.4. State of the art methods

In this work, the performance of the proposed G-SICAMM and UG-SICAMM procedures are compared with Bayesian Networks and Dynamic Bayesian Networks [140] that are related state-of-the-art methods. These methods were chosen because of the similarities to G-SICAMM, although Bayesian Networks are very varied in nature: in fact, HMM and CHMM can be seen as particular kinds of (dynamic) Bayesian Networks. Thus, in this section, we include a brief review of these methods.

Bayesian Networks and Dynamic Bayesian Networks have gathered much attention during the last decade. They have been used for many applications, including data mining [279], biological sequence analysis [102], and biosignal processing, including that of EEG data [107,47].

### 4.4.1. Bayesian Networks

Bayesian Networks (BN) are graphical structures that allow us to represent and rationalize an uncertain domain [140]. A BN comprises a directed graph, $G$, and several conditional probability distributions, $\Theta$. The graph is itself composed of two kinds of elements, nodes and vertices; nodes represent random variables modeled by the network, while vertices state direct dependences between the nodes (i.e., variables) they link. Nodes corresponding to discrete random variables are usually drawn as squares, while those corresponding to continuous random variables are drawn as circles. In some cases, observed variables are shadowed in gray. An example of such a graph is shown in Figure 4.4.

One characteristic of these graphs is that there can be no closed circles - that is to say, one cannot return to a previously-visited node by following the directed vertices. Such a graph is called a directed acyclic graph (DAG), and it greatly simplifies the task of calculating the joint probability density of the network.

A vertex from node $\chi_{i}$ to node $\chi_{j}$ implies a direct dependence of node $j$ with respect to node $i$. In BN theory, $\chi_{i}$ is usually named a "parent node" of $\chi_{j}$; likewise, $\chi_{j}$ is known as a


Figure 4.4. Sample graph of a Bayesian Network with discrete nodes $\left(\chi_{1}, \chi_{2}\right)$ and continuous nodes $\left(\chi_{3}, \chi_{4}, \chi_{5}\right)$.

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"children node" of $\chi_{i}$. These definitions can be extended to define the "ancestors" or "descendants" of a given node.

The graph of a BN shows conditional dependences and assumes that any given variable is conditionally independent of all of its non-descendants, given the parents of the variable. These dependences are modeled by the conditional probability density functions of the $\mathrm{BN}, \Theta$. Thus, the $i$-th node is defined by its $P_{B}\left(\chi_{i} \mid \pi_{i}\right)$ functions, where $\pi_{i}$ is the set of parent nodes of $i$. For discrete nodes, these probabilities are usually represented as a table.

Given the above, a Bayesian Network allows to easily define the joint probability density of a set of $K$ random variables $\chi_{k}, k=1, \ldots, K$ :

$$
\begin{equation*}
P_{B}\left(\chi_{1}, \chi_{2}, \ldots, \chi_{K}\right)=\prod_{k=1}^{K} P_{B}\left(\chi_{k} \mid \pi_{k}\right) \tag{4.44}
\end{equation*}
$$

### 4.4.2. Dynamic Bayesian Networks

Dynamic Bayesian Networks are an extension of regular BN that deals with stochastic processes with time dependences. In this case, time is discretized as a series of regularly-placed time instants, $n$, at which the modeled variables are measured. The graph $G$ is extended to include time dependences and the joint probability function of the system becomes

$$
\begin{equation*}
P(\chi(0: N))=\prod_{n=0}^{N-1} P(\chi(n+1) \mid \chi(0: n)) \tag{4.45}
\end{equation*}
$$

where $\chi(n)$ is the set of variables that define the system at time $n$, and $\chi(0: n)$ is the set of all variables at times $0,1,2, \ldots, n$. The above joint probability density is still very complex, but it can be simplified by making the Markov assumption, i.e., future data are conditionally independent from past data given the current observation. Therefore, future states of the DBN are dependent only on the current state. In that case, (4.45) becomes

$$
\begin{equation*}
P(\chi(0: N))=\prod_{n=0}^{N-1} P(\chi(n+1) \mid \chi(n)) \tag{4.46}
\end{equation*}
$$

One common assumption of many DBN is stationarity, i.e., any temporal dependence remains the same for all time. In this case, the network can be adequately modeled by considering the dependences within the initial values, $P(\chi(0))$, and the dependences during the transition between any two time instants, $P(\chi(n) \mid \chi(n-1))$. This is usually known as a Two-slice Temporal Bayes Network (2TBN). Hidden Markov models are the most common instances of 2TBN (see Figure 4.5), since they are extremely useful despite their simplicity, are broadly used in several applications, such as speech recognition [91] and biological sequence analysis [140].

Time $n$


Time $n+1$

Figure 4.5. Graph of a HMM, one instance of a 2TBN.

### 4.5. Simulations

The proposed procedures were tested on simulated data before their application on real data that will be studied in Chapter 6.

### 4.5.1. Measuring the distance between two G-SICAMMs

Some of the applications in this work require measuring the distance or difference between two sets of G-SICAMM parameters, e.g., to compare two G-SICAMM calculated at different times. However, given the novelty of these procedures, there is no commonly-used measure of the similarity of two given models. Considering their parameter structure, it seems appropriate to combine the similarity measures for Hidden Markov Models with those for ICA.

Any similarity measure used to compare ICA mixture models, including sequential models like G-SICAMM, should take into account the indeterminacies or unknowns of ICA, i.e., the sources are recovered in no particular order, and the sources are identified up to a scale factor (including a sign), $\alpha$. In this work, two indicators were considered, the Amari index and the SIR. Both indicators are typical in the comparison of ICA models. A third indicator, the probabilistic distance, was considered in order to compare transition probabilities, thus completing the comparison of G-SICAMM parameters.

In the following, the G-SICAMM parameters at time instants $n_{i}$ and $n_{j}$ will be denoted by the super-indices ${ }^{(i)}$ and ${ }^{(j)}$, respectively, while the models will be referred to as $\Theta^{(i)}$ and $\Theta^{(j)}$, respectively. Note that, even though the formulation will assume two G-SICAMM, these indicators can be used to compare two sets of SICAMM parameters by setting $L=1$.

### 4.5.1.a. Amari index

The Amari index is used to calculate the similarity of a given matrix and any permutation matrix, $\mathbf{P}$ [7]. In the case of ICA, this estimator can be used to attest the performance of an estimated de-mixing matrix, $\hat{\mathbf{W}}_{k_{l}}$, if we know the true mixing matrix, $\mathbf{A}_{k_{l}}$. The more similar the product $\hat{\mathbf{W}}_{k_{l}} \cdot \mathbf{A}_{k_{l}}$ is to a permutation matrix, the better the source extraction is. Conversely, we can use the Amari index to calculate the similarity between two de-mixing matrices if we invert the first one, $\mathbf{A}_{k_{l}}{ }^{(1)}=\left(\mathbf{W}_{k_{l}}{ }^{(1)}\right)^{-1}$, and consider the product $\left(\mathbf{W}_{k_{l}}{ }^{(1)}\right)^{-1} \cdot \mathbf{W}_{k_{l}}{ }^{(2)}$. The definition of the Amari index is

$$
\begin{equation*}
a\left(\mathbf{W}_{k_{l}}{ }^{(1)}, \mathbf{W}_{k_{l}}{ }^{(2)}\right)=\sum_{i=1}^{M}\left(\sum_{j=1}^{M} \frac{\left|p_{i j}\right|}{\max _{k}\left|p_{i k}\right|}-1\right)+\sum_{j=1}^{M}\left(\sum_{i=1}^{M} \frac{\left|p_{i j}\right|}{\max _{k}\left|p_{k j}\right|}-1\right) \tag{4.47}
\end{equation*}
$$

where $P=\left\{p_{i j}\right\}=\left(\mathbf{W}_{k_{1}}{ }^{(1)}\right)^{-1} \cdot \mathbf{W}_{k_{l}}{ }^{(2)}$ and $M$ is the number of sources in the ICA model. The index can range from 0 (perfect match) to a maximum value of $M \cdot(M-1) / 2$ (constant matrix). In this work, values were normalized to range between 0 and 1.

The Amari index between two models is calculated by comparing their classes one by one using (4.47) and then averaging the results:

$$
\begin{equation*}
a\left(\Theta^{(1)}, \Theta^{(2)}\right)=\frac{1}{L} \sum_{l=1}^{L}\left\lfloor\frac{1}{K_{l}} \sum_{k_{l}=1}^{K_{l}} a\left(\mathbf{W}_{k_{l}}{ }^{(1)}, \mathbf{W}_{k_{l}}{ }^{(2)}\right)\right\rfloor \tag{4.48}
\end{equation*}
$$

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The Amari index is not affected at all by the value of the sources, ignoring the second unknown in the ICA model. The index is also robust with respect to the first unknown, since any change in the order of the sources would only result in a different permutation matrix with the same index. It is also possible to estimate the nearest permutation matrix using this index, thus allowing us to set the same source ordering in both models and removing that unknown during the calculation of the other indicators.

### 4.5.1.b. Signal-to-interference ratio

The most classical definitions of the SIR are sensitive to the scale factor $\alpha$, but an indicator robust to this unknown was introduced in [101]. In that work, the SIR is defined as

$$
\begin{equation*}
\operatorname{SIR}\left(\mathbf{s}_{k_{l}}{ }^{(1)}(n), \mathbf{s}_{k_{l}}{ }^{(2)}(n)\right)=\frac{1}{M} \sum_{m=1}^{M} \frac{\left.\| s_{k_{l}, m}{ }^{(1)}(n), s_{k_{l}, m}{ }^{(2)}(n)\right\rangle\left.\right|^{2}}{s_{k_{l}, m}{ }^{(1)}(n)\left\|^{2} \cdot\right\| s_{k_{k}, m}{ }^{(2)}(n) \|^{2}-\left|\left\langle s_{k_{l}, m}{ }^{(1)}(n), s_{k_{l}, m}{ }^{(2)}(n)\right\rangle\right|^{2}} \tag{4.49}
\end{equation*}
$$

where $s_{k_{l}, m}{ }^{(i)}$ is the value of the $m$-th source, $m=1, \ldots, M$, from class $k_{l}$ in model $i$, and $\langle x, y\rangle=\sum_{n=1}^{N} x(n) \cdot y(n)$ is the interior product of two sources $x, y$. Same as we did with the Amari index, the SIR is first calculated separately for each class and then averaged:

$$
\begin{equation*}
\operatorname{SIR}\left(\Theta^{(1)}, \Theta^{(2)}\right)=\frac{1}{L} \sum_{l=1}^{L}\left\lfloor\frac{1}{K_{l}} \sum_{k_{l}=1}^{K_{l}} \operatorname{SIR}\left(\mathbf{s}_{k_{l}}^{(1)}(n), \mathbf{s}_{k_{l}}^{(2)}(n)\right)\right\rfloor \tag{4.50}
\end{equation*}
$$

### 4.5.1.c. Probabilistic distance

The SIR and the Amari indexes allow us to compare ICA mixture models, but G-SICAMM also include temporal dependences which those two indicators do not consider. Thus, the transition probabilities are compared using a third indicator, the probabilistic distance, which was proposed as a distance measure between Hidden Markov Models [281]. This indicator is used considering the similarities between G-SICAMM and a CHMM model.

Usually, the difference between HMM models are estimated using the Kullback-Leibler divergence between transition probabilities. Unfortunately, the required calculations are complex and have no closed form ( [201]), thus the Kullback-Leibler divergence is estimated using Monte Carlo experiments. However, this can be computationally complex and slow. To avoid this problem, the probabilistic distance is considered instead, since it is much simpler to calculate ( [201]). The probabilistic distance is calculated using the information from each combination of states:

$$
D P\left(\Theta^{(1)}, \Theta^{(2)}\right)=\lim _{n \rightarrow \infty} \frac{1}{n} \cdot \log \left\{\begin{array}{l}
\left(\begin{array}{l}
K_{1} \\
\sum_{k_{1}=1}^{K_{2}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L}=1}^{K_{k}} \mu_{k}{ }^{(1)}(n) \\
\sum_{k_{1}=1}^{K_{2}} \sum_{k_{2}=1}^{K_{2}} \cdots \sum_{k_{L}=1}^{K_{L}} \mu_{\mathrm{k}}{ }^{(2)}(n)
\end{array}\right) \tag{4.51}
\end{array}\right\}
$$

where $\mu_{\mathrm{k}}{ }^{(i)}$ is the information in model $i(i=1,2)$ in the combination of states $\mathbf{k}=\left[k_{1}, k_{2}, \ldots, k_{L}\right]$ at time $n$. This information can be recursively calculated at each time as

$$
\begin{equation*}
\mu_{\mathbf{k}}^{(i)}(n)=\sum_{k_{1}^{\prime}=1}^{K_{1}} \sum_{k_{2}^{\prime}=1}^{K_{2}} \cdots \sum_{k_{L^{\prime}}=1}^{K_{L}} p\left(\mathbf{x}(n) \mid \mathbf{c}_{\mathbf{k}}(n)\right) \cdot P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1)\right) \cdot \mu_{\mathbf{k}}^{(i)}(n-1) \tag{4.52}
\end{equation*}
$$

where the initial value is equal to the prior probability of each state combination, $\mu_{\mathbf{k}}{ }^{(i)}(0)=\prod_{l=1}^{L} P\left(C_{k_{l}}\right)$. Note that nlike the SIR and the Amari index, the probabilistic distance is calculated for the two compared models, not for any single class.

### 4.5.2. Simulation of UG-SICAMM for semi-supervised training

The convergence of UG-SICAMM for semi-supervised training was studied using a Monte Carlo experiment with synthetic data. These data were simulated using a G-SICAMM with two chains $(L=2)$, two classes $(K=2)$, and observations of dimension two $(M=2)$. The mixing matrices for each class were randomly initialized using values drawn from a uniform distribution in the range $[0,1]$. The centroids were the same for both chains, and they were set relatively close, $\mathbf{b}_{1}=\left[\begin{array}{ll}1 & 1\end{array}\right]^{T}$ and $\mathbf{b}_{2}=\left[\begin{array}{ll}1.5 & 1.5\end{array}\right]^{T}$. The sources followed a uniform distribution with zero mean and unit standard deviation. Finally, the classes $\mathbf{c}_{\mathbf{k}}(n)$ were randomly generated using a CHMM which was modeled as a super-HMM with $L \cdot K=4$ states. The transition probabilities of this super-HMM were initialized as follows. It was decided that both chains would show the same time dependences, and the transition probabilities for each chain were initialized as

$$
\left.\begin{array}{l}
\left.\begin{array}{l}
\pi_{11}(n)=\pi_{22}(n)=\alpha \\
\pi_{12}(n)=\pi_{21}(n)=1-\alpha
\end{array}\right\} \text { if the other chain was in class } 1 \text { at time } n-1  \tag{4.53}\\
\pi_{11}(n)=\pi_{22}(n)=\alpha-\beta \\
\pi_{12}(n)=\pi_{21}(n)=1-(\alpha-\beta)
\end{array}\right\} \text { if the other chain was in class } 2 \text { at time } n-1
$$

where $\alpha$ and $\beta$ are two parameters which regulate the sequential dependence in the GSICAMM. $\alpha$ is the intra-chain dependence parameter, since it sets the time dependence of each chain with respect to past values of the same chain; and conversely, $\beta$ is the inter-chain dependence parameter, since it sets the time dependence of each chain with respect to past values of the other chain. From (4.53), it can be seen that $0 \leq \alpha \leq 1$ and $\alpha-1 \leq \beta \leq \alpha$. For $\beta=0$ the transition probabilities of each chain are independent from the other chain; furthermore, if $\beta=0, \alpha=0.5$ there is no time dependence. Once the $\pi_{k_{1} k_{2}}, k_{1}=1 \ldots K, k_{2}=1 \ldots K$ for each chain have been initialized, the transition probabilities of the equivalent super-HMM, $\pi_{\mathrm{k} \mathrm{k}^{\prime}}$, are calculated from the probabilities for every possible combinations of classes in (4.53) using results from probability theory. In the experiments shown in this section, $\alpha=0.8$ and $\beta=0.1$.

For each iteration of the experiment, the parameters were randomly set as explained above and $N=1024$ observations, $\mathbf{x}(n), n=1 \ldots N$, were generated from the model, along with their respective classes, $\mathbf{c}_{\mathbf{k}}(n)$. It was considered that only some of the observations were labeled, and the amount of labeled data was called the supervision rate. A supervision rate of $100 \%$ indicates that all labels are known, and thus, we perform supervised training. Conversely, a supervision rate equal to $0 \%$ indicates that no labels are known, and thus, we perform unsupervised training. The labels were selected at random, and each $\mathbf{x}(n)$ could be unlabeled,

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partly labeled (we know either $C_{k_{1}}(n)$ or $C_{k_{2}}(n)$ ), or totally labeled (we know $\mathbf{c}_{\mathbf{k}}(n)$ ). After the generation process, the observations and the labels were passed to UG-SICAMM for estimating the G-SICAMM. Finally, we calculated the distance between the estimated model and the true model using the indexes shown in Section 4.5.1. This process is summarized in Figure 4.6; the procedure was repeated 100 times and results were averaged. The Monte Carlo experiment was repeated for values of supervision rate from $0 \%$ to $100 \%$ in steps of $10 \%$.

UG-SICAMM is compared with G-SICAMM estimated using the supervised training algorithm explained in Section 4.2.2. The supervised training data were obtained by removing unlabeled observations from the record; therefore, there is no result for the $0 \%$ supervision rate. The ICAMM parameters were estimated using the MIXCA procedure [231] (with JADE as the embedded ICA algorithm), and the transition probabilities were estimated by counting.

Figure 4.7 shows the results of the experiment. The performance of UG-SICAMM and GSICAMM increased with the supervision rate. In the case of G-SICAMM, this improvement was steady. UG-SICAMM improved at a slower pace after the supervision rate surpassed $50 \%$. Particularly, the probabilistic distance (Figure 4.7.c) of UG-SICAMM increased for a supervision rate above $40 \%$. The results for both methods are similar, although the supervised training used for G-SICAMM obtained the best results in all distance indicators for supervision rates above $40 \%$. This is due to the good convergence properties of the embedded ICA algorithm, JADE, which obtained de-mixing matrices closer to the true ones. However, UGSICAMM obtains good results in all cases, and it is able to achieve a result for unsupervised data.


Figure 4.6. Diagram showing an iteration of the simulation with semi-supervised training. This process is repeated a number of times during each Monte Carlo experiment.


Figure 4.7. Results for the simulation with semi-supervised training data: a) Amari index; b) SDR; c) probabilistic distance.

### 4.5.3. Simulation of SICAMM and G-SICAMM variants

The classification performance of the proposed methods was tested with several Monte Carlo experiments similar to the one presented in Section 4.5.2, except the following. The experiments in this section use a slightly modified iteration process, shown in Figure 4.8. Once the model was randomly initialized and the data were generated, the first half of the data was used for estimating the parameters for each one of the proposed methods using supervised training; this is explained in detail later on. After training, the performance of the methods was tested by performing classification on the second half of the data; it was measured using the classification error rate.

G-SICAMM was configured in the same way as the model used for data generation, with two chains and two classes per chain ( $K=2$ and $L=2$ ). For the other ICA-based methods (SICAMM and ICAMM) a single model was used for the data of both chains, $\mathbf{x}(n)=\left[\mathbf{x}_{1}(n)^{T}, \mathbf{x}_{2}(n)^{T}\right]^{T}$. To compare these models with the one obtained with G-SICAMM, SICAMM and ICAMM considered four classes $\left(K^{\prime}=4\right)$, one class per combination of classes in the G-SICAMM: $\mathbf{k}_{1}=[1,1]^{T}, \mathbf{k}_{2}=[1,2]^{T}, \mathbf{k}_{3}=[2,1]^{T}$, and $\mathbf{k}_{4}=[2,2]^{T}$. The graphs for these methods are shown in Figure 4.9.a, Figure 4.9.c and Figure 4.9.e for ICAMM, SICAMM and GSICAMM respectively. The parameter estimation for the ICA-based methods was performed using the training algorithm explained in Section 4.2.2. The ICAMM parameters were estimated using the MIXCA procedure [231] (with JADE as the embedded ICA algorithm) and the transition probabilities were estimated by counting.

Three types of Bayesian networks were considered, each one similar to one of the ICA-based methods: a network without temporal dependence (BNT); a network with dependence similar to a HMM (DBN); and a network with two-chain dependence similar to a CHMM (DBN2). The configuration of these methods was similar to that of the ICA-based methods: for the DBN2, two chains were considered, each one with two classes ( $K=2$ and $L=2$ ); DBN and BNT were adjusted considering four classes, $K^{\prime}=4$, one for each combination of classes from the DBN2 method. The node probabilities were modeled using Gaussian Mixture Models (GMM). The number of mixtures for each node was determined by training several GMM with an increasing number of classes ( 3 to 20) and selecting the best fit. This selection was performed using the Akaike Information Criterion ( [4]), a commonly-used criterion to test the quality of a model. The AIC is a relative estimation of the information lost by representing the data with a given model, and it is defined as

$$
\begin{equation*}
A I C(\Theta)=2 k-2 \log (p(\mathbf{x} \mid \Theta)) \tag{4.54}
\end{equation*}
$$



Figure 4.8. Diagram showing the process of each iteration of the simulation. This process is repeated several times during each Monte Carlo experiment.

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c) SICAMM



Figure 4.9. Graphs for the proposed methods: a) ICAMM with four classes; b) BNT with four classes; c) SICAMM with four classes; d) DBN with four classes; e) G-SICAMM with two chains and two classes per chain; f) DBN2 with two chains and two classes per chain.
where $k$ is the number of parameters in model $\Theta$. Figure 4.10 shows an example of this selection process; in this case, the lowest AIC value corresponded to a Gaussian Mixture Model with eleven components. The graphs for these methods are shown in Figure 4.9.b, Figure 4.9.d and Figure 4.9.f for BNT, DBN and DBN2 respectively.

For the first experiment, the inter-chain dependence parameter was set to $\beta=0.1$ and the intrachain dependence parameter was changed between $\alpha=0.5$ (no dependence) to $\alpha=0.99$ (almost complete dependence) in steps of 0.025 . The Monte Carlo experiment was repeated 300 times for each value of $\alpha$, for a total number of 6,000 iterations.

Figure 4.11 shows the average classification error rate of the proposed methods. The results are split into three sub-Figures. Figure 4.11.a compares the performance of SICAMM using MAP estimation with that of SICAMM using its proposed variants, the Baum-Welch and Viterbi algorithms (denoted as SICAMM+BW and SICAMM+VI respectively). Figure 4.11.b is similar, but compares G-SICAMM and its variants. For readability, Figure 4.11.c shows the results for all the proposed methods except for the variants of SICAMM and G-SICAMM.

It can be seen that the static methods (ICAMM and BNT) maintained or decreased their performance when the intra-chain dependence increased; conversely, most of the dynamic methods (DBN, SICAMM and G-SICAMM) increased their performance as $\alpha$ increased. SICAMM and G-SICAMM performed better than DBN, and G-SICAMM achieved the best classification performance due to its exploitation of the time cross-dependences between chains.


Figure 4.10. Sample of the calculation of AIC used for the estimation of the number of GMM components for modeling node probabilities: a) AIC values, with the optimal value denoted by an asterisk; b) PDF fit corresponding to the optimal value.


Figure 4.11. Classification results with respect to the intra-chain dependence parameter, $\alpha:$ a) SICAMM versus its proposed variants; b) G-SICAMM versus its proposed variants; c) comparison of all the proposed methods.

As a matter of fact, G-SICAMM yields the best result in every point of the simulation. The low performances of DBN2 and BNT were due to problems with estimating the model from the training data. Furthermore, the two variants proposed for classification (the Baum-Welch algorithm and the Viterbi algorithm) have achieved better classification performance than MAP estimation for SICAMM (Figure 4.11.a) and for G-SICAMM (Figure 4.11.b). This improvement is negligible for low values of the dependence parameter ( $\alpha<=0.7$ ), but it increases consistently with temporal dependence, up to half the error rate of MAP estimation for very high values of dependence. Both variants obtained similar results, although the BaumWelch algorithm performed slightly better than Viterbi.

A second Monte Carlo experiment was performed to test the performance of the proposed methods with respect to changes in the inter-chain dependence. In this case, the intra-chain dependence parameter was set to $\alpha=0.8$ and the inter-chain dependence parameter was changed between $\beta=0$ (no dependence) and $\beta=\alpha=0.8$ (maximum dependence) in steps of 0.06 . The simulation was repeated 300 times for each value of $\beta$ and the results were averaged, for a total number of 3,900 iterations.

Figure 4.12 shows the results of the experiment. As with Figure 4.11, the results of the proposed variants to SICAMM and G-SICAMM are separated into sub-Figures in order to make the results clearer. Figure 4.12.c shows that G-SICAMM consistently outperformed the other proposed methods, and SICAMM achieved a slightly worse result. The dynamic Bayesian Networks (DBN and DBN2) improved as the inter-chain dependence increased, while GSICAMM and SICAMM worsened for very small values of $\beta$ and only improved their performance when $\beta>0.3$; however, SICAMM and G-SICAMM outperformed DBN and DBN2 for all the considered values of $\beta$. ICAMM achieved a stable result since it does not consider dependence. BNT obtained the worst result, which worsened as the dependence increased due to problems during model estimation.

Figure 4.12.a and Figure 4.12.b for SICAMM and G-SICAMM, respectively, show that both of the proposed variants achieved a lower error than the base methods. This improvement remained stable for low values of $\beta$ and increased for higher values of dependence, up to a maximum of half the value of MAP estimation. This is consistent with the results in Figure 4.11.a and Figure 4.11.b, where the improvement also increased with the dependence parameter. The Baum-Welch algorithm achieved the lowest error for both SICAMM and G-SICAMM, although the difference with Viterbi was small and, in fact, decreased as the dependence


Figure 4.12. Classification results with respect to the inter-chain dependence parameter, $\beta:$ a) SICAMM versus its proposed variants; b) G-SICAMM versus its proposed variants; c) comparison of all the proposed methods.
increased. The behavior shown in Figure 4.12 can be explained from (4.53). If $\alpha>0.5$, positive values of $\beta$ will actually reduce the time dependence in the model as long as $\alpha-\beta>=0.5$. If we keep increasing the inter-chain dependence parameter so that $\alpha-\beta<0.5$, the overall time dependence in the model rises again. This explains the results in Figure 4.11 and Figure 4.12, where the effect of the time dependence is more pronounced the more $\alpha-\beta$ steps away from 0.5 .

### 4.5.3.a. Dynamic experiments

We performed further experiments to test the resilience of the proposed methods with respect to alterations of the base assumptions of ICA mixture models: in particular, if the probability density functions of the data change with time. To this effect, the dependence parameters were set to $\alpha=0.8, \beta=0.1$ and the probability density function of the sources was altered. The sources were split into two groups: stationary sources, which kept a constant probability density during the experiment; and dynamic sources, which changed their density with time. The stationary sources followed a uniform distribution, while the dynamic sources followed a beta distribution with shape parameters $a=1$ and $b$ changing with time (the values of $b$ are shown in Figure 4.13). All the sources had zero mean and unit variance. The beta distribution was selected because it is a parametric distribution that enables to gradually change its shape in time (see Figure 4.13.b), and because it is equivalent to the uniform distribution when $a=b=1$. The number of dynamic sources was changed from 0 (all sources stationary) to 8 (all sources dynamic). Dynamic sources were distributed evenly between the chains and the classes.

Other than the different sources, the classification experiment followed the steps shown in Figure 4.8. Note that the models were trained using static data, since even dynamic sources did not change during the first half of the data, as seen in Figure 4.13.a, and were then tested on partially dynamic data that were progressively more different from the training data. The simulation was repeated 300 times for each number of dynamic sources and the results were averaged, for a total number of 2,700 iterations.

The classification results are shown in Figure 4.14. All the methods showed a similar increase in error as the number of dynamic sources increased, i.e., as the underlying model became less and less stationary. The behavior of the methods is consistent with that in Figure 4.11 and Figure 4.12: i) G-SICAMM obtained the best result; ii) ICAMM-based methods (ICAMM, SICAMM and G-SICAMM) obtained a lower error, in general, than Bayesian networks (BNT, DBN and DBN2); iii) the proposed variants to SICAMM and G-SICAMM obtained a better result than the base method.


Figure 4.13. Evolution of $b$ : a) value for each observation and resulting skewness and kurtosis of the beta distribution; b) beta density for five values of $b$; in all cases, $a=1$.

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Figure 4.14. Classification results with respect to the number of dynamic sources: a) SICAMM versus its proposed variants; b) G-SICAMM versus its proposed variants; c) comparison of all the proposed methods. The sequential dependence parameters were $\alpha=0.8$ and $\beta=0.1$.

We performed a second experiment with a different probability density. The only change with respect to the first experiment is the probability densities of the sources. Static sources followed a K distribution (see Table 3.3) with shape parameter $K=1$ and dynamic sources followed a K distribution with $K$ ranging from one to five and changing with time (see Figure 4.15.a).

The classification results of this second experiment are shown in Figure 4.16. The error increased with the number of dynamic sources, in concordance with the results in Figure 4.14. With the K distribution, however, there was a greater dependence on the number of dynamic sources: the results were better when all sources were static, but worsened at a faster rate, and became much worse (almost double the balanced error rate) when all sources were dynamic. Another difference is that DBN and DBN2 slightly changed their behavior with respect to the experiment with the beta distribution. This was probably due to the larger differences introduced by the changes in the K distribution, whose high-order statistics change more than those of the beta distribution (compare Figure 4.13.a with Figure 4.15.a). DBN2 performed better than DBN (i.e., obtained lower error), yet slightly worse than ICAMM. ICAMM-based methods obtained the best results, and G-SICAMM+BW obtained the lowest error rate.


Figure 4.15. Evolution of $K$ : a) value for each observation and resulting skewness and kurtosis of the K distribution; b) probability density for five values of $K$.


Figure 4.16. Classification results with respect to the number of dynamic sources: a) SICAMM versus its proposed variants; b) G-SICAMM versus its proposed variants; c) comparison of all the proposed methods. The sequential dependence parameters were $\alpha=0.8$ and $\beta=0.1$.

### 4.5.3.b. Changes in the G-SICAMM parameters

A further test was performed to test the effect of the dynamic sources on the G-SICAMM parameters. In the experiment shown in Section 4.5.3.a, we considered "batch training," i.e., the model is trained once using training data and then applied once on test data. This was appropriate to test the degradation of the model as the number of non-stationary sources increased. To test the effect of these non-stationary sources on G-SICAMM estimation, we applied "semi-batch training," i.e., performed batch training several time, once for each timeconsecutive subset of the whole dataset. These local models can be examined to determine changes in the G-SICAMM parameters using the distance indicators defined in Section 4.5.1. The semi-batch training was performed using windows of length 512 samples, with $90 \%$ overlap between windows.

Figure 4.17 shows the average distance indicators between the G-SICAMM obtained during semi-batch training of every pair of consecutive windows. All indicators remained stable for the stationary part of the data, i.e., the first half of the data (see Figure 4.15). Once the windows entered the second half of the data, however, all indicators worsened as the number of nonstationary sources increased. This effect is more noticeable when the number of dynamic sources is high. Therefore, it can be seen that the G-SICAMM parameters were sensitive to changes in the underlying model, even at a local level. This effect could be used to determine non-stationary areas of interest, or even to perform classification, as will be seen in Chapter 6.


Figure 4.17. Distance indicators between consecutive pairs of local G-SICAMM: a) Amari index; b) SDR; c) probabilistic distance.

### 4.6. Conclusions

This chapter has introduced two extensions of Sequential ICAMM, a dynamic model based on ICA mixture modeling that takes into account the temporal dependences in the data that the basic ICAMM does not consider [230]. The first one of these extensions is based on the similarities between SICAMM and Hidden Markov Models. Because of these similarities, when SICAMM is used for classification, the result can be improved by considering two classical classification algorithms, Baum-Welch and Viterbi. The Baum-Welch algorithm performs a forward-backward estimation of the class probabilities while making use of all available data, while the Viterbi algorithm is a classical decoding algorithm that can find the most likely sequence of classes in the data without performing an exhaustive search. The second extension of SICAMM is a generalization of the concept of SICAMM to work with any number of parallel chains which are inter-related, each one a SICAMM on its own. This extension has been named Generalized SICAMM (G-SICAMM). Such a method can be used to work simultaneously with several datasets in parallel, or to split the data into multiple sub-chains. Furthermore, both the Baum-Welch and the Viterbi algorithms can be used to improve the results of G-SICAMM as well, combining both proposed extensions to SICAMM.

If labeled data are available for training, the estimation of the time dependence parameters can be performed separately from the estimation of the ICAMM parameters, both for SICAMM and G-SICAMM. In that case, the parameters can be estimated using known methods. However, if some training data is unlabeled (i.e., we perform semi-supervised or unsupervised training), all of the G-SICAMM parameters have to be estimated simultaneously. This chapter presents an algorithm for semi-supervised or unsupervised training of SICAMM and G-SICAMM, which we have named UG-SICAMM.

The performance of UG-SICAMM was tested by assessing the distance between the estimated model and the true model using a Monte Carlo experiment with an increasing number of labeled data, from unsupervised (all of the data are unlabeled) to fully-supervised (all of the data are labeled) training. To this effect, three distance indicators were proposed: i) the Amari index, which calculates the distance between de-mixing matrices; ii) the signal-to-interference ratio, which measures the similarity between the recovered sources and the true sources; iii) the probabilistic distance, which determines the difference between the dynamic behavior of two given models. The results show that the distance to the true model decreased as the amount of supervised data increased; although this improvement was faster for low supervision rates than it was for high supervision rates. Out of the considered indicators, the SIR and Amari indices were the ones that improved the most when the amount of labeled data increased, while the probabilistic distance did not improve for high amounts of supervision.

The performance of SICAMM and G-SICAMM was tested by performing classification on several sets of simulated data, and compared with that of Bayesian Networks (BNT) and Dynamic Bayesian Networks (DBN and DBN2). This study was performed using several Monte Carlo experiments, considering changes in the time dependence of the simulated data; this dependence was modeled with two values, the intra-chain dependence parameter ( $\alpha$ ) and the inter-chain dependence parameter $(\beta)$. The results show that the dynamic methods (DBN, DBN2, SICAMM and G-SICAMM) performed better than the static ones (BNT and ICAMM) because they exploit the time dependences between observations. The ICA-based methods always obtained a better classification than the similar Bayesian-network-based methods, i.e., ICAMM performed better than BNT, and SICAMM and G-SICAMM performed better than DBN and DBN2. Furthermore, G-SICAMM always obtained the best result because it was able to exploit more time dependences than the other methods. Furthermore, it has been shown that SICAMM and G-SICAMM improve their results if the classification is performed using the Baum-Welch or the Viterbi algorithms. The improvement was negligible for small dependence values, but it increased with the dependence in the data up to a maximum result of half the error
of the base methods. The behavior of the proposed methods was the same for both types of dependence, although it was more pronounced for changes in the inter-chain dependence.

Finally, we tested the behavior of the proposed methods when the basic ICAMM assumptions could not be met; particularly, when the probability density of the sources was not stationary, but rather changed over time. This was done using two Monte Carlo experiments with an increasing number of non-stationary sources, i.e., sources that changed in distribution after training. In the first experiment, the sources were originally uniformly distributed, but then changed according to a beta distribution. In the second experiment, the sources were Kdistributed and the $K$ parameter changed with time. In both cases, all the proposed methods worsened at a similar rate as the number of non-stationary sources increased. The performance of the methods was consistent with that of the previous simulations, and G-SICAMM+BW obtained the best result, followed by G-SICAMM+VI and SICAMM+BW. It was found that the performance on the K-distributed data was more affected by the non-stationarity than the performance on beta-distributed data. Furthermore, it was shown that the G-SICAMM parameters are sensitive to these changes in the model. Local estimations of the G-SICAMM were found to be similar if the data were stationary, and became more and more different as the data became more dynamic.

The results in this chapter show the potential of the proposed G-SICAMM procedure. The classification performance was the best out of the considered methods, and it was further improved by the use of the Baum-Welch algorithm. The parameters of the model can be obtained from semi-labeled or unlabeled data, which increases the range of possible applications for the procedure. Furthermore, although it was not considered in this chapter, the G-SICAMM parameters can be interpreted on their own and provide a structured result which can model the local behavior of the data without compromising its generalization capabilities.

> Application of PREDICAMM to nondestructive testing and EEG signal processing applications

## Chapter 5 - Application of PREDICAMM to non-destructive testing and EEG signal processing applications

This chapter presents three applications of signal prediction using the proposed PREDICAMM and E-ICAMM methods explained in Section 3.1 and 3.2, respectively. The results of PREDICAMM are compared with those of Kriging, Wiener structures, and spherical splines (also explained in Section 3.3). The proposed methods were tested on one set of simulated ground-penetrating radar data and three applications on real data: recovery of GPR data of real scale replicas of historical walls, reconstruction of data from a seismic survey, and interpolation of missing electroencephalographic data from a memory task.

The first application is based on non-destructive testing (NDT) signals from a groundpenetrating radar survey on real scale replicas of historical walls. In NDT applications, the signals are usually spatially distributed, forming two-dimensional sets of data or B-Scans. As explained in Chapter 3, PREDICAMM and E-ICAMM are able to perform prediction in data of any shape, even spatial data, depending on how the ICAMM is calculated. However, in this work, spatial data were preprocessed to be converted into time-distributed signals. This is a common preprocessing step in image processing applications, including several methods based on ICA such as Topographical ICA [111] and hierarchical ICA mixture models [240].

The second application performs prediction on data from a reflection seismology survey, where the subsurface is explored by a careful study of reflected seismic waves. The proposed methods were tested on a set of true seismic data from an underwater exploration.

The third application consists of the reconstruction of artifacted or missing data from an electroencephalogram, a record of the electrical activity of the brain taken on the scalp. PREDICAMM and E-ICAMM were applied to EEG data captured on subjects that were performing the Sternberg memory task, a classical procedure for evaluation of the short-term memory function. Prediction performance was estimated by means of a Monte Carlo experiment with a growing number of missing channels. The proposed methods were compared with spherical splines, a commonly-used interpolation method for EEG data.

In all three applications, the performance of the proposed methods will be quantified using the four error indicators introduced in Section 3.4.2. These indicators are: i) the signal-to-

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interference ratio, which quantifies the average squared error in the prediction; ii) the KullbackLeibler divergence, a measure of the distance between the probability density function of the original data and of the PDF of the reconstructed data; iii) the cross-correlation between the original data and the reconstructed data, an indicator of the temporal similarity of both sets of data; and iv) the mean structural similarity, a similarity measure between two images that compares their structures.

### 5.1. Non-destructive testing simulations

Non-destructive testing is a set of techniques that allow the structure of a material to be analyzed without damaging it. They are usually used to characterize a material or to test its integrity in cases where there is no option to sample or affect the material under test; this can happen for a number of reasons, mainly:

- The material under test must remain undamaged and it cannot be duplicated, e.g., the testing of archaeological objects [229,62] or historical buildings [99,212].
- The material under test is unreachable and no sample can be obtained, e.g., seismic exploration of underground environments [177,105] or remote sensing [71].
- There are many objects under test and taking samples out of every single one of them is unfeasible, e.g., quality testing of products before they leave the production chain [205].
- The material is hazardous, e.g., landmine detection [90].

When any element of a NDT system fails, some information can be lost, resulting in missing data (also known as missing traces). The reconstruction of this information from the rest of captured data is not a straightforward work; in fact, this reconstruction is an ill-posed problem. Field studies are particularly exposed to this kind of problem, since they usually involve an amount of sensors spread over a hostile area; it is quite usual that several traces are lost or miscaptured for any number of reasons. Furthermore, reconstruction methods can be used even if there is no actual data loss. For instance, they can be used to interpolate data and achieve the same resolution with a lower number of sensors (e.g., by considering that every other trace is missing).

The reconstruction scenario is well-known in the literature and several algorithms have been proposed to deal with it. Nevertheless, data reconstruction remains an interesting research topic (given its difficulty) and it is the subject of current research. Most of the algorithms proposed for this task make use of low-order statistical properties of the signals involved, e.g., linear predictors [163,116].

In particular, in this thesis, we will consider NDT signals in the areas of ground penetrating radar and seismic exploration surveys. There are only a few examples of the application of ICA and ICAMM to problems related with seismic and GPR signal processing. The motivation of using ICAMM to these application areas is the degrees of freedom provided by ICAMM, which allow for linear local projections that can be adapted to partial segments of a data set while maintaining generalization (capability for nonlinear modeling) given the mixture of several ICAs. Furthermore, the normal method to represent the results in seismic exploration and GPR is using images (B-Scans) called seismograms and radargrams, respectively. ICA has been extensively applied to image processing in problems such as filtering [19], segmentation [152], face recognition [135,16], and processing of biomedical images [168,255]. Briefly, images patches values taken from the pixels of the image are considered as variables for ICA processing, and the estimated basis functions (mixing matrix) and sources are used for image application. Thus, we will process radargrams and seismograms as images applying the proposed methods based on ICAMM explained in Chapter 3.

### 5.1.1. Ground-penetrating radar

Ground penetrating radar is a non-destructive testing technique that transmits high-frequency pulsed electromagnetic waves into the ground surface [68]. There is a detailed description of GPR and its applications in [68,43], but a brief explanation is given here to make the chapter more self-contained. The description here will focus on GPR working in the time domain, which is more common than those that work in the frequency domain (stepped-frequency systems). Most commercial GPR systems actually use two antennas, one for transmission and one for reception; in practice, however, they are usually referred to as one single antenna.

GPR operation is quite similar to that of conventional radar, as shown in Figure 5.1. First, the device emits a pulse which is transmitted through the medium under test. When the electromagnetic waves reach an interface between two materials (changes in dielectric permittivity for non-ferromagnetic materials), part of the signal is reflected back to the surface. These reflections are captured by the GPR device; the captured one-dimensional signal is called a trace or an A-Scan (each one of the signals shown in Figure 5.1.b). The device is then moved along a trajectory, capturing data at multiple locations or "shifts." Multiple GPR A-Scans corresponding to different shifts are usually organized in a B-Scan (also known as radargram) format to afford a 2D description of the medium [68] (see Figure 5.1.b). The B-Scan is studied to characterize the internal structure of the medium under test, like the geometry of buried objects or the presence of geological structures.

There are a number of parameters which affect the detection of objects in the GPR signal, chiefly the time resolution (the length of each pulse), the lateral resolution (the ability to discern between two separate nearby objects), and the reflected power.

To increase the time resolution (or "vertical" resolution) of the system, the transmitted waves usually have a bandwidth as great as possible. Typically, antennas with higher center frequency also have greater bandwidth and therefore shorter pulse length. Since higher frequencies attenuate faster, antennas with lower center frequencies have a greater depth of penetration. Thus, the correct choice of the center frequency is a critical part of a GPR survey. Commercial GPR systems have antennas with center frequencies ranging from several MHz (low resolution, high penetration depth, used in geological applications) to several GHz (high resolution, low penetration depth, used in NDT applications).

On the other hand, the lateral resolution of GPR is limited by the size of the Fresnel region (which characterizes the area where reflected waves add together constructively). Single points within this region cannot be separated in the signal. Assuming that the distance between the


Figure 5.1. Typical ground-penetrating radar scenario: a) depiction of the medium under test, with one interface between layers (A) and one buried object (B), and the device that is being carried along the surface; b) captured BScan.

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transmission antenna and the reception antenna is negligible with respect to their distance to the target, $D$, the radius of the first Fresnel region is $r \cong \sqrt{D \cdot v / 2 f}$, where $v$ is the speed of electromagnetic waves in the medium and $f$ is the frequency of the pulse. GPR is not used in ferromagnetic materials because electromagnetic waves in conducting materials lead to stray currents, thus increasing the noise and sharply reducing the depth of penetration of GPR signals. Therefore, GPR waves travel at speed $v=c_{0} / \sqrt{\varepsilon_{r}}$, where $c_{0}$ is the speed of light in vacuum and $\varepsilon_{r}$ is the relative dielectric permittivity of the material. Thus, lateral resolution decreases with depth and increases with frequency and dielectric permittivity.

Finally, the reflected power at every interface depends on the dielectric permittivity of both materials. Let us assume a plain electromagnetic wave traveling in a low-loss material with dielectric permittivity $\varepsilon_{1}$ that is normally incident on the interface with another material with dielectric permittivity $\varepsilon_{2}$. Then, the power of the reflected wave is directly proportional to the square of the reflection coefficient $R=\left(\sqrt{\varepsilon_{1}}-\sqrt{\varepsilon_{2}}\right) /\left(\sqrt{\varepsilon_{1}}+\sqrt{\varepsilon_{2}}\right)$. Thus, GPR will only show interfaces between materials of a high enough difference in dielectric permittivity.

Given these limits, GPR surveys attempt to obtain data from as many shifts as possible from the terrain. The resolution in the shift domain is limited by practical constraints like duration of inspection, volume of recorded data and accessibility to specific areas. Moreover, uncontrolled failures during the signal acquisition step may lead to missing relevant information, thus degrading the final quality of the data. A possible solution not requiring reacquisition of the GPR signals is given by interpolation methods, which can recover the missing data from the available ones. The interpolation of missing or corrupted traces is a common processing step in ground-penetrating radar interpretation [43], and is not limited to B-Scans. Currently, C-Scans and 3D imaging and pseudo-3D imaging are common GPR issues and, in those cases, interpolation is also needed when imaging is reconstructed from parallel or non-parallel radargrams. However, this study is limited to the interpolation of GPR B-Scans. In this context, there are three common issues that require interpolation: i) recovery of traces lost due to sampling errors, particularly in difficult terrain; ii) de-clipping of saturated GPR signals; and iii) re-sampling of data acquired in continuous trigger mode to a fixed sampling rate, also known as rubber-band interpolation. In GPR, these issues are usually solved using spline interpolation [69]. Some works explore the possibility of using interpolation to increase the resolution of the acquired GPR signals, a problem that is still under research [252]. This improvement could help with the development of techniques that benefit from high data resolution [149].

The most common GPR applications are location of underground structures [62,90,105] and identification of material properties [212], with less common applications such as remote sensing [71]. There have been some attempts to perform hyperbola detection on GPR data robust to missing or anomalous data (for instance, [280]). However, these attempts are performed on simulated data and in highly controlled conditions, whereas this section studies both simulated and real data in realistic conditions. The GTS has used ground penetrating radar to search for cracks in historical walls [218,212,227,89,98, 100, 210,226,216]. In particular, the results in this Section have been reported in [219,220].

### 5.1.2. Preprocessing of the B-Scan for ICAMM: data alignment

As stated in Section 5.1.1, GPR signals (and, indeed, a lot of NDT signals) are usually taken as B-Scans or two-dimensional images. In these B-Scans, one dimension is time and the other is space. However, many B-Scans are too high-dimensional to directly work with them given the complexities of most of the ICA algorithms. This is important in the cases where there are more traces than time samples, since in that case no significant model can be calculated from the data.

The usual preprocessing in these cases consists of dimensionality reduction using methods such as PCA [124]. Briefly, PCA is applied to obtain a reduced subset of principal components and the ICA mixture model is calculated from these components; then, the ICAMM parameters are adjusted to include the information from the PCA. This results in non-square de-mixing matrices where the $M$ observations are mapped to $L<M$ sources. However, the ICAMMbased methods in this thesis require square de-mixing matrices, since we perform probability transformations that are only defined for unique mappings (i.e., square matrices) for PREDICAMM in (3.3). Therefore, we did not apply dimensionality reduction in this thesis.

The B-Scans from GPR signals were treated as images. In this case, we can consider that the image is composed of "patches" or squares of the same size, and that each patch is a linear combination of underlying basis functions; this is known as the Blind Linear Image Synthesis model [188]. These basis functions can be viewed as independent "image sources" that can be estimated by using ICA [19,111]. We used the procedure defined in [114], dividing the image into patches and then estimating their underlying ICA mixture model. Briefly, the B-Scans were preprocessed by following the steps shown in Figure 5.2. Each B-Scan from the GPR signals is divided into squares of fixed size or "patches." Thus, if the size of a patch is [ $L \times L$ ], each patch comprises $L$ consecutive time samples from $L$ adjacent traces. Then, each patch is transformed into a column vector with $M=L^{2}$ components by vertically concatenating the columns of the patch. Each one of these vectors is considered an observation $\mathbf{x}$. In this thesis, this preprocessing is called "alignment." Once the data are aligned this way, the parameters of the ICA mixture model can be estimated using any of the available methods (e.g., [153,231]). The definition of the partition of known and unknown data $\mathbf{x}=\left[\mathbf{y}^{T}, \mathbf{z}^{T}\right]^{T}$ depends on the particular experiment, as shown in the following sections.


Figure 5.2. Diagram of the alignment preprocessing applied to B-Scans. In the example, the size of the patch is [ $3 \times 3$ ].

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### 5.1.3. Simulations

The performance of the proposed methods was tested on a set of simulated data. The synthetic GPR data were obtained from the simulation of the 2D model shown in Figure 5.3.a. This model was a homogeneous wall surrounded by air with five discontinuities inside the wall. This model was designed so that it was similar to the real data. The simulated radargram was obtained by applying a ray tracing algorithm in MATLAB®. The resulting B-Scan is shown in Figure 5.3.b. The wall had dielectric permittivity $\varepsilon_{r, g r o u n d}=8$ (e.g., old cement), and the discontinuities had dielectric permittivity: $\varepsilon_{r, 1}=\varepsilon_{r, 4}=20$ (wet cement, in gray in Figure 5.3.a); $\varepsilon_{r, 2}=\varepsilon_{r, 3}=1$ (air, in black); and $\varepsilon_{r, 5}=81$ (water, in white). The final B-Scan had 512 traces, and each trace was 1024 samples long. Other parameters were: inline spacing distance 5 mm , time sampling period 10 picoseconds, center frequency of the GPR antenna 1.5 GHz with 1 GHz bandwidth, and signal-to-noise ratio $S N R=30 \mathrm{~dB}$ with K1 noise (see Table 3.3). The SNR corresponds to a low-noise signal, and was chosen to improve the representation of reflections. The noise was modeled with a K-distribution because it is often the distribution that best fits radar clutter [202].

The results of E-ICAMM and PREDICAMM were compared with those of several of the methods proposed in Section 3.3. Out of all proposed methods, we selected Kriging, Wiener structures and Splines for the comparison. Kriging and Wiener structures have been already used for the prediction of spatially-distributed GPR data, whereas Splines are commonly used for interpolation of GPR data. SRF was not selected because it yielded poor results in a preliminary test. Out of the considered possible initial values for PREDICAMM, we considered only that with the best results, PREDICAMM+E-ICAMM (as seen in Section 3.4.3.b).

Kriging and Splines are suited to work with spatially-distributed data, whereas the other methods require data alignment as shown in Section 5.1.2. Hence, we considered two patch sizes, $[8 \times 8]$ and $[16 \times 16]$ samples, which were converted to column vectors of $M=64$ and 256 variables, respectively. These patch sizes are typical in image processing applications, particularly $[8 \times 8]$, which gained popularity due to the importance of JPEG compression and other methods related to the discrete cosine transform (DCT). Fast implementation of such methods requires patch sizes that are powers of 2 [156]. However, patch size is usually determined using rather empirical methods.

It was assumed that $l$ out of every $L$ GPR traces were corrupted or not captured at all in the experiment $(l<L)$. Thus, the proposed prediction methods were used to interpolate missing information in these traces. Such a scenario could arise while increasing the horizontal scanning rate (i.e., the number of "sampled" locations) by interpolating new traces from the available


Figure 5.3. Simulated GPR data: a) initial model of the ground; b) simulated radargram.
ones; in this case, the new traces can be considered missing traces and can be interpolated. A similar scenario would arise when problems during the data measure process occur; for instance, if the antenna is moved too fast across the surface and the measure device is unable to properly sample the underlying terrain. In the latter case, however, missing traces would be located at random intervals, depending on the speed of the antenna.

The experiment setup is shown in Figure 5.4. First, the simulated data are aligned if necessary and then any model parameters (such as the covariance function for Kriging or the ICAMM parameters) are calculated from the complete original radargram. In general, the number of classes for ICAMM is determined from the data, either from data with several known classes or by testing several models with an increasing number of classes. However, estimation of the ICAMM parameters was complicated because of the high dimensionality of signals and the high correlation between radargram patches. In the end, we opted for an ICAMM with a single class whose parameters were found using Topographic Independent Component Analysis (TICA [111]). TICA is an ICA algorithm which is commonly used to model natural images, and it employs the same data alignment as Section 5.1.2.

Once the data model parameters required for the implementation of predictors were estimated from the full data, $l$ out of every $L$ traces were marked as erroneous or missing $(l<L)$. The result is shown in Figure 5.5, where marked traces are shown in red. Marked traces were centered within their patches in order to ensure that there was always some information at the first and last traces of the radargram. This process avoided extrapolation. The missing data were then predicted with each proposed method. Therefore, a substantial number of data were removed from each affected patch because even a single missing trace causes at least $L$ missing data from every affected patch, where $L$ is 8 or 16 .


Figure 5.4. Diagram showing steps followed in the prediction experiment on simulated GPR data. This process is repeated for every number of missing traces per patch.



Figure 5.5. Selection of missing or erroneous traces for the prediction experiment: a) original data; b) data with missing traces shown in red.

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The radargram with missing traces was aligned and the proposed prediction methods were used to interpolate these erroneous data. Afterward, the similarity between the interpolated data and the true data was measured using the error indicators defined in Chapter 3: SIR, KullbackLeibler divergence, cross-correlation, and MSSIM. The above experiment was repeated multiple times, each time increasing the number of missing traces around each selected position. The number of missing traces ranged from 1 to the number of traces per patch minus 2 (e.g., 6 traces for $[8 \times 8]$ patches). This range was decided to keep at least some information available within each patch.

It could be argued that the regularly-distributed missing traces and the high number of missing data make this a very particular experimental situation. However, this case can be split into several local sub-cases in which a group of $l$ consecutive traces were erroneous or missing and had to be reconstructed. This corresponds to a more normal experimental situation, where only a few of the traces are missing or damaged. Here, we removed multiple sub-cases at the same time (at regular intervals) across the whole radargram to find out the average prediction performance on the complete B-Scan. This average will avoid local optima and yield more significant and robust results. In practice, local results oscillate around the average values. Another reason for the equal intervals is to simulate a case where we attempt to increase the resolution of the captured data. In that case, the "missing data" (i.e., the data to be interpolated) would be located at equal intervals.

The results for patches of size $[8 \times 8]$ are shown in Figure 5.6. These results can be split into two regions, depending on the amount of reconstructed data. For low amounts of missing traces per patch, Splines performed slightly better than E-ICAMM and PREDICAMM, Kriging yielded the next best result, and Wiener structures achieved the worst result. For higher amounts of missing traces, the performance of E-ICAMM and PREDICAMM matched that of Splines, and even exceeded it for 6 missing traces per patch. Furthermore, Wiener structures obtained a better result than Kriging when the number of missing traces was high. This performance owed to the fast worsening of Kriging as the number of missing traces increases, since Wiener structures were more resistant to the amount of unknown data. Finally, both PREDICAMM and E-ICAMM yielded practically identical results. This result implied that the reconstruction by EICAMM was already very close to the maximum in the probability density function. This was confirmed by the low number of iterations in the PREDICAMM gradient step.


Figure 5.6. Error indicators for prediction of the simulated radargram for patches of size [ $8 \times 8]$.

Figure 5.7 shows the result for patches of size $[16 \times 16]$. Both PREDICAMM and E-ICAMM improved their performance with higher patch size, while the other methods obtained similar results than for $[8 \times 8]$ patches. The ICAMM-based methods obtained the best result for all considered amounts of missing traces in SIR, correlation and MSSIM. Splines obtained the second best result, followed by Kriging, and then Wiener structures. This result might indicate that the ICA mixture model is more appropriate for $[16 \times 16]$ patches. As with Figure 5.6, PREDICAMM and E-ICAMM obtained almost identical results, confirming the idea that the reconstruction yielded by E-ICAMM is already very close to the maximum in the probability density function. However, this might not be the case in other applications. As it will be seen in Section 5.4.3, some applications benefit greatly from the optimization procedure in PREDICAMM.

In terms of processing time, the proposed methods can be sorted in descending order of time cost: PREDICAMM, Wiener structures, Kriging, E-ICAMM, and Splines. Although E-ICAMM interpolation itself is faster than Splines, E-ICAMM requires a previously-estimated ICAMM, which is a costly procedure. The same ICAMM can be used multiple times, even if the number of missing traces changes or these traces are moved around, which reduces the difference in computational cost. Furthermore, this model is also used for the gradient method in PREDICAMM.

Figure 5.8 shows the reconstruction results for [ $16 \times 16$ ] patches with 9 missing traces per patch: a) simulated data; b) simulated data with missing traces; c-f) reconstructed B-Scans; and g-j) prediction error obtained by the proposed methods. PREDICAMM was not included because the reconstruction is almost identical to that of E-ICAMM. In concordance with the values in Figure 5.6, Kriging achieved the worst result, Wiener structures improved with respect to Kriging, and E-ICAMM and PREDICAMM obtained the best quality interpolation, outperforming the results of Splines. The ICAMM based methods and Splines perfectly reconstructed the reflections at the beginning and end of the wall, and the hyperbolas were better reconstructed by PREDICAMM and E-ICAMM. This is particularly true for the hyperbolas for defects 2 and 5 , at the right end of the wall relative to Figure 5.8. Out of the four error indicators in Figure 5.7, the MSSIM (Figure 5.7.d) is the closest fit to perceived quality of


Figure 5.7. Error indicators for prediction of the simulated radargram for patches of size [16×16].

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the results in Figure 5.8. The MSSIM values were $0.87,0.90,0.93,0.95$ and 0.95 respectively for Kriging, Wiener structures, Splines, E-ICAMM and PREDICAMM. The result for Wiener structures (Figure 5.8.d and Figure 5.8.h) is more similar to the original simulated data than the result for Kriging, but the other indicators would seem to indicate a closer result between Kriging and Wiener structures.


Figure 5.8. Results for $[16 \times 16]$ patches with 9 missing traces per patch: a) simulated data; b) simulated data with missing traces; c-f) reconstructed B-Scans; and g-j) prediction error obtained by the proposed methods. PREDICAMM was not included because the reconstruction is almost identical to that of E-ICAMM.

### 5.2. Application on GPR data from a survey on historical walls

The experiment was carried out on data obtained from a multidisciplinary study on replicas of historical walls; these data have been used by the GTS in previous studies [212,218,227,89,98,100,210]. The walls were built in a laboratory to control their composition and introduce certain defects or discontinuities at specific locations. They were built using travertine ashlars from the Godella quarry (Spain), each ashlar being $40 \times 30 \times 20 \mathrm{~cm}$. The mix was $0: 1: 3$, with no cement and one part of sand for every three parts of hydraulic lime (NHL5 class). This impoverished mortar is typical of historical buildings, and achieves low compressive strength ( $<4 \mathrm{MPa}$ ). The total dimensions of the walls were 287 cm length, 220 cm height and 20 cm thickness. A picture of one of the walls is shown in Figure 5.9.a.

The GPR equipment consisted of a SIR-3000 data acquisition system and a 1.6 GHz center frequency antenna (model 5100B) from Geophysical Survey Systems, Inc (see Figure 5.10). The dimensions of the antenna were $3.8 \times 10 \times 16.5 \mathrm{~cm}$; it was fitted to an encoder cart built $a d$ hoc for the experiment. The encoder and cart were used for two reasons: a) to ensure a uniform sampling of the wall, capturing data at a constant rate; and b) to help with displacing the antenna across the (uneven) surface of the wall.


Figure 5.9. Picture of the wall under test: a) studied wall, with a green line indicating the scanned trajectories considered for this work; b) captured GPR radargram for the scanned trajectory of vertical radar line 1 . The reflections corresponding to front and back faces of the wall are indicated in the radargram. The wave velocity used to estimate distances was equal to $92.56 \cdot 10^{6} \mathrm{~m} / \mathrm{s}$, which is equivalent to a dielectric permittivity of $\varepsilon_{r}=10.50$.


Figure 5.10. Picture of the GPR equipment used to scan the historical walls.

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Each wall was scanned with the GPR in order to detect any significant flaw, crack or discontinuity. This survey was performed following a grid of trajectories with 7 vertical lines and 4 horizontal lines, placed more or less uniformly along the surface of the wall (see Figure 5.9.a). Thus, in total, eleven B-Scans were obtained for each of the two walls. All 11 radargrams were used for this prediction experiment, and results were averaged. Figure 5.9.b shows an example radargram obtained for vertical radar line 1 of Figure 5.9.a. Each B-Scan was composed by between 330 and 450 traces, each one 1024 samples long. The inline spacing distance was 6 mm , the time sampling period was approximately 10 picoseconds, and the total time for each trace was 10 nanoseconds.

The procedure was the same as that explained for simulated data (see Section 5.1.3); including alignment, interpolation methods, and patch sizes. Results for prediction using [ $8 \times 8$ ] patches are shown in Figure 5.11. All proposed methods achieved better performance with real data than with simulated data (see Figure 5.6). This was due to differences in the GPR data. The real data included planar targets (wall discontinuities) and thus several structures of the real radargrams were spread over many patches, resulting in higher redundancies. Improvement of real data analysis over simulated data was greater for ICAMM-based methods and Splines, which yielded much better results than Kriging and Wiener structures. The performances of ICAMM-based methods and Splines were similar, and PREDICAMM and E-ICAMM obtained a slightly higher SIR for a high amount of missing traces (see Figure 9.a). Wiener structures performed better than Kriging except for very low amounts of missing traces, indicating a higher presence of nonlinearities in real data with respect to simulated data. In concordance with the results for simulated data, PREDICAMM+E-ICAMM and E-ICAMM yielded almost identical reconstructions.

Results for $[16 \times 16]$ patches are shown in Figure 5.12. As with the simulated data, the performance of ICAMM-based methods was improved with the larger patch size. PREDICAMM, E-ICAMM and Splines performed similarly for low amounts of missing traces, but the relative result of ICAMM-based methods became better for higher concentrations of missing traces per patch. This is more noticeable in the SIR and MSSIM indicators (Figure 5.12.a and Figure 5.12.d, respectively). The maximum difference was for the case with 12 missing traces per patch. The difference was lower for 13 and 14 missing traces due to the larger


Figure 5.11. Error indicators for the prediction of the real radargram for patches of size [8 $\times 8$ ].


Figure 5.12. Error indicators for the prediction of the real radargram for patches of size [16 $\times 16$ ].
number of missing data in the patch. With 13 or 14 missing traces, the ICAMM no longer had enough information about the structure of the data to reconstruct the signal with high accuracy. The performance of Kriging and Wiener structures was similar to their performance for [8×8] patches (Figure 5.11). Finally, the results of E-ICAMM and PREDICAMM+E-ICAMM are almost identical, in concordance with the results for simulated data (Figure 5.7). As for the processing times for each method, results were almost identical to those for the simulated data.

Figure 5.13 shows the reconstruction results for vertical radar line 1 of the wall in Figure 5.9, for [ $16 \times 16$ ] patches with 10 missing traces per patch: a) real data; b) real data with missing traces; c-f) reconstructed B-Scans; and $\mathrm{g}-\mathrm{j}$ ) prediction error obtained by the proposed methods. PREDICAMM was not included because the reconstruction is almost identical to that of EICAMM. The highest errors are for interpolation using Kriging and Wiener structures methods; Splines performed better than Kriging and Wiener structures; and E-ICAMM achieved the best interpolation (i.e., minimum prediction error), outperforming the other methods. The error was higher around the borders of the wall. This effect was more marked for Splines, PREDICAMM and E-ICAMM (Figure 5.13.e and Figure 5.13.f, respectively). Error for ICAMM-based methods was negligible, however, and the reconstruction is very close to the real data, even more so for the inside of the wall.

To extend testing of the proposed methods in an application-oriented context, we performed a simple detection experiment on the real radargrams. The radargrams from wall 2 were used to detect two discontinuities within the wall. The first one was a hollow filled with cement near the upper-left corner of the wall, of size $8 \times 6 \times 2 \mathrm{~cm}$ (width, height and length). The second discontinuity was a vertical crack near the right end of the wall, of size $0.15 \times 5 \times 8 \mathrm{~cm}$ (width, height and length). The detection algorithm consisted of the following steps: i) band-pass filtering to remove noise; ii) background removal using the local mean; iii) calculation of the envelope of the signals; and iv) thresholding. This algorithm was valid for our study. Developing an optimum detection algorithm on a set of real GPR data is a challenging task, and was therefore beyond the scope of this study.

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The detection algorithm was used on the full data set, and with the reconstructed results for the case with $[16 \times 16]$ patches and 12 missing traces per patch. The detection results, summarized by the area under the ROC (Receiver Operating Characteristic) curve, were as follows: 0.6588 (real data), 0.6586 (reconstruction with PREDICAMM+E-ICAMM), 0.6586 (reconstruction with E-ICAMM), 0.6323 (reconstruction with Splines), 0.5546 (reconstruction with Kriging), and 0.5259 (reconstruction with Wiener structures). E-ICAMM yielded results that were consistently almost identical to those of the data without missing traces. Splines yielded the next best result, and Kriging and Wiener structures yielded the worst detection rates. These results are in concordance with results in Figure 5.13, showing that a good interpolation can help with subsequent GPR processing steps.


Figure 5.13. Results for vertical radar line 1 of the wall in Figure 5.9 , for [ $16 \times 16$ ] patches with 10 missing traces per patch: a) real data; b) real data with missing traces; c-f) reconstructed B-Scans; and $g-j$ ) prediction error obtained by the proposed methods. Amplitude was normalized to unit power. PREDICAMM was not included because the reconstruction is almost identical to that of E-ICAMM.

### 5.3. Application on seismic signals for underground surveying

Exploration seismology is a discipline that analyzes the behavior of captured seismic waves to study the underground terrain; i.e., the propagation of these waves is studied to characterize the properties of the underground [241]. Careful examination of seismic data can be used to detect, locate and analyze points of interest such as wells, layers or reservoirs. The basic technique of seismic exploration consists of generating seismic waves and measuring the time required for the waves to travel from the source to a series of geophones, usually disposed along a straight line directed toward the source. The time of arrival of each wave is the most important feature; but there is also interest in the variations in amplitude, frequency, and waveform.

There are two main categories of seismic surveys: refraction seismology, in which the principal portion of the path is along the interface between two rock layers (hence, it is approximately horizontal); and reflection seismology, in which the wave travels downward initially and, at some point, is reflected back to the surface (the path being essentially vertical). The main difference between both categories is that for refraction, the distance between source and geophones is large relative to the depths being mapped; whereas for reflection, the distance between source and geophones is smaller than the depths being mapped. Our description will consider reflection seismology, since it is more widely used than refraction seismology.

A typical reflection seismology survey has a single source event or "shot" that emits elastic waves using an energy source such as a controlled explosion, thumper truck, or air gun (depending on the medium under test). Once the shot is generated, the elastic waves travel through the medium under test and reflect off the boundaries between materials with different acoustic properties. These reflections are then captured at the surface by groups of receivers (usually geophones or hydrophones); the receivers are usually laid out in a straight line, spreading over a large area of terrain (see Figure 5.14). The signal captured by each receiver is an A-Scan or trace; groups of A-Scans are usually combined to form B-Scans or "seismograms" for the user to interpret.

The interpretation of the captured seismograms is usually based on the detection of "events," arrivals of energy that vary from trace to trace. The study of the time of arrival of these events is used to estimate the underlying underground structures, though other parameters of the data can be used as well. Typically, the recorded signals are subject to signal processing techniques to enhance their quality and to improve their interpretation by the user [283,179]. The processing of seismic data is still a significant area of research, e.g., to reduce the computational costs [23] or to improve data interpretation [82]. One of the typical processing steps is the treatment of missing traces. Missing traces are relatively common in seismic studies, since they involve large amounts of devices over a large area of terrain; furthermore, most studies take place in hostile environments (underwater, underground, etc.) or under unfavorable meteorological conditions.


Figure 5.14. Sample of a reflection seismology scenario: a) medium under test and experiment setup; b) recovered signals. The shot is emitted from the transmitter (Tx) and travels underground until it finds a discontinuity between layers; part of the incident energy is reflected back at the surface, where it is captured by an array of receivers (Rx). The captured reflection, the interface between layers 1 and 2, is shown in b). Each trace shows a different time of arrival because the traveled distance is different for each receiver.

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A complete review on seismic exploration and its applications is treated in [241]. Although there are multiple applications for seismic exploration, such as the exploration of deep underground structures [6], the most important is the exploration of the underground to locate mineral and oil deposits [241,179]. The GTS has already performed some studies on seismic signals [222,211].

Reflection seismology is somewhat similar to ground-penetrating radar (compare Figure 5.14 with Figure 5.1), but their respective non-destructive systems operate at different frequencies and seismic studies involve several reception antennas at once. Furthermore, since seismic surveys operate on much lower frequencies, they usually involve greater depths and span large breadths of terrain. In fact, one could say that reflection seismology is to sonar and echolocation what GPR is to conventional radar.

### 5.3.1. Reconstruction of seismic data

The proposed prediction methods were tested on a public dataset from BP Amoco [79]. One half of the dataset is a cross-section through the Carpathian thrust belt from the Straciccina area of Poland, where Amoco acquired a swath seismic survey in 1996, while the other half of the model represents North Sea-type salt ridge structures contained in much lower velocity sediments than are present on the left. This set was artificially built to test the limits of migration methods, but it is composed of real data. The resulting model was 2.5D model, that is, a 3D model with variations in only two of its axes. Out of the whole data set, a single 2-D slice of data was chosen for this experiment; these data are shown in Figure 5.15. The selected Bscan comprises 240 traces, each one 352 samples long. The vertical sample rate is 9.9 ms and the horizontal sample rate is 25 m .

Like in Sections 5.1 and 5.2, it was assumed that $l$ out of every $L$ traces were completely or partially corrupted, or not captured at all during testing $(l<L)$. Thus, the proposed prediction methods were used to interpolate missing information in these traces. The procedure was the same as that explained for GPR data (see Section 5.1.3), including alignment, interpolation methods, and patch sizes. As mentioned in Section 5.1.3, the selection of the traces at regular intervals along the B-Scan was performed to find out the average prediction performance of the proposed methods. This average will avoid local optima and yield more significant and robust results.

Figure 5.16 shows the prediction results when using patches of size [ $8 \times 8$ ]. E-ICAMM obtained the best result in all cases, with PREDICAMM obtaining a very similar result. The behavior of the other methods depended on the considered error indicator. Splines yielded the third best


Figure 5.15. Seismic signals used for the prediction experiment. Possible reflections appear as white, black and white.
result in terms of KLD, CORR and MSSIM, while Kriging yielded the third best result in terms of SIR. Wiener structures obtained a middle ground between Kriging and splines for the SIR, KLD and CORR indicators, although they also yielded the lowest MSSIM out of all the proposed methods. The difference between the performances of E-ICAMM and PREDICAMM and those of the other methods is larger for low amounts of missing traces $(l<4)$.

The results obtained for patches of size $[16 \times 16]$ are shown in Figure 5.17. E-ICAMM, PREDICAMM and Wiener structures all yielded better SIR and KLD than in the [ $8 \times 8$ ] case ICAMM and PREDICAMM yielded the best overall performance, with the best SIR and CORR for all cases, the best MSSIM for most of the cases $(l<12)$, and the best KLD for low amount (see Figure 5.16.a and Figure 5.16.b, respectively) for low amounts of missing traces $(l<6)$.


Figure 5.16. Error indicators for the prediction of the real seismic data for patches of size $[8 \times 8]$.

a) Number of missing traces per patch
b) Number of missing traces per patch

c) Number of missing traces per patch

d) Number of missing traces per patch

Figure 5.17. Error indicators for the prediction of the real seismic data for patches of size [ $16 \times 16$ ].

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Thus, it seems like the larger patch size increased the performance of the nonlinear methods. Es of missing traces ( $l<6$ ). Splines obtained the worst result with respect to SIR and CORR, but it obtained the best KLD and MSSIM for high amounts of missing traces $(l>9$ and $l>12$, respectively). The results for seismic data were worse than those obtained for simulated and real GPR data, both for $[8 \times 8]$ and for [ $16 \times 16$ ] patches (see Sections 5.1.3 and 5.2). This owed to the lower correlations in the B-Scan due to the longer distances involved in the capture process.

Figure 5.18 shows the reconstruction results for $[8 \times 8]$ patches with 4 missing traces per patch: a) real data; b) real data with missing traces; c-f) reconstructed B-Scans; and g-j) prediction error obtained by the proposed methods. PREDICAMM was not included because the reconstruction is almost identical to that of E-ICAMM. The results are in concordance with the error indicators in Figure 5.16. This is particularly noticeable in the first reflection in the data, which shows irregularities for Kriging, Wiener structures and splines (Figure 5.18.c, .d and .e, respectively). Note the "ribbing" effect in the prediction using Wiener structures, which explains their significantly lower MSSIM in this case (see Figure 5.16.d). E-ICAMM yielded the best prediction, as can be seen both from the reconstructed B-Scan and the very low reconstruction error.


Figure 5.18. Results for [ $8 \times 8$ ] patches with 4 missing traces per patch: a) real data; b) real data with missing traces shown in red; c-f) reconstructed B-Scans; and g-j) prediction error obtained by the proposed methods. PREDICAMM was not included because the reconstruction is almost identical to that of E-ICAMM.

### 5.4. Application on electroencephalographic signals

Electroencephalographic signals are recordings of surface brain electrical activity taken at the scalp, where each sensor captures the combined signal from multiple neurons of the brain [185]. The study of EEG signals is a useful clinical tool because some illnesses, typically seizures and sleep disorders, produce abnormal electric patterns in the electrical activity of the brain that can be identified by an expert. Even though there are other techniques for the exploration of the human brain, such as magnetic resonance (MRI), functional magnetic resonance (fMRI) and positron emission tomography (PET), EEG remains the subject of much research on brain activity and a valuable tool for clinical analysis. The main reasons for the use of EEG are the lower hardware cost of the device, the higher temporal resolution of EEG when compared to other available techniques, and the maturity of EEG analysis. Research on EEG data started in the late years of the $19^{\text {th }}$ century, although digital processing techniques were not used until the late 1990s [258].

Independent component analysis and other blind source separation techniques have been successfully used for the modeling and processing of EEG and other biological signals. For instance, ICA has been used to separate fetal and maternal electrocardiograms (ECG) [286,285,233], detect atrial fibrillation [284,92], and analyze high-density ECG [292].

The first applications of ICA to EEG signals took place during the late 1990s [258]. These works introduced the assumption that each EEG channel is composed by the mixture of a number of non-Gaussian sources [159,160]. Furthermore, it is assumed that this mixture is generated by the mixture of signals from several neurons due to the own conductivity of the head, and that this mixing is almost instantaneous in nature. In ICA, EEG signals are modeled as a mixture of independent but spatially fixed sources, with each source being either a point source or a distributed source spanning over an area of the brain. Later works seem to confirm that not only is it possible to separate time signals, but it is also possible to locate them on the surface of the head [190]. This spatial location is far from perfect, but it has been shown to be a very useful pre-processing step for other source location algorithms (for instance, [291]).

Another important application of ICA makes use of the recovered sources to model the EEG signal, allowing the extraction of sources of a given kind, e.g., evoked potential signals [161,162]. This source separation method is statistical in nature and therefore it can correctly separate signals that overlap across time and/or frequency (a probabilistic filter, as it were). This application can be used to remove unimportant signals and reduce the workload of the expert during exploration. Moreover, it can also be used for automatic diagnosis of illnesses such as ADHD (Attention Deficit Hyperactivity Disorder) or sleep disorders [180,230]. There are also works on the application of ICA to the separation of fMRI signals [168]. In this thesis, however, we will only consider EEG signals.

Source separation by ICA can also be used for artifact removal, since there are several artifacts that can be safely assumed to be independent from EEG data [128]. There are several works on this topic, ranging from supervised artifact removal [128] to fully automatic artifact detection and removal [186]. A good review of the applications of ICA to EEG signal processing can be found in [127].

One of the main research topics on the application of ICA to EEG signals is the dynamic modeling of brain oscillations in humans [230,189,109,61] and lab rats [232,10]. This research attempts to combine the advantages of independent component analysis with the capabilities of certain dynamic models to deal with the temporal variability of the EEG. For instance, some representative examples are the study of developmental differences in the saccadic contingent negative variation [138], EEG and event-related potential (ERP) data [162,277], and removal of artifacts in the EEG signal [44]. The GTS has already published some works in this area [230]. EEG data will also be explored in Chapter 6, where we will apply the methods proposed in

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Chapter 4 to the dynamical modeling of EEG data. These data were obtained from subjects performing cognitive tasks and neuropsychological tests for the evaluation of the memory function and learning in epileptic subjects.

In the EEG prediction application presented here, it was assumed that one or several channels have been partially corrupted or missing; thus, the proposed methods were used to complete these EEG. This kind of scenario is relatively common in EEG processing, for instance, for artifact removal from EEG data. In that case, artifacted data are removed and then reconstructed from neighboring electrodes. The results in this section have been reported in [224,215].

### 5.4.1. Data capture

The EEG data that were used in this experiment were captured using an ActiveTwo system by BioSemi. This device uses active electrodes and a water-based gel to increase coupling with the skin, and thus increasing data quality. The data capture was performed using the ActiveView600 software freely available at BioSemi’s web site.

The device was connected to 66 electrodes, 64 EEG data electrodes and 2 ground electrodes (CMS and DRL); EMG, EOG and other types of channels were not measured. These ground electrodes are used to increase the quality of captured data, since they form a feedback loop that drives the average potential of the subject as close as possible to the reference of the device. Furthermore, this loop decreases noise and protects the user against high currents. Electrodes were positioned following the $10-10$ system (see Figure 5.19 .a) with the help of a measuring cap, and the 64 data channels were captured at a sampling rate of $2,048 \mathrm{~Hz}$. All electrodes are referenced with respect to channel Cz in order to reduce noise levels.

The signal acquisition process started with the explanation of the experiment to the subject, which had already given his or her consent. Then, the subject was seated and the measuring cap was adjusted, taking particular care to place Cz correctly (halfway between the nasion and the inion and halfway between the left pre-auricular and right pre-auricular points). Once the cap was in position, the electrodes were placed one by one, ensuring their correct coupling with the scalp. This check was performed by verifying that the offset between any electrode and CMS was low and stable, removing and re-attaching any offending electrode. Then, the subject was seated in front of a computer screen and a sample test was shown to confirm that they understood the memory task. Afterwards, the EEG data were captured while the subject


Figure 5.19. EEG capture process: a) spatial distribution of the 66 electrodes (10-10 system) for the capture of EEG signals; b) picture of one of the subjects undertaking the memory task. The electrodes are attached to the subject beforehand so they capture data during the memory task.
performed the task (see Figure 5.19.b). Once the capture process was finished, the electrodes and the measuring cap were cleaned and dried up.

After the acquisition stage, the EEG signals were filtered to remove noise caused both by the environment (electronic devices, ambient noise, machinery, line noise, etc.) and by the capture device itself. These filters used for this pre-processing are typical in EEG processing:

* A high-pass Butterworth filter of order 6 with cutoff frequency $f_{c}=0.2 \mathrm{~Hz}$. This filter attenuates the very-low-frequency noise generated by the capture device, as well as slow drifts in the data.
* A low-pass Butterworth filter of order 6 with cutoff frequency $f_{c}=70 \mathrm{~Hz}$. This filter removes frequencies outside of the EEG range of interest, reducing high-frequency noise.
* A notch Butterworth filter of order 2 centered at 50 Hz with quality factor $Q=50$. This filter removes line noise (i.e., coupled noise from the power line).


### 5.4.2. Sternberg memory task

The electroencephalograms were captured while subjects performed the Sternberg memory task, a classical memory test that measures multi-object short-term memory [251]. The task is composed of 30 trials or repetitions, each one following the pattern shown in Figure 5.20.


Figure 5.20. Description of one trial of the Sternberg memory task.
During each trial, the subject is shown between one and five symbols, chosen at random from the available 20 -symbol set (see Figure 5.21); the number of symbols changed between trials. Each symbol is displayed on screen for 200 milliseconds (display stage) and then followed by a blank screen during 1000 milliseconds (pause stage) before showing the next symbol. Once the last symbol has been shown, the screen remains blank for a further 1000 milliseconds (retention interval), after which there is a warning and the participant is presented with the test symbol. The subject must decide whether this test symbol was part of the series of shown symbols (test stage). The correct answer is set beforehand to have the same number of affirmative and negative answers. After the subject answers the question, there is a further delay of 500 milliseconds before continuing with the next trial. For this particular experiment, each subject performed 30 trials.


Figure 5.21. Available symbol set for the Sternberg memory task.

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### 5.4.3. Reconstruction of missing EEG data

Data were captured from three healthy human subjects, with 60 to 300 trials per subject. The subjects answered correctly $98 \%$ of the trials with an average response time of 1.17 s. Figure 5.22 displays one of the captured EEG, with the stages of the Sternberg memory task marked as red and blue lines.

In order to test the predictive capabilities of the method, it was assumed that the values at one or more of the electrodes were unusable and had to be discarded. Thus, the proposed methods were used to reconstruct these corrupted data. As mentioned at the beginning of Section 5.4, such a scenario could happen, for instance, if some of the electrodes had been disconnected during data capture. The proposed ICAMM-based methods were compared with spherical splines, a classical method for EEG prediction that was already introduced in Section 3.3.4 [199]. The other methods considered in Section 3.3 were discarded after a previous study, in which they obtained bad results when used to predict EEG data.

Since the choice of channels affects the result of any predictor and the number of possible was too large to perform an exhaustive search, performance was calculated with a Monte Carlo experiment, as shown in Figure 3.8. First, the parameters necessary for each predictor are calculated using the first half of the EEG data. After estimation, one of the EEG channels (chosen at random for each iteration) was removed and the proposed methods were used to interpolate these missing data on the second half of the data. Prediction performance was measured using the error indicators introduced in Section 3.4.2: SIR, Kullback-Leibler divergence, correlation and MSSIM. This process was repeated 1,000 iterations and results were averaged. The Monte Carlo experiment was repeated several times, each time with an increasing number of missing channels, $l=1, \ldots, 12$. Therefore, the end result was obtained with 12,000 iterations in total.

The ICA mixture model in the EEG data was estimated with the on-line ICAMM algorithm shown in [157]. A single-class ICA model was selected, and its parameters are shown in Figure 5.24 .


Figure 5.22. Sample of the captured data during the experiment. The starting point of each trial is shown as a solid red line, while the beginning of each "Probe item" stage is indicated by a dashed blue line. The shown data span four trials.


Figure 5.23. Diagram showing the process of the Monte Carlo experiment used to calculate performance on EEG data. This process was repeated for an increasing number of missing channels, $l$.


Figure 5.24. Sample of the ICA parameters estimated from the EEG data: a) recovered sources; b) scalp map for an eye artifact; c) and d) scalp maps for two non-artifacted EEG sources.

Figure 5.25 shows the scalp maps corresponding to the prediction results for an increasing number of missing channels for spherical splines, E-ICAMM and PREDICAMM initialized with the result of E-ICAMM (PREDICAMM+E-ICAMM). Spherical splines performed at a similar level as the ICAMM-based methods for one missing channel. As the number of channels increased, however, the performance E-ICAMM and PREDICAMM increases above that of spherical splines. The optimization procedure in PREDICAMM improved the result of EICAMM by a wide margin in all cases, particularly in the case of the SIR error indicator (Figure 5.25.a), with a difference of almost 10 dB in favor of PREDICAMM. Furthermore, the performance of the proposed ICAMM-based methods was more resistant to the number of missing channels, and in fact, barely degrades up to $l=12$ missing channels.

To further showcase the performance of the proposed methods, Figure 5.26 shows the prediction for a given time instant from a case with $l=32$ missing channels. It can be seen that both proposed ICAMM-based methods achieve much lower prediction error than spherical splines, and their predictions are more similar to true data. More importantly, the general distribution of the channel amplitudes (as indicated by the contour lines in Figure 5.26) with spherical splines is different from the true one, while E-ICAMM yields a spatial distribution more similar to the true one, and PREDICAMM improves this result even further.

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Figure 5.25. Average error indicators for the prediction on real EEG data.


Figure 5.26. Scalp maps of the prediction and prediction error for a case with 32 missing channels. Missing channels are indicated by stars $(*)$, while known channels are marked by dots $(\cdot)$.

### 5.5. Conclusions

This chapter presents the application on real data of the prediction methods introduced in Chapter 3, PREDICAMM and E-ICAMM. Both methods make the assumption that the data can be modeled using a mixture of independent component analyzers (ICA). Each of these methods is the optimal predictor with respect to one particular characteristic: PREDICAMM is optimal with respect to the log-likelihood of the data, while E-ICAMM is optimal with respect to the mean square error. Both predictors are general-purpose and they can be used in many signal processing fields. Because of this flexibility, they were tested for the reconstruction of missing data from three quite different signal processing fields: non-destructive testing, seismic exploration, and electroencephalography.

First, the proposed methods were tested on a set of simulated NDT data, a synthetic radargram. In this case, the methods were used to reconstruct several missing traces from the radargram. This application required the transformation of the two-dimensional signal (B-Scan) to a onedimensional signal by a decomposition of the original image into square patches, a process that we have named alignment. After alignment, E-ICAMM and PREDICAMM were compared with the state-of-the-art method (Splines), a classical predictor (Kriging), and a nonlinear predictor (Wiener structures). Two patch sizes were considered, [ $8 \times 8$ ] and [ $16 \times 16$ ], and the behavior of the proposed methods changed slightly with patch size. For [ $8 \times 8$ ] patches, the reconstruction yielded by PREDICAMM and E-ICAMM was similar to that obtained by the state-of-the-art method (Splines), and was better than that of the competing methods for high amounts of missing traces. The performance of the ICAMM-based methods increased for [ $16 \times 16$ ] patches, in which case both E-ICAMM and PREDICAMM over-performed Splines across all estimators (e.g., the SIR obtained by both methods was 3 dB higher, on average, than the SIR obtained by Splines). The proposed methods and Splines always performed better than the classical predictor, Kriging, and a nonlinear predictor, Wiener structures. This improved reconstruction was shown by a better reconstruction of the shape of the recovered hyperbolas in the simulated radargram. For this application, the gradient used in PREDICAMM did not obtain any significant difference with respect to the initial value provided by E-ICAMM.

The first application of the proposed methods on real data consisted of the reconstruction of real GPR data from a study on replicas of historical walls. As with the simulated data, the data had to be aligned prior to prediction, and the result proved to depend on patch size. In this case, however, performance was different because of the larger presence of planar targets in the real data. PREDICAMM, E-ICAMM and Splines performed better on the considered set of real data ( 9 dB average increase in SIR), while Kriging and Wiener structures performed worse on real data ( 8 dB average reduction in SIR). Thus, the difference in performance between both groups of methods was larger for real data, and the difference between Splines and the proposed ICAMM-based methods was smaller. Other than these differences, the relative behavior of the methods was in concordance with the results on simulated data. E-ICAMM and PREDICAMM performed at a similar level to Splines for $[8 \times 8]$ patches, and performed better than Splines for [ $16 \times 16$ ] patches.

The second application was the reconstruction of missing data from a seismic B-Scan or seismogram, which was obtained from a public dataset from BP Amoco. Again, the performance of E-ICAMM and PREDICAMM was compared with that of Splines, Kriging and Wiener structures. The basic structure of the seismogram is similar to that of the radargram, and therefore, alignment was required to predict missing data with the proposed methods. The real seismogram, however, was more complex than the radargram and all the proposed methods achieved lower performances than they did for the first application. E-ICAMM and PREDICAMM always performed better than the other considered methods, and Splines usually performed better than Kriging and Wiener structures. The difference between the proposed methods and Splines was higher for $[16 \times 16]$ patches ( 8 dB average increase in SIR) than it was for [ $16 \times 16$ ] patches ( 4 dB average increase in SIR). Finally, PREDICAMM performed at a

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very similar level to E-ICAMM. Other than the general decrease in performance, which was more marked in the case of Splines, these results are consistent with those obtained on GPR data.

Finally, E-ICAMM and PREDICAMM were tested for the reconstruction of missing information from EEG data. These EEG were obtained from healthy human subjects performing the Sternberg memory task. The proposed methods were used to reconstruct missing data from one or more EEG channels, a scenario simulating the disconnection of the corresponding electrodes. In this application, the performance of the proposed methods was compared with that of the classical interpolator for EEG data, Spherical Splines, which was introduced in Section 3.3.4. Results showed that PREDICAMM performed better than E-ICAMM, which in turn performed better than Spherical Splines. These differences were small for one missing channel, but increased rapidly with the number of missing channels. This behavior owed to the faster decrease of performance of Spherical Splines, whereas both E-ICAMM and PREDICAMM were shown to be resistant to the number of missing channels. This point was shown with an extreme case where half the channels were missing. Even in this case, the reconstruction yielded by E-ICAMM and PREDICAMM was similar to the true data.

In the results presented in this chapter, PREDICAMM was always initialized with E-ICAMM. When used on GPR or seismic data, however, PREDICAMM obtained a result that was very similar to that of E-ICAMM. In these cases, the initial value was already very close to a (possibly local) maximum in the log-likelihood and PREDICAMM did not iterate, or iterated only shortly. Conversely, the performance of PREDICAMM did improve greatly over that of the initial value, E-ICAMM, for the reconstruction of EEG data. ICA techniques have been used on EEG data for a wide variety of applications, and the estimation of the ICA parameters in this case is well known. Therefore, it would seem that PREDICAMM performed better in the case where the ICA mixture model was best fit (EEG data), and not as well when the model was more complex or less applicable (radargram, seismogram). In the former, the probability densities estimated from the model were more precise and the maximization procedure in PREDICAMM was optimal. In the latter, the densities were not as precise and the initial value was usually close to a local maximum, reducing the usefulness of the gradient optimization step.

Furthermore, the ICA mixture model allows us to model local dependences without compromising the modeling of global structure. This behavior increases the performance of the proposed predictors and, at the same time, describes the structure in the data, since the ICAMM parameters can be studied to gain further knowledge on the data. This will be expanded upon in Chapter 6, where we will present the application of dynamic modeling methods to cognitive tasks and neuropsychological tests for the evaluation of the memory function and learning in epileptic subjects.

## Application of G- and UG-SICAMM to EEG signal processing

# Chapter 6 - Application of G- and UG-SICAMM to EEG signal 

processing
This chapter presents three applications of classification and dynamic analysis using the proposed SICAMM variants and G-SICAMM and UG-SICAMM procedures explained in Chapter 4. The results the proposed methods are compared with those of SICAMM, ICAMM, and several types of Bayesian networks (explained in Section 4.4). The proposed methods were tested on three sets of real data from biomedical applications: hypnogram records from sleeping subjects, stage detection in memory tasks, and evaluation of data from subjects performing several neuropsychological tests. In all cases, the application deals with electroencephalographic data. The interested reader can find a brief introduction on EEG data in Section 5.4.

The first application consists of the detection of very brief periods of wakefulness during sleep, also known as microarousals, from a set of electroencephalographic and biomedical data known as a polysomnogram (PSG). Microarousal detection can be used for differential diagnosis of several disorders and diseases [2]. The proposed methods were trained on a set of PSG from six patients and the accuracy was estimated by the balanced error rate (BER) of the classification and Cohen's kappa coefficient ( [58]). Both indicators were selected to compensate for the large difference in prior probability between the classes, which might interfere with less robust indicators (e.g., the error rate). The relation between microarousals and changes in the GSICAMM parameters was studied as well.

The second application is the classification of EEG signals from subjects performing the Sternberg memory task, a classical neuropsychological test that measures delays in working memory. The proposed methods were used to model the EEG data and then studied to find a correspondence between said models and the stages of the task. The performance of this correspondence was measured by the BER of the classification. The relation between changes in the G-SICAMM parameters and the stages of the task was also explored.

The third application is the evaluation of EEG data from epileptic patients. For this application, multiple neuropsychological tests were automated using graphic user interfaces (GUI) and distributed architectures. The EEGs of the participants were registered while they were taking the tests. The synchronicity between the task and the data capture was ensured by the automated

GUI. The proposed methods were used to classify the data from six patients. Depending on the type of test, the classification considered two classes (stimulus / response) or three classes (stimulus / retention / response). Performance was estimated by the BER of the classification and Cohen's kappa coefficient ( [58]).

Wherever two models are compared, the distance between them will be quantified using the three indicators introduced in Section 4.5.1. Those indicators are: (i) the Amari index, which is used to measure the distance between the de-mixing matrices of both models; (ii) the signal-tointerference ratio of the recovered sources, which quantifies the average squared error in the extraction; and (iii) the probabilistic distance, an approximation of the Kullback-Leibler divergence between the sequential distributions of the classes in two models.

### 6.1. Automatic classification of hypnogram data

In the clinical environment, human sleep is usually split in several stages: (i) stage 0 , awakening; (ii) non-rapid eye movement (NREM) sleep, which is further classified into stages 1-4 in increasing order of deepness, i.e., difficulty to awaken the sleeper; and (iii) stage 5, rapid eye movement (REM) sleep. REM sleep is also known as paradoxical sleep because the brain activity of subjects in REM sleep closely resembles that of awakened subjects [144]. Stages 1-5 follow each other in cycles that last for about an hour and a half (see Figure 6.1.a). Healthy subjects complete four or five of these cycles during a typical night's sleep.

The record of the different sleep stages during a given period of time is called a "hypnogram." The sequence of sleep stages displayed in the hypnogram can be used to diagnose different sleep disorders, illnesses (e.g., depression), and some drug addictions. Figure 6.1 shows two sample hypnograms, one from a healthy subject (Figure 6.1.a) and another from a patient with a sleep disorder (Figure 6.1.b). The hypnogram of the patient is markedly different from that of the healthy subject in several ways: (i) the sleep cycle is very different from that of a healthy subject; (ii) the hypnogram lacks any REM sleep, which is related to narcolepsy [144]; and (iii) there were multiple short periods of wakefulness through the night. Hypnograms are usually obtained in a non-automated manner by an expert performing visual inspection of the polysomnogram, a set of EEG and other biological records obtained from the sleeping patient. There have been some advances towards the automation of the hypnogram [2,230], but a fully automatic system remains a challenge.

One of the most common features extracted from the hypnogram is the absence or presence of very short periods of wakefulness [123], also called "microarousals," since their rate of appearance is linked with sleep disorders such as apnea and epilepsy. Microarousals appear in



Figure 6.1. Sample hypnograms covering all six sleep stages (1-4 plus REM and awakening): a) healthy subject; b) patient with a sleep disorder. Due to its nature, REM sleep is usually placed between stages 0 and 1 .
the hypnogram as short stays in stage 0 , as seen in Figure 6.1.b. In this section, we show a practical application of the methods proposed in Chapter 4 for automatic detection of microarousals in real EEG data from apnea patients. The results shown in this section have been reported in [223,215,221,213].

### 6.1.1. Data and pre-processing

In this experiment, the proposed methods were applied to perform automatic detection of microarousals. Hence, the classification will only consider two classes: (i) class 1, which corresponds to any stage of actual sleep (NREM and REM); and (ii) class 2, which corresponds to microarousals (i.e., stage 0 from the hypnogram). Six 8 -hour records were considered for the experiment, each from a different apnea patient. The records and their respective reference hypnograms were obtained by an expert using conventional, non-automated, procedures. As in Section 4.5.3, the results of SICAMM and its variants will be compared against those of ICAMM and several types of Bayesian networks. These automatic classifications will be compared with the non-automated classifications made by the expert, which we will assume to be the ground truth.

The recorded PSG were composed by 24 channels each, 11 EEG channels and 13 other channels measuring muscle signals, breathing, and other physiological characteristics. For this experiment, however, only the EEG channels were considered. The 11 EEG channels were sampled at 256 Hz , band-pass filtered using a Butterworth filter of order 6 between 0.2 and 70 Hz , and then a notch filter at 50 Hz was used to remove line noise. The filtered signals were split in 1-3 seconds long epochs ( 256 to 768 samples) without overlapping, and four features were calculated at each epoch. These features where then averaged for 30 -second segments, which were used by the proposed methods for training and testing. Thus, a decision about the sleep stage of the subject is taken every 30 seconds.

### 6.1.1.a. Extracted features

The four features extracted from the PSG signals were: amplitude, dominant rhythm (centroid frequency), and theta-slow-wave index (TSI) from channel C3-A2; and alpha-slow-wave index (ASI) from EEG channel O2-A1. These features are commonly used in PSG analysis [2,123], and their definitions are included in the following.

## Average amplitude

The average amplitude is the average absolute value of the voltage at every electrode during an epoch. It was calculated as the sample average of the absolute value of the EEG signal; thus, the average amplitude of the $i$-th channel is

$$
\begin{equation*}
\bar{x}_{i}=\frac{1}{N} \sum_{n=1}^{N}\left|x_{i}(n)\right| \tag{6.1}
\end{equation*}
$$

where $x_{i}(n)$ are the data from the $i$-th channel $(i=1, \ldots, 64)$ at time sample $n$, and with each epoch being $N$ samples long ( $N$ ranged from 256 to 768 samples).

## Centroid frequency

The centroid frequency is the "center of gravity" of the frequency transform of the data from every channel during an epoch. It was calculated as the frequency of the first pole of the AR model,

$$
\begin{equation*}
x_{i}(n)=\sum_{j=1}^{p} w_{j} \cdot x_{i}(n-j) \tag{6.2}
\end{equation*}
$$

where $w_{j}, j=1, \ldots, p$, are the parameters of the AR model. In this work, a second-order model $(p=2)$ was considered. This method of calculation of the centroid frequency is common in sleep staging [2].

## Alpha Slow-wave Index (ASI)

The ASI is the ratio of power in the alpha band $(8-11 \mathrm{~Hz})$ with respect to the power in the delta and theta band $(0.5-3.5 \mathrm{~Hz}$ and $3.5-8 \mathrm{~Hz}$, respectively):

$$
\begin{equation*}
\text { A SI at channel } i: \quad A S I_{i}=\frac{\bar{P}_{i, a l p h a}}{\bar{P}_{i, \text { delta } a}+\bar{P}_{i, \text { theta }}} \tag{6.3}
\end{equation*}
$$

where $\bar{P}_{i, a l p h a}$ is the power at the $i$-th channel during the epoch, considering only the power at the frequencies within the alpha band; and $\bar{P}_{i, \text { detta }}, \bar{P}_{i, \text { theta }}$ are defined likewise.

## Theta Slow-wave Index (TSI)

The TSI is the ratio of power in the theta band with respect the power in both the alpha and the delta bands:

$$
\begin{equation*}
\text { TS I at channel } i: \quad T S I_{i}=\frac{\bar{P}_{i, \text { theta }}}{\bar{P}_{i, \text { delta } a}+\bar{P}_{i, a l p h a}} \tag{6.4}
\end{equation*}
$$

### 6.1.1.b. Estimation of SICAMM parameters

The first half of the data was used to estimate the parameters of each method (ICAMM, SICAMM and Bayesian networks) in a supervised form, considering the labels provided by the expert. Due to the low number of features, G-SICAMM was not used. The ICAMM parameters, $\mathbf{W}_{k}, p\left(\mathbf{s}_{k}\right), \mathbf{b}_{k}$, were estimated from the training record by the JADE algorithm ( [231]) embedded in the MIXCA procedure. The transition probabilities between classes were also estimated from the training record, and they are shown in Table 6.1. Note that all the probabilities of permanence in the same class are clearly above 0.5 , justifying the use of sequential dependence in this application.

| Subject 1 | Subject 2 |  |  |  |  | Class 1 | Class 2 |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Class 1 | Class 2 |  | Class 1 | Class 2 |  |  |  |  |  |  |  |  |  |  |  |
| Class 1 | 0.98 | 0.02 | Class 1 | 0.96 | 0.04 | Class 1 | 0.97 | 0.03 |  |  |  |  |  |  |  |
| Class 2 | 0.31 | 0.69 | Class 2 | 0.20 | 0.80 | Class 2 | 0.06 | 0.94 |  |  |  |  |  |  |  |
| Subject 4 | Subject 5 |  |  |  |  |  |  |  |  |  | Class 1 | Class 2 |  | Class 1 | Class 2 |
|  | Class 1 | Class 2 |  | Class 1 | 0.97 | 0.03 | Class 1 | 0.99 |  |  |  |  |  |  |  |
| Class 1 | 0.91 | 0.09 | Class | 0.01 |  |  |  |  |  |  |  |  |  |  |  |
| Class 2 | 0.31 | 0.69 | Class 2 | 0.21 | 0.79 | Class 2 | 0.14 | 0.86 |  |  |  |  |  |  |  |

[^1]
### 6.1.2. Classification results

The performance of each method was initially measured by the error rate and the recall (or sensitivity) of the classification. However, the microarousals only occur during a very small amount of time every night. Since the proportion of class-2 segments is much smaller than the proportion of class-1 segments, the error rate and the recall were heavily dominated by class-1 errors. In sleep staging, this effect is usually compensated by using the balanced error rate. The BER is the average of the error rates for each class, and thus is more resistant with respect to classes with very different prior probabilities. Conversely, the recall was replaced by Cohen's kappa coefficient ( $\kappa,[58]$ ), a commonly-used tool to assess accuracy. Cohen's kappa takes into account different class probabilities, and is thus much more robust than the recall. In this work, the following definition of $\kappa$ for a classification with $K$ classes was used ( [41]):

$$
\begin{equation*}
\kappa=\frac{N \cdot \sum_{i=1}^{K} c_{i i}-\sum_{i=1}^{K} c_{i+} \cdot c_{+i}}{N^{2}-\sum_{i=1}^{K} c_{i+} \cdot c_{+i}} \tag{6.5}
\end{equation*}
$$

where $N$ is the number of classified samples; $c_{i i}$ is the number of correctly classified samples from class $i, i=1, \ldots, K ; c_{i+}$ is the number of samples that truly belong to class $i$; and $c_{+i}$ is the number of samples that were classified as class $i$.

The BER is bound in the interval $[0,1]$, and a low value is better than a high value. On the other hand, Cohen's kappa is bound in the interval $[-1,1]$ and a high value is better than a low value. Thus, a perfect result would have BER $=0$ and $\kappa=1$.

Table 6.2 shows the BER and kappa for the proposed methods for each subject, and Figure 6.2 shows the average results. Overall, the dynamic methods (SICAMM, DBN) performed better than the non-dynamic methods (BNT, ICAMM). SICAMM and its variants achieved the best result for all subjects, having the lowest BER and highest $\kappa$ in all cases. ICAMM obtained the second best result, although DBN performed at a similar level for some subjects. Finally, BNT achieved the worst results, particularly for Cohen's kappa coefficient. The proposed variants to SICAMM improved the base method and yielded better values of BER and $\kappa$, which is particularly noticeable in Figure 6.2. SICAMM+VI achieved the best results out of the two variants, and the best result out of all the proposed methods.

|  |  | ICAMM | SICAMM | SICAMM <br> +BW | SICAMM <br> +VI | BNT | DBN |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Subject <br> $\mathbf{1}$ | BER | 0.310 | 0.251 | 0.213 | 0.209 | 0.374 | 0.303 |
|  | Kappa | 0.145 | 0.326 | 0.333 | 0.351 | 0.259 | 0.255 |
| Subject | BER | 0.475 | 0.435 | 0.416 | 0.371 | 0.477 | 0.441 |
|  | Kappa | 0.026 | 0.098 | 0.112 | 0.180 | 0.058 | 0.103 |
| Subject | BER | 0.352 | 0.298 | 0.224 | 0.221 | 0.430 | 0.399 |
|  | Kappa | 0.326 | 0.400 | 0.534 | 0.543 | 0.152 | 0.221 |
| Subject | BER | 0.452 | 0.404 | 0.355 | 0.321 | 0.500 | 0.500 |
|  | Kappa | 0.116 | 0.213 | 0.309 | 0.380 | 0.000 | 0.000 |
| Subject | BER | 0.493 | 0.492 | 0.461 | 0.445 | 0.500 | 0.500 |
|  | Kappa | 0.020 | 0.024 | 0.115 | 0.158 | 0.000 | 0.000 |
| Subject | BER | 0.466 | 0.429 | 0.407 | 0.341 | 0.479 | 0.496 |
|  | Kappa | 0.117 | 0.204 | 0.200 | 0.286 | 0.020 | 0.013 |

Table 6.2. BER and Cohen's kappa for each subject.


Figure 6.2. Average BER and Cohen's kappa for all subjects.
The classifications achieved for each subject are compared with their respective reference hypnograms in Figure 6.3. The results are consistent with those in Table 6.2, with non-dynamic methods showing more false alarms than dynamic methods, as indicated by their BER and Kappa values. SICAMM and its variants obtained a result closer to the reference hypnogram than DBN. In particular, the proposed variants to SICAMM further reduce the number of false alarms of SICAMM while maintaining the good classification rate of the original method. This effect is more noticeable for subject 3 , since the hypnograms obtained by SICAMM+BW and SICAMM+VI were cleaner than the one obtained by SICAMM, and all three were in turn cleaner than the hypnogram returned by ICAMM.

### 6.1.3. Sensitivity analysis

The sensitivity of the parameters of the model with respect to time was measured using the procedure outlined in Section 4.5.3.b. In brief, SICAMM was trained using semi-batch learning on several overlapping windows of the data from each subject. The model for each window was then compared against the model from the previous window, in order to detect changes in the parameters of the model. Distances were measured using the three indicators presented in Section 4.5.1: the Amari index, the signal-to-interference ratio, and the Kullback-Leibler divergence (approximated by the probabilistic distance).

The obtained distance indicators for each time-consecutive pair of SICAMM models are shown in Figure 6.4. Since a high SIR implies a short distance between models, unlike the Amari index and the probabilistic distance, the Figure shows the value 1/SIR instead of the SIR. All of the indicators show some dependence on the presence or absence of microarousals, i.e., with the reference hypnogram. The estimated correlation with the reference hypnogram was 0.4362 , 0.3628 and 0.2828 for the $1 /$ SIR, Amari index and probabilistic distance, respectively; in all cases, $p \ll 0.05$. This demonstrates the sensitivity of the SICAMM parameters with respect to the sleep stages. Out of the three, the inverse of the SIR seemed to be the most sensitive to the presence of microarousals, since it had the greatest correlation with the reference hypnogram.

### 6.2. Analysis of EEG data captured during a working memory task

Working memory (WM) is defined as the temporary storage and manipulation of information, necessary for the performance of other cognitive tasks such as reading, problem-solving or learning [13]. The concept of WM evolved from that of short-term memory (STM), but the former is more involved than the latter. Research on WM is very popular in the field of cognitive psychology owing to its relation to memory and learning. WM is also very common in research, particularly in neuroimaging.


Figure 6.3. Microarousal detection for the examined subjects: a) subject $1 ; b$ ) subject 2 ; c) subject 3 ; d) subject 4 ; e) subject 5 ; f) subject 6 . For each method, a high value corresponds to a microarousal.

WM was conventionally considered to only hold temporary information, making it similar to STM and a separate system from the long-term memory (LTM) [13]. There are studies, however, that demonstrate the important role of WM during text comprehension and expert performance, thus involving several properties that are more akin to LTM than STM [78]. This is also considered in skill memory theory [51]. Recent WM models consider the connections between WM and LTM in a number of ways: a) through the existence of multiple biological links between WM and LTM [13]; b) modeling WM as an active subset of LTM [65]; or c) merging WM and LTM in a more complicated model [125].

The most commonly accepted model of WM is Multicomponent WM (M-WM, [13]). M-WM divides the working memory into four main components (see Figure 6.5): (i) phonological loop, which controls verbal STM and language; (ii) visuo-spatial sketch-pad, which stores visual and spatial information; (iii) episodic buffer, which holds entire experiences, episodes or events in STM and acts as storage for other WM and LTM elements; and (iv) central executive, which controls attentional focus, task switching, and decision making. Some criticisms of the M-WM are the high complexity of the central executive component and the evidence suggesting a separation between the visual and spatial components of WM [247].

Chapter 6- Application of G- and UG-SICAMM to EEG signal processing


Figure 6.4. Distance between time-consecutive pairs of SICAMM models for the six subjects: a) subject 1 ; b) subject 2 ; c) subject 3 ; d) subject 4 ; e) subject 5 ; f) subject 6 .


Figure 6.5. Multicomponent Working Memory model. Shadowed areas are part of the LTM rather than the WM.

Working memory and cognitive control functions have been associated most commonly with the prefrontal cortex (PFC) [34]. This idea is supported by PET studies that have shown activation of this region during a variety of cognitively demanding tasks, all of which can be thought to invoke short-term working memory. These tasks seem to activate similar regions of the PFC despite the fact that different types of information are involved. However, fMRI studies show that other areas do activate during WM tasks, particularly in prefrontal and parietal areas [34]. The fMRI studies provide more precise location, determining areas that relate to different WM tasks [272].

Studies on working memory test the subjects with different cognitive tasks. In this experiment, the subjects were performing the Sternberg memory task [251], one of the most well-known working memory tests. The Sternberg memory task was introduced in Section 5.4.2.

### 6.2.1. Experiment configuration

The data processing for this experiment can be split into a series of stages or modules, as shown in Figure 6.6. The process initiates with the capture of electroencephalographic data while the subject performs a working memory task. Once captured, data are pre-processed to remove noise and extract several features from them. These extracted features are used for data labeling by determining the activity of each hemisphere at each particular time sample. After the labels are calculated, the parameters of each method are estimated from the first half of the data. These parameters are used afterward to classify the second half of the data, i.e., to attempt to automatically determine the level of brain activity in each hemisphere. Finally, these classifications are compared against the previously-estimated labels to test the classification performance of our system. Each of these stages will be studied in depth in the following sections.


Figure 6.6. Diagram of the EEG data processing stages.

### 6.2.1.a. Data capture and EEG signal pre-processing

The data capture process was the same that was explained in Section 5.4.1. The captured signals were filtered to remove noise caused both by the environment and by the capture device. The filters are explained in Section 5.4.1 as well, and the locations of each one of the 64 electrodes is shown in Figure 5.19. After filtering, data are split into data segments of a short duration, known as epochs, to obtain local estimates of the features and improve the classification. Epochs were windowed prior to feature extraction to avoid high-frequency artifacts caused by the artificial separation of the data, attenuating the values of all channels at the beginning and
the end of the epoch. For this application, we considered epochs of length 0.1 seconds, which corresponds to 205 samples, and Hamming windows. Each epoch is treated as a separate observation with respect to the models and classifiers. Thus, a decision on the state of the subject was taken every 0.1 seconds.

### 6.2.1.b. Feature extraction

Twelve features were extracted from each epoch of the EEG data (see Table 6.3), and each was calculated separately for each channel and for each epoch. The features are explained in detail below. Note that the average amplitude, the centroid frequency, the TSI and the ASI were already introduced in Section 6.1.1.a.

| Kind of feature | Feature |
| :---: | :---: |
| Amplitude | Average amplitude |
|  | Maximum amplitude |
|  | Average power |
| Spectral | Centroid frequency |
|  | Peak frequency |
|  | Spindles ratio |
|  | TSI |
|  | ASI |
| Statistical | Skewness |
|  | Kurtosis |
|  | Time reversibility |
|  | Third-order autocovariance |

Table 6.3. List of features calculated from each epoch.

## Maximum amplitude

The maximum amplitude is the maximum absolute value of the voltage at every electrode during an epoch. It was calculated as

$$
\begin{equation*}
\text { maximum amplitude at channel } i: \quad x_{i}{ }^{M A X}=\max \left(\left|x_{i}(n)\right|\right), n=1, \ldots, N \tag{6.6}
\end{equation*}
$$

## Average power

The average power is the average quadratic value of the EEG signal during an epoch. It is calculated as

$$
\begin{equation*}
\text { average power at channel } i: \quad \overline{P_{i}}=\frac{1}{N} \sum_{n=1}^{N} x_{i}{ }^{2}(n) \tag{6.7}
\end{equation*}
$$

## Peak frequency

The peak frequency is the frequency which concentrates the maximum amount of energy in each channel for an epoch. Note that it is not necessarily equal to the centroid frequency, since the maximum frequency only searches for the energy at a single frequency, while the centroid frequency considers all points of the frequency spectrum. It is calculated as

$$
\begin{equation*}
\text { peak frequency: } \quad f_{i}^{M A X}=\max _{f}\left|X_{i}(f)\right|^{2} \tag{6.8}
\end{equation*}
$$

where $X_{i}(f)$ is the frequency spectrum of the $i$-th channel.

## Spindles ratio

Spindles are oscillatory bursts of brain activity in the sigma band $(11.5-15 \mathrm{~Hz})$. The spindles ratio is calculated as the ratio of power in the sigma band with respect to the power of the other EEG bands:

$$
\begin{equation*}
\text { Spindles ratio at channel } i: \quad I S_{i}=\frac{\bar{P}_{i, \text { sigma }}}{\bar{P}_{i}-\bar{P}_{i, s i g m a}} \tag{6.9}
\end{equation*}
$$

where $\bar{P}_{i, s i s m a}$ is the average power of the $i$-th channel during the epoch, considering only the power at the frequencies within the sigma band.

## Skewness

The skewness or asymmetry is a statistical indicator of how asymmetrical a probability density function is with respect to its mean. A skewness close to zero indicates a symmetrical PDF, while a skewness far from zero (be it negative or positive) indicates an asymmetrical PDF. It is calculated as

$$
\begin{equation*}
\text { Skewness at channel } i: \quad \gamma_{1, i}=\frac{1}{N} \sum_{n=1}^{N} \frac{\left(x_{i}(n)-\bar{x}_{i}\right)^{3}}{\sigma_{i}{ }^{3}} \tag{6.10}
\end{equation*}
$$

where $\sigma_{i}$ is the standard deviation at the $i$-th channel.

## Kurtosis

Kurtosis is a statistical indicator of how "peaked" a probability density function is. It is usually normalized with respect to a Gaussian distribution, which corresponds to an un-normalized kurtosis of 3. A PDF that is very sharp around its mean, but shows very long tails, will have a kurtosis greater than that of a Gaussian distribution; it is known as "super-Gaussian". Conversely, a distribution that is smoother around its mean, with smaller tails, will have a kurtosis lower than that of a Gaussian distribution and be known as "sub-Gausian". It is calculated as

$$
\begin{equation*}
\text { Kurtosis at channel } i: \quad \gamma_{2, i}=\left\{\frac{1}{N} \sum_{n=1}^{N} \frac{\left(x_{i}(n)-\bar{x}_{i}\right)^{4}}{\sigma_{i}^{4}}\right)-3 \tag{6.11}
\end{equation*}
$$

where the 3 is a normalization factor, and is equal to the kurtosis of a Gaussian distribution.

## Time reversibility

The time reversibility of a signal is an indicator of how symmetrical with respect to time is the signal in each channel during an epoch. A symmetrical signal has time reversibility equal to zero, and an asymmetrical signal has larger time reversibility. It is calculated as

$$
\begin{equation*}
\text { Time reversibility at channel } i: \quad T R E V_{i}=\frac{1}{\sigma_{i}{ }^{3}} \cdot \frac{1}{N-\tau} \cdot \sum_{n=1+\tau}^{N}\left[x_{i}(n)-x_{i}(n-\tau)\right]^{3} \tag{6.12}
\end{equation*}
$$

where $\tau$ is the considered lag (in this work, $\tau=1$ ).

## Third-order autocovariance

The third-order autocovariance (ACOV3) is an extension to high-order statistics of the classical self-covariance of a signal, and equally considers temporal dependences in the signal. It is calculated as a sliding average of the third-order moment,

$$
\begin{align*}
& \text { Third-order autocovariance at channel } i \text { : } \\
& A \operatorname{CoV} 3_{i}=\frac{1}{N-2 \tau} \sum_{n=1+2 \tau}^{N} x_{i}(n) \cdot x_{i}(n-\tau) \cdot x_{i}(n-2 \tau) \tag{6.13}
\end{align*}
$$

where $\tau$ is the considered lag (in this work, $\tau=1$ ).

### 6.2.1.c. Epoch labeling

After feature extraction, each epoch is assigned to one class, i.e., gets labeled. This process is necessary for supervised or semi-supervised estimation. Although it is possible to train some methods with fully unlabeled data (unsupervised estimation), the performance increases with known labels. In most cases, data are labeled by an expert so they are ready for training and testing, or the labels are previously known due to the nature of the experiment (for instance, if they are the stages of a test). In this work, all epochs were automatically labeled using the process outlined in the following.

Each epoch was assigned two labels, one for each brain hemisphere, representing the level of activity in the corresponding brain region. The process was performed separately for each brain hemisphere, i.e., the channels on the left hemisphere were only used to label the left side of the brain, and the channels on the right hemisphere were only used to label the right side of the brain (Figure 5.19 shows the location of each of the capture electrodes). The central channels of the captures EEG $(\mathrm{FPz}, \mathrm{AFz}, \mathrm{Fz}, \mathrm{FCz}, \mathrm{Cz}, \mathrm{CPz}, \mathrm{Pz}, \mathrm{POz}, \mathrm{Oz}, \mathrm{Iz})$ were ignored for the purposes of labeling. This assignment results in 27 channels per hemisphere for labeling purposes.

At each epoch, the features of each group of channels are combined together using a fusion algorithm. Then, this fused channel is compared with its own time average for all epochs. Epochs above the average were labeled as active (class 2), and epochs below the average were labeled as inactive (class 1). This process is performed separately for each hemisphere, as explained before. After this process was finished, the resulting labels were used for training, and testing the proposed methods.

The fusion algorithm itself does not have any particular restriction, other than having a singlechannel output and returning one value per epoch. In this work, we considered the sample average of the features of the selected input channels. That is, we take the values of one or more of the extracted features for all the channels of a given hemisphere and average them to obtain the fused channel.

The training procedure is summarized in Figure 6.7.


Figure 6.7. Diagram of the behavior of the labeling stage at each epoch.

In the case of methods that cannot work with multiple labels per observation (ICAMM, SICAMM, BNT and DBN), the labels were converted into four equivalent labels, each one equivalent to a combination of the labels of each hemisphere ( $00,01,10$ and 11).

### 6.2.1.d. Labeling results

In this section, we will present a selection of the labels assigned from captured data by using the process described in Section 6.2.1.c. The labels are shown in Figure 6.8 for five healthy subjects. The stages of the experiment have been simplified into two classes, memorization (class 1) and response (class 2).

For all subjects, the obtained labels show small but significant correlation with the stages of the experiment. Numerically, correlations ranged between 0.06 and 0.3 , though they were statistically significant $(p<0.05)$ in all cases. It can be seen that the labels change much faster


Figure 6.8. Sample of the labels for five of the subjects, using different features in each case.


Figure 6.9. Detail of the labels for one of the subjects (subject from Figure 6.8.b).
than the stages of the experiment but are still correlated with them, as shown in Figure 6.9. This faster variation persists even if we change the fusion algorithm or the threshold, and even if we change the features selected for labeling.

### 6.2.1.e. Training and testing

The EEG data of each subject were split into two sets. The central $30 \%$ of the data was used for training, and the remaining $70 \%$ was used for testing the classification performance of the proposed methods (see Figure 6.10). The selection of the central $30 \%$ of the data was done so as to minimize any possible difference caused by a lack of concentration of the subject at the beginning or at the end of the experiment.


Figure 6.10. Diagram of the data split into classification and testing sets.
As in the case of the labeling process, the system can use one or more of the extracted features in order to classify data. If more than one feature is selected, the system considers the features as extra channels. Note that the features selected for training and for classification must be the same, but can be different from the ones selected for labeling.

For the methods with two chains (G-SICAMM and DBN2), the channels from each feature were separated according to their hemisphere. The channels from the left side of the brain were assigned to the left hemisphere and channels from the right side of the brain were assigned to the right hemisphere. Central channels ( $\mathrm{FPz}, \mathrm{AFz}, \mathrm{Fz}, \mathrm{FCz}, \mathrm{Cz}, \mathrm{CPz}, \mathrm{Pz}, \mathrm{POz}, \mathrm{Oz}, \mathrm{Iz}$ ) were ignored with respect to data training and classification. Thus, G-SICAMM and DBN2 considered 27 channels per hemisphere. The rest of the proposed methods worked with all 64 channels.

Once training and classification data were selected, we performed PCA on the selected features [124]. The number of components to keep, $M^{\prime}$, was estimated so the sum of the explained variances of the selected components was at least $95 \%$ of the total variance in the original data. This selection means that the number of components changes depending on the subject, as well as the number of selected features for training and testing. In the case of methods with two chains (G-SICAMM and DBN2), since they have different datasets for each hemisphere, a different PCA was calculated for each hemisphere.

The parameters for each of the proposed methods were estimated as follows. G-SICAMM was with two chains and two classes per chain ( $K=2$ and $L=2$ ). For the SICAMM and ICAMM, a single model was fitted for the data from both hemispheres, that is, the model is fit to $\mathbf{x}(n)=\left[\mathbf{x}_{1}(n)^{T}, \mathbf{x}_{2}(n)^{T}\right]^{T}$. As explained in Section 6.2.1.c, in order to compare these models with the one obtained with G-SICAMM, SICAMM and ICAMM considered four classes ( $K=$ 4), one class per combination of classes from each chain (both hemispheres inactive, left hemisphere active, right hemisphere active, and both hemispheres active). In all cases, parameter estimation was performed with supervised training using the estimated labels with the JADE algorithm ( [231]) embedded in the MIXCA procedure.

The configuration of the dynamic Bayesian network was dynamically adjusted to the data. Three types of DBN were considered, each one similar to one of the ICA-based methods: a network without temporal dependence (BNT), a single network with a HMM (DBN1), and a network with a two-chain CHMM (DBN2). The configuration of these methods was similar to that of the ICAMM-based methods: for the DBN2, two chains were considered, each one with two states ( $K=2$ and $L=2$ ); and DBN1 and BNT were adjusted considering four states, $K=4$. Node probabilities were modeled using a Gaussian Mixture Model (GMM) with a variable number of mixtures for each node. The number of mixtures for each node was determined by testing several GMM with an increasing number of classes (3 to 20) and choosing the model with a lower Akaike Information Criterion. In this work, most GMM ended up with seven to ten components.

### 6.2.2. Classification results

The performance of the classification of the state of each brain hemisphere can be evaluated in one of two ways. The first would be to determine the number of samples which are correctly classified for both hemispheres at the same time. In practice, this is a classification problem with four classes, since there are four possibilities: (i) both hemispheres inactive; (ii) left active and right inactive; (iii) left inactive and right active; and (iv) both hemispheres active. However, the performance of the classification could also be evaluated separately for each hemisphere, i.e., counting how many times has a hemisphere been correctly classified as active or inactive. This second case is thus a two-class classification case. This Section explores both evaluations of the performance of each classification.

Regardless of the number of classes, classification performance is usually estimated from their confusion matrix (or error matrix), a matrix defined such that its element $(i, j)$ is equal to the number of observations that truly belong to class $i$ and have been labeled as class $j$ by the method. A good classifier should have a diagonal or close-to-diagonal confusion matrix. Table 6.4 and Table 6.5 show two examples of confusion matrices for four-class and two-class classification, respectively. Note the largely uneven distribution of the true classes. For instance, the case shown in Table 6.4 had 1483 values that belonged to class 00 (both hemispheres inactive), but only 112 that belonged to class 11 (both hemispheres active). Therefore, the performance of the classification was estimated with the balanced error rate, an indicator that is robust with respect to differences in class probability.

Table 6.6 shows the BER of the four-class classification obtained by each of the proposed methods. To unify results, all subjects were labeled using the same feature (average power) and classified using the same two features (centroid frequency and spindles ratio). Although the BER is somewhat large, note that the average BER of a trivial classifier would be $75 \%$ because of the four classes. Out of all the proposed methods, only SICAMM, G-SICAMM and their variants performed significantly better than the base performance. G-SICAMM+VI achieved the best result, an average BER of $54.49 \%$ across all subjects. Overall, dynamic methods yielded better results than non-dynamic methods.

Performance increases if we consider two-class classification (i.e., the success rate in determining if a hemisphere is active or not). In this case, there are only two classes and the trivial classifier would yield a $50 \%$ average BER. The results for this second case are shown in Table 6.7. Other than the decrease in BER, the relative performance of all methods is in concordance with that for the case with four classes. Again, the best result was obtained by one of the variants of G-SICAMM, in this case, G-SICAMM+BW with an average BER of $25.91 \%$. The proposed variants to SICAMM and G-SICAMM generally improve the result of their respective basic methods.

Besides classification, ICAMM-based methods can also be used to obtain a generative model for EEG data that can be interpreted on its own. Figure 6.11 shows the obtained model after

|  |  | Estimated classes |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  | $\mathbf{0 0}$ | $\mathbf{0 1}$ | $\mathbf{1 0}$ | $\mathbf{1 1}$ |
| True |  |  |  |  |  |
| classes | $\mathbf{0 0}$ | 1154 | 118 | 30 | 181 |
|  | $\mathbf{0 1}$ | 107 | 135 | 11 | 126 |
|  | $\mathbf{1 0}$ | 24 | 4 | 130 | 13 |
|  | $\mathbf{1 1}$ | 19 | 2 | 4 | 87 |

Table 6.4. Typical confusion matrix for G-SICAMM (subject 1), depending on the state of both hemispheres.

|  | Estimated class |  |  |
| :---: | :---: | :---: | :---: |
| True class |  | $\mathbf{0}$ |  |
|  | $\mathbf{0}$ | 2854 |  |
|  | $\mathbf{1}$ | 190 |  |
|  | 1964 |  |  |

Table 6.5. Typical confusion matrix for G-SICAMM (subject 2), considering only within-hemisphere transitions.

| Method | Subject 1 | Subject 2 | Subject 3 | Subject 4 | Subject 5 | Average |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ICAMM | 76.07 | 61.57 | 72.70 | 69.52 | 75.66 | 71.11 |
| SICAMM | 63.60 | 55.78 | 64.91 | 64.17 | 65.46 | 62.78 |
| SICAMM+BW | 64.09 | 56.06 | 63.60 | 63.96 | 63.65 | 62.27 |
| SICAMM+VI | 64.13 | 55.99 | 64.85 | 63.96 | 62.88 | 62.36 |
| G-SICAMM | 52.96 | 51.42 | 54.86 | 57.83 | 57.23 | 54.86 |
| G-SICAMM+BW | 51.76 | 51.86 | 54.60 | 58.24 | 56.19 | 54.53 |
| G-SICAMM+VI | 51.94 | 51.64 | 54.49 | 58.20 | 56.20 | 54.49 |
| BNT | 75.00 | 75.00 | 75.00 | 75.00 | 75.00 | 75.00 |
| DBN | 75.02 | 75.00 | 75.00 | 74.72 | 75.00 | 74.95 |
| DBN2 | 73.43 | 62.74 | 75.00 | 59.74 | 75.02 | 69.19 |

Table 6.6. BER for four-class classification of the data from all the subjects. The EEG were labeled using one feature (average power) and classified using two features (centroid frequency and spindles ratio).

| Method | Subject 1 | Subject 2 | Subject 3 | Subject 4 | Subject 5 | Average |
| :---: | ---: | :---: | :---: | :---: | :---: | :---: |
| ICAMM | 51.91 | 35.38 | 36.52 | 38.98 | 59.67 | 44.49 |
| SICAMM | 42.17 | 17.48 | 45.31 | 38.62 | 45.22 | 37.76 |
| SICAMM+BW | 42.45 | 17.39 | 45.27 | 38.42 | 45.56 | 37.82 |
| SICAMM+VI | 42.45 | 17.39 | 45.74 | 38.42 | 45.69 | 37.94 |
| G-SICAMM | 30.18 | 11.71 | 34.32 | 21.77 | 33.36 | 26.27 |
| G-SICAMM+BW | 29.14 | 11.89 | 34.40 | 21.94 | 32.17 | 25.91 |
| G-SICAMM+VI | 29.98 | 11.89 | 34.18 | 21.94 | 32.17 | 26.03 |
| BNT | 50.00 | 50.00 | 50.00 | 50.00 | 50.00 | 50.00 |
| DBN | 50.04 | 50.00 | 50.00 | 49.85 | 50.00 | 49.98 |
| DBN2 | 48.78 | 36.43 | 49.15 | 30.32 | 48.97 | 42.73 |

Table 6.7. Balanced error rate for each hemisphere when classifying data from several subjects. The EEG were labeled using one feature (average power) and classified using two features (centroid frequency and spindles ratio).
estimating the G-SICAMM for one of the subjects using a one-second data window as training data. The de-mixing matrices for both hemispheres have 23 channels, since the PCA preprocessing reduced the 27 EEG channels to 23 components. Figure 6.12 is similar, but it shows the model obtained for SICAMM during the same time interval. Note that de-mixing matrices are larger for SICAMM, since it works with both hemispheres at the same time, while GSICAMM considers each hemisphere separately, resulting in smaller de-mixing matrices and less sources. In both cases, the model was trained as explained in Section 6.2.1.e.


Figure 6.11. De-mixing matrices (first row) and sources (subsequent rows) extracted after training the G-SICAMM. For each source, both the amplitude values (blue) and the histogram (black) are shown. The values indicated over each histogram are the kurtosis of each source. De-mixing matrices were composed of 23 rows and columns (reduced from the 27 EEG channels using PCA), so 23 sources were recovered - the Figure plots only the first three sources from each class for the sake of brevity. The number of samples in each source was different for each class, since the 2068 epochs available for training were not equally distributed between classes. The sources from inactive classes have 1622 and 1634 samples (left and right hemisphere, respectively), while the sources from active classes have 446 and 434 samples (left and right hemisphere, respectively).


Figure 6.12. De-mixing matrices (first row) and sources (subsequent rows) extracted after training the G-SICAMM. For each source, both the amplitude values (blue) and the histogram (black) are shown. The values indicated over each histogram are the kurtosis of each source. De-mixing matrices were composed of 52 rows and columns (reduced from the 64 EEG channels using PCA), so 52 sources were recovered - the Figure plots only the first three sources from each class for the sake of brevity. The number of samples in each source was different for each class, since the 2068 epochs available for training were not equally distributed between classes. From left to right, each class was composed of $940,569,366$, and 193 samples.

The plots in Figure 6.11 and Figure 6.12 show that the the activity in the right hemisphere was more diffuse (their de-mixing matrices are more diffuse), indicating a higher spatial dispersion in the brain activity. They also show that when a hemisphere did activate, its sources became less Gaussian (their kurtoses rose), indicating a change in the probability densities of the recovered sources.

### 6.2.3. Sensitivity analysis

Besides the proposed analysis system, a test was carried out to measure the changes in the parameters of the model with respect to time. To this end, the G-SICAMM was trained multiple times, each time using a higher number of training data until all available data were used for training. Then, we calculated the distances between the parameters in each time step, looking for significant differences in the estimated models.

The G-SICAMM parameters, as explained previously, are the following: the de-mixing matrices $\mathbf{w}_{k_{l}}$, sources $p\left(\mathbf{s}_{k_{l}}(n)\right)$, and centroids $\mathbf{b}_{k_{l}}$, for each class $k_{l}=1, \ldots, K_{l}$ from each chain $l=1, \ldots, L$; and the transition probabilities between states of the system, $P\left(\mathbf{c}_{\mathbf{k}}(n) \mid \mathbf{c}_{\mathbf{k}^{\prime}}(n-1)\right)$. The sources, $s_{k_{1}}(n)$, can be considered as activation functions, in which case the mixing matrices $\mathbf{A}_{k_{1}}=\mathbf{W}_{k_{1}}{ }^{-1}$ could be taken as activation patterns or "scalp maps." These parameters can thus be used to locate and characterize EEG activity using the model. Accordingly, differences in the model should allow us to identify changes in the brain activity of the subject.

The G-SICAMM parameters for each epoch were estimated as explained above, and then we calculated the distances between each consecutive pair of these models. The best results for a single subject are shown in Figure 6.13 (Amari index) and Figure 6.14 (SIR). It is shown that the variations in the Amari index show some correlation with the changes in class in the subject, while the SIR does not seem to be dependent on these classes or on their changes. To better show the correlation of the Amari index and class changes, Figure 6.15 displays just a small amount of distances, in order to better interpret the results. It is shown that changes in the class usually correspond to increments in the Amari index, particularly in the case of changes to and from class 4 (both hemispheres active).

From the three considered distance indicators, the Amari index (i.e., the distance between demixing matrices) is the one that resulted more sensitive to changes in the classes - that is,


Figure 6.13. Distance between de-mixing matrices (Amari index) of each pair of consecutive models. The training data for the second model were one epoch longer that the training data for the first model. Four classes were considered: 1- both hemispheres inactive; 2 - left hemisphere active, right hemisphere inactive; 3-left hemisphere inactive, right hemisphere active; 4 - both hemispheres active.
changes in the brain activity of the subject. This outcome matches the result from previous sections (see Figure 6.11 and Figure 6.12), where the G-SICAMM parameter that changed the most between classes was indeed the de-mixing matrix. At any rate, these results suggest that there is a dynamic variation in the model, variation which is related to the brain activity of the subject during the memory task. A future line of work is the application of these indicators to the rest of the subjects, in order to confirm the detection capabilities of the Amari index.


Figure 6.14. Distance between recovered sources (SIR) of each pair of consecutive models. The training data for the second model were one epoch longer that the training data for the first model. Four classes were considered: 1- both hemispheres inactive; 2- left hemisphere active, right hemisphere inactive; 3- left hemisphere inactive, right hemisphere active; 4- both hemispheres active.


Figure 6.15. Sample section of the distance between de-mixing matrices (Amari index).

### 6.3. Analysis of EEG data from neurophysiological tests

In this section, we model the dynamics of brain waves using multimodal data from electroencephalographic, electrocardiographic and electromyographic (EMG) signals. These signals were taken from subjects that were performing memory tests. In particular, we search for changes in the connectivity between brain areas during the memory tasks. This kind of tests is an essential area of clinical neurophysiology. The evaluation of the learning and memory functions of the patient is an unavoidable part of their neuropsychological assessment. Information cannot be processed if the brain is unable to store a certain amount of it in shortterm (working) memory or to recall past experiences, events and strategies from long-term memory. Conversely, information stored in short- or long-term memory is useless without the means to properly access and activate it.

Most of our day-to-day activities require that we make use of information stored in our brains, such as previous knowledge and successful strategies. Any problem while accessing that information will disrupt the flow of the activity. Conversely, learning is a vital part of many situations in life, from childhood to professional life. The inability to learn new concepts interferes not only with the subject's academic learning, but also with their capability to adapt to new environments. For instance, a worker with learning disabilities would find it harder to adapt to a new job, thus reducing his performance and limiting his career development [1]. Similarly, students with learning disabilities experience a much higher dropout rate than non-disabled students [235].This kind of problems motivate the development and maintenance of tests to evaluate the memory function.

Memory and learning disabilities can be produced by a number of conditions, from normal aging to a vast array of neurological or psychiatric pathologies, such as dementia, brain tumors, alcoholism, depression, and schizophrenia. Brain damage in particular will usually result in memory and learning impairments. Furthermore, the rehabilitation process of any patient is dependent on his ability to retain new information. Therefore, it is imperative that memory and learning alterations are diagnosed as soon as possible in order to cure or mitigate the underlying cause(s). This diagnosis requires detailed evaluation of the cognitive functions of the patient, including his memory system. To recapitulate, careful study of the learning and memory systems of the brain can help to determine the causes of problems such as low academic performance, dropping out of school or college, job problems and failure when adapting to new jobs or new environments. Furthermore, the obtained information can help to determine the best rehabilitation program for the patient.

Memory tests are usually split in two stages, presentation/retention and test. In the first stage, the subject is shown several stimuli that he must memorize. These stimuli can be visual (characters, symbols, figures...) or auditory (words, tones...). Nowadays, the tests are performed manually under the direct supervision of a neuropsychologist. Therefore, the data capture process is not synchronized with the test or with the annotations on the test. Since data analysis requires that all these kinds of information be synchronized with each other, we have automatized a number of these neurophysiological tests, as seen in Figure 6.16.


Figure 6.16. Diagram of the memory and learning testing system.
From the many available neuropsychological tests (see [253,142] for an exhaustive collection), we selected the ones shown in Table 6.8 for implementation. The implemented tests were the ones most commonly used by the Neuropsychology Unit in the Hospital Universitari $i$ Politècnic (HUP) La Fe, Valencia (Spain). Table 6.8 shows three levels of process automation
for the tests: full, partial, and synch-only. Fully-automated tests are completely implemented on the computer and require no work from the neuropsychologist. Partially-automated tests are also automated, but they require some degree of collaboration on the part of the neuropsychologist. Only-synchronized ("synch-only") tests are not implemented on the computer, which is only used to synchronize the test with the data and the annotations.

### 6.3.1. Neuropsychological tests

The implemented tests are explained in brief in this Section in order to make this chapter more self-contained. The Sternberg test, also known as Sternberg memory task, was presented in Section 5.4.2.

Most of the implemented tests include both the immediate and the delayed "conditions" or paradigms. In the immediate condition, the stimulus is presented to the participant just before the task. In the delayed condition, there is a longer delay (typically 20 minutes) after the stimuli are presented and before the participant is told the task to perform. Typically, the immediate condition is used to assess working or short-term memory, whereas the delayed condition is more appropriate to evaluate long-term memory.

| Name |  | Stimuli | Automation | Studied brain functions |
| :---: | :---: | :---: | :---: | :---: |
| Test de Aprendizaje Verbal EspañaComplutense (TAVEC, [20]) |  | Auditory | Full | Auditory memory |
| Wechsler Memory Scale-R (WMS-R) | Visual Paired Associates | Visual | Full | Visual memory |
|  | Figural Memory | Visual | Full | Visual working memory |
| Wechsler Memory Scale III (WMSIII) | Verbal Paired Associates | Auditory | Full | Auditory memory |
|  | Visual Reproduction | Visual | Full | Visual memory |
|  | Mental Control | Auditory | Synch-only | Executive |
| Wechsler Adult Intelligence Scale (WAIS-III) | Digit Span | Auditory | Full | Auditory working memory |
|  | $\begin{gathered} \hline \text { Digit } \\ \text { Symbol- } \\ \text { Coding } \\ \hline \end{gathered}$ | Visual | Full | Processing speed |
|  | Symbol Search | Visual | Full | Processing speed |
| Barcelona Neuropsychological Test (TB, [197]) | Visual Memory | Visual | Full | Visual working memory |
| Stroop Color Word |  | Visual | Synch-only | Executive |
| Trail Making |  | Visual | Full | Attention |
| Boston Naming |  | Visual | Partial | Language |
| Verbal Fluency | Phonemic | Auditory | Synch-only | Executive |
|  | Semantic | Auditory | Synch-only | Executive |
| Sternberg [251] |  | Visual | Full | Visual working memory |

Table 6.8. Implemented neuropsychological tests. Tests were taken from [253] unless otherwise noted.

### 6.3.1.a. Test de Aprendizaje Verbal España-Complutense (TAVEC)

The Test de Aprendizaje Verbal España-Complutense (TAVEC, [20]) is a neuropsychological test of auditory working memory and long-term memory. Based on the Rey Fifteen-Item Test (FIT, [142]), the TAVEC introduces knowledge about neurocognitive models of the memory function to interpret the results of the test [20]. This interpretation surpasses the "multi-storage" model and integrates into modularity-of-mind theories. The TAVEC allows determining the "normality" of a patient when compared against a similar normed sample and determining the possible causes of any deviation. It is used for differential diagnosis of memory alterations such as dementia, cognitive loss, traumatic brain injuries (TBI), and epilepsy.

The TAVEC comprises three different lists, Learning (list A), Interference (list B), and Recall. In this work, only the Learning and Interference lists were implemented. Lists A and B are composed of 16 words from four semantic categories, two in common for both lists ("spices" and "fruit") and two exclusive to each list: "tools" and "clothing" for list A; "fish" and "kitchen utensils" for list B. In the immediate condition, the Learning list is read and the participant is asked to repeat as many words as possible in any order. This process is repeated 5 times. The Interference list is then read and the participant is required to repeat as many words as possible from it. Finally, the participant is asked to recall the words from list A without listening to it. In the delayed condition, the participant is asked to repeat as many words as possible from list A. Scoring is calculated depending on the number of recalled items and the number of errors.

### 6.3.1.b. Wechsler Memory Scale

The Wechsler Memory Scale (WMS, [253]) is a neuropsychological test developed to detect and evaluate memory disorders in adults and older adolescents. The original WMS was published by Dr. David Wechsler in 1945, and it has been revised several times through the years. The first revision, WMS-R, includes nine sub-tests and five indices that measured different types of memory: Verbal Memory, Visual Memory, Delayed Recall, Attention/Concentration, and General Memory. The next revision, WMS-III, added sub-tests to assess delayed recognition memory and replaced abstract visual designs with pictures of everyday stimuli (e.g., the Faces sub-test). The test includes eleven sub-tests, from which eight primary index scores are derived. The WSM can be used to assess the clinically relevant aspects of memory functioning. For example, it can be used to detect and localize cerebral dysfunction and it can aid in detecting dementias and neurodegenerative disorders. Research suggests that the primary indices of the WMS-III can accurately identify malingering of neurocognitive dysfunction in mild TBI.

As shown in Table 6.8, five sub-tests were implemented: Visual Paired Associates and Figural Memory (from WMS-R), and Verbal Paired Associates, Visual Reproduction and Mental Control (from WMS-III).

The Visual Paired Associated sub-test evaluates visual memory and cued recall. It includes six pairs of an abstract figure and a color. In the immediate condition, the participant is shown the six pairs in succession. Afterward, the figures are shown one by one and the participant is told to provide the corresponding color for each figure. There are three trials of the same pairs in different orders. In the delayed condition, the examinee is shown the same figures and is asked to choose the corresponding colors. Scoring is calculated from the number of correct pairs.

The Figural Memory sub-test is an immediate recognition test of abstract designs. The participant is shown a set of three abstract figures, rectangles with a pattern of shapes inside them, for 10 seconds. Afterward, the examinee is shown a set of nine similar figures from which they have to select the three figures they were shown before. There are three trials of increasing difficulty. Scoring is calculated from the number of correctly-selected figures.

The Verbal Paired Associates sub-test evaluates auditory memory and cued recall. It is composed of 10 to 14 word pairs; half of these pairs are semantically related (e.g., rose-flower) and the other half are unrelated (e.g., cauliflower-pencil). In the immediate condition, after the word pairs are read, the first word of each pair is read and the participant is told to provide the corresponding word. There are three to six trials of the same list in different orders. In the delayed condition, the examinee is orally presented with the first word of each pair learned in the immediate condition and asked to provide the corresponding word. Scoring is calculated from the number of correct pairs.

The Visual Reproduction sub-test assesses memory for non-verbal (i.e., abstract) visual stimuli. In the immediate condition, the participant is shown a series of five designs for 10 seconds each. After each design is presented, the participant is asked to draw the design from memory. In the delayed condition, the examinee is asked to draw the designs shown during the immediate condition from memory in any order. The result of the sub-test is calculated by a methodical comparison of the copied figures and the original ones.

In the Mental Control sub-test, the participant is asked to perform seven verbal tasks of increasing difficulty: i) counting from 1 to 20 ; ii) reciting the alphabet; iii) listing the days of the week; iv) saying the months of the year; v) counting down from 20 to 1 ; vi) saying the days of the week in reverse order; vi) saying the months of the year in reverse order; vii) counting from 0 to 36 by sixes and reciting the days of the week in alternating order ( 0 -Monday, 6-Tuesday, and so on until 36 -Sunday). Scoring is calculated from the number of mistakes and the time taken to complete each task.

### 6.3.1.c. Wechsler Adult Intelligence Scale

The Wechsler Adult Intelligence Scale (WAIS, [253]) is a test designed to measure intelligence in adults and older adolescents. The first edition of the test was created in 1939, and it was named the Wechsler-Bellevue intelligence scale (WB); later editions changed the name of the test. It was developed by Dr. David Wechsler to replace the then-dominant Stanford-Binet scale of intelligence. The third edition of the test (WAIS-III), unlike previous editions, measures intelligence based on four factorially-derived indices. These indices enhance its clinical relevance for differential diagnosis of conditions that are linked with intelligence, such as brain injuries or learning disabilities. In neuropsychological assessment, the WAIS-III can: a) diagnose cognitive disorders and identify brain dysfunction; b) track changes in cognitive function over time; c) identify cognitive strengths and weaknesses important for daily functioning. The test comprises seven verbal sub-tests and six non-verbal (performance) subtests. Out of these, one verbal sub-test and two performance sub-tests were implemented, as shown in Table 6.8: Digit Span, Digit Symbol-Coding, and Symbol Search.

The Digit Span sub-test is split in two stages. In the first one, called Digit Span Forward, the participant is read a sequence of numbers and then recalls the numbers in the same order. During the second stage, Digit Span Backward, the participant is read a sequence of numbers and recalls the numbers in reverse order. In both stages, the objective is recalling correctly as many sequences as possible.

In the Digit Symbol-Coding sub-test, the numbers 1 to 9 are paired with symbols on a key. The participant is given the key and asked to go through a grid numbers and select the correct symbols for each number. The sub-test is timed and scoring is given depending on the amount of correct responses and the number of mistakes.

In the Symbol Search sub-test, the participant indicates whether one of the symbols in the target group matches any of the symbols in the search group. This process is repeated as many times as possible within a specified time limit, and scoring is given depending on the amount of correct responses.

### 6.3.1.d. Barcelona Neuropsychological Test

The Barcelona Neuropsychological Test (TB, [197]) or Programa Integrado de Exploración Neuropsicológica (PIEN) is a battery of tests designed in Spain in 1977 to evaluate higher mental functions in such a way as to advance clinical knowledge of neuropsychological patients. It is one of the first neuropsychological tests developed in Spain. It is a comprehensive test that considers a high number of mental functions, such as: attention, language, orientation, visual memory, and abstraction capability. It comprises 106 subtests split in 42 categories, and the whole TB takes about 3 hours to complete. Successive revisions of the TB have reduced the run time and complexity of the test, such as the abbreviated Barcelona test (TB-A, [198]). Only the Visual Memory sub-test of the TB was implemented, as shown in Table 6.8.

In the Visual Memory sub-test, the participant is shown an abstract line figure during 10 seconds. Afterward, the participant is told to select the shown figure out of a group of four similar figures. There are ten series in this sub-test, and scoring is given depending on the number of correct responses.

### 6.3.1.e. Stroop Color Word Test

The Stroop Color Word Test (SCWT, [253]) is based on the Stroop effect, discovered in 1935 by its namesake, Dr. John Ridley Stroop. In brief, the Stroop effect consists in that we are able to read words more quickly and automatically than we can name colors. For instance, if one is presented with the word "blue" printed in red ink, he will say the word "blue" more readily than he can name the color in which it is printed, red. The SCWT uses this effect to assess the ability of an individual to inhibit a habitual response for one that is less readily available. It provides insight into cognitive effects that are experienced as a result of attentional fatigue. Also, performance in the SCWT is lower in patients with dementia and in individuals with frontal lobe versus posterior lesions and left versus right hemisphere lesions.

The SCWT is composed of three stages, Color, Word, and Color-Word. In the first stage, Color, the participant is given a sheet of paper with a $5 \times 20$ grid of bars that are colored red, green or blue. Participants are instructed to say the color of each bar going down the columns. In the Word stage, the bars are replaced with color words (red, green, blue) in black type, and the participant is required to read the words. Finally, in the Color-Word stage, each word is printed in a color that differs from the written word (e.g., the word "red" will be printed in blue or green, not in red). The participant is instructed to say the color of the item, not the written word. Participants are given 45 seconds for each stage, with scoring being given by the number of correct responses.

### 6.3.1.f. Trail Making Test

The Trail Making Test (TMT, [253]) is a neuropsychological test of attention, processing speed, and task switching. It was developed in 1938 by US Army psychologists, and adapted to civil use in 1955. The TMT is one of the best measures of attention and one of the most popular neuropsychological tests. The test is highly sensitive to brain injury, and it can be used for differential diagnosis of several conditions, such as alcoholism and learning disabilities.

The TMT has two parts, A and B. In part A, participants are instructed to connect 25 encircled numbers that have been randomly placed on a page. The numbers have to be connected in proper order within 5 minutes, without making mistakes or lifting the pencil from the paper. In part B , the participants are required to connect 25 encircled numbers and letters in alternating order, again within 5 minutes. In both parts, participants are instructed to connect the circles as fast as they can. The test is scored based on the time taken to complete each part. The number of errors may be clinically relevant, but it is not a separate score.

### 6.3.1.g. Boston Naming Test

The Boston Naming Test (BNT, [253]) is a visual confrontation naming test used to measure confrontational word retrieval in individuals. This ability is diminished in patients with strokes, Alzheimer's disease, and other dementing disorders. However, there is limited normative data, and the BNT is usually used as a supplement to other neuropsychological tests.

The BNT contains 60 line drawings graded in ascending difficulty, that is, frequency of use. The drawings are shown one at a time and the participant is asked to name each of them within 20 seconds. The examinee may be presented with cues when there is a mistaken response; these cues can be descriptive or phonemic. The total score is the number of accurate responses, disregarding those following a phonemic cue.

### 6.3.1.h. Verbal Fluency

Verbal fluency is a cognitive function that facilitates information retrieval from memory. There are a number of verbal fluency tests that date back to the 1960 's. The two most commonlymeasured parameters are ( [142]): a) semantic fluency, tested by asking the participant to generate as many words from a given category as possible (animals, clothing...); b) phonemic fluency, which is tested by asking the participant to generate words beginning with a single letter (f, a, s...). Neuroimaging studies suggest that the two types of fluency tasks may engage different cognitive processes and are differentially affected in clinical populations. Results show a number of consistent characteristics across types and subjects, such as the production of bursts of semantically-related words and a hyperbolic decline in the rate of production of new words.

In this work, three verbal fluency tasks were considered: two phonemic fluency tasks (word beginning with " f " and with "a") and one semantic fluency task (animals). In all cases, the participant was asked to provide as many words as possible within 60 seconds.

### 6.3.2. Experiment configuration

The experiment was performed on six epileptic patients, between 32 and 67 years old. Each patient was fitted with several electrodes with which to record the EEG, ECG and EMG signals for the duration of the neuropsychological testing. The location of the EEG electrodes is shown in Figure 6.17; note that they are different from the locations of the electrodes in Figure 5.19. Two ECG electrodes were placed in a modification of Lead II of the American Heart Association. One of the electrodes was placed on the right hemithorax and the other on the left inframammary region, close to the sixth intercostal space. This lead was selected because we were more interested in the sequence of the EEG, rather than in its fine detail.

The recorded signals were composed by 18 bipolar EEG channels and one bipolar electrocardiographic channel. The data were captured with a sampling frequency of 512 Hz , and then band-pass filtered between 1.6 and 35 Hz using clinical-purpose software. The data recording and filtering process was performed by specialists of the Neurology Unit of the LaFe hospital. The signals and the test results were registered by different devices, and special care was taken to ensure the correct synchronization between the capture devices and the computer performing the tests. A neuropsychologist was present at all times to guide and supervise the participant during the test taking process.

The implementation of each test was different depending on whether the test requires visual or auditory stimuli, as indicated in Table 6.8. The visual tests were built as graphical user interfaces using MATLAB®, a high-level language and interactive environment for numerical computation. Each GUI is composed of a graphical front end and a numerical back end. The front end for the WAIS-III Symbol Search sub-test is shown in Figure 6.18; the rest of the front ends look very similar to it. The tests were presented on a large touchscreen in order to simplify


Figure 6.17. Location of the EEG electrodes according to the $10-20$ system.


Figure 6.18. Front end for the WAIS-III Symbol Search sub-test.
the testing process and make it as similar as possible to the traditional process. This was done because many patients are not habituated to work with computers (particularly, mouse and keyboard), which might impact their test results. The GUI were designed so the buttons and images were large and recognizable, and the distance between buttons was maximized to avoid any accidental or incorrect clicking. The front ends featured neutral colors and images were presented on a white background which helped them stand out from the rest of the GUI, as shown in Figure 6.18. The numerical back end was similar for all the tests. It was used to check the responses given by the participant, calculate neuropsychological scoring, and annotate each response with the exact date and time. This information was used to synchronize the responses with the multimodal data.

The auditory tests were implemented using distributed programming, following the architecture shown in Figure 6.19. The main program for each test was implemented using Voice Extensible Markup Language (VXML). VXML is a digital document standard for specifying interactive media and voice dialogs between humans and computers [87]. The participant accesses the VXML program using any Voice-over-IP (VoIP) software such as Skype ${ }^{\mathrm{TM}}$. At that moment, the VXML server dynamically calls the instructions for the corresponding test from a database in a Swiss server and executes them in real time. The test is taken using the VoIP software, and the process depends on the particular test. Figure 6.20 shows the testing process for the TAVEC test, but other tests are similar. Every step of the process is annotated by the VXML server with the exact date and time in order to ensure synchronicity with the multimodal data. This information, as well as the responses of the participant, is stored in the database. All of these
transmissions are undertaken automatically by the program using JavaScript and they require no input by the examinee or the neuropsychologist. The application server runs ASP.NET, using the programming language $\mathrm{C} \#$, and the database server runs MS-SQL-Server. Finally, the synch-only tests were implemented using a MATLAB GUI similar to the one used for the visual tests. In the case of synch-only tests, however, this computer interface was used only to synchronize the test with the multimodal data. The test itself was administered by a neuropsychologist in the traditional fashion.


Figure 6.19. Distributed architecture for the auditory tests.


Figure 6.20. Flowchart of the testing process for the TAVEC auditory test.

### 6.3.3. Classification results

### 6.3.3.a. Two-class classification

The performance of the proposed methods was tested using the EEG data from the experiments. For the purposes of this experiment, two classes were considered $(K=2)$. The first class corresponds to stimuli presentation, whether visual (e.g., showing a picture to the subject) or auditory (e.g., reading a list of words to the subject). The second class corresponds to the response of the participant after each set of stimuli. This includes both the actual response time, plus the latency until this response. Some of the implemented neuropsychological tests, however, show no separation between stimuli presentation and user response. In these cases, the user responds while the stimulus is being shown, thus overlapping both classes. The tests that correspond to this category, and thus were not considered for the classification experiment, were the following: Stroop Color Word test, Boston Naming test, and the Digit Symbol-Coding and Symbol Search sub-tests in WAIS-III.

For the experiment, each test and each subject was treated separately. The proposed dynamic modeling methods were trained using the first half of the data for each test and then used to classify the second half of the data. This process was repeated for each test and for each subject. The filtered signals were split into epochs of length 0.25 seconds (approximately 125 samples long). This short length was selected in order to ensure that all stages of each test (some of which are very short) were spread over multiple epochs, thus improving parameter estimation. The eleven features shown in Table 6.3 were calculated for each epoch, and for each test, the best feature was selected with a cross-validation method.

The parameters of the ICAMM, SICAMM and G-SICAMM methods were estimated using supervised training on the first half of the data. The ICA parameters were estimated with the JADE algorithm ( [231]) embedded in the MIXCA procedure, and transition probabilities were estimated by counting. ICAMM and SICAMM considered all channels. G-SICAMM used two chains ( $L=2$ ), one for each hemisphere. Each chain considered the 8 channels on the corresponding side of the head, plus the central channels ( $\mathrm{Fz}, \mathrm{Cz}$ and Pz in Figure 6.17). Both chains considered the same classes: in this case, the G-SICAMM structure is used to isolate the contributions of each hemisphere. The configuration of the Bayesian networks was dynamically adjusted to the data. Three types of DBN were considered, each one similar to one of the ICAMM-based methods: a network without temporal dependence (BNT), a single network with a HMM (DBN1), and a network with a two-chain CHMM (DBN2). The configuration of these methods was similar to that of the ICAMM-based methods. Node probabilities were modeled using a Gaussian mixture model (GMM) with a variable number of mixtures for each node. The number of mixtures for each node was determined by testing several GMM with an increasing number of classes ( 3 to 20) and choosing the model with a lower Akaike Information Criterion. In this work, most GMM ended up with seven to ten components.

Classification performance was initially measured with the balanced error rate and the recall (or sensitivity) of the user response class. The BER was selected because of the uneven distribution of the stimuli/response classes across tests and subjects, and the recall is commonly used in pattern recognition and information retrieval scenarios. Initial results, however, proved the recall to be unreliable for this experiment. This owed to the high recall values obtained for obviously bad classification results, e.g., a classifier that always returned "user response" would obtain $100 \%$ recall. Therefore, the recall was replaced by Cohen's kappa coefficient ( $\kappa,[58]$ ), which was defined as (6.5) in Section 6.1.2.

The average values of BER and $\kappa$ of each method across all subjects and tests are shown in Table 6.9. In concordance with the results in Chapter 4, ICAMM-based methods obtained a better overall performance than Bayesian networks. Non-dynamic methods performed worse than their respective dynamic methods, which is more noticeable in the case of ICAMM-based
methods. G-SICAMM performed better than SICAMM, and the variants with the Baum-Welch and Viterbi algorithms performed better than the base methods. The best average result, both in BER and $\kappa$, was yielded by G-SICAMM+VI. In all cases, it can be seen that this classification is a difficult problem that required the use of powerful dynamic models.

Let us consider the result for each individual combination of test and subject. Due to the high number of results (six methods, ten tests, six subjects, and two performance indicators), we only show here the BER and $\kappa$ of the classification experiment for the G-SICAMM+VI and DBN methods (Table 6.10 and Table 6.11 , respectively). These methods were selected because they obtained the highest average performance (lowest BER and highest kappa) of all ICAMM-based methods (G-SICAMM+VI) or of all Bayesian networks (DBN). The rest of the tables are included in Appendix 1. It can be seen that G-SICAMM+VI obtained the best performance in almost all cases. Even in the few cases were DBN achieved the best performance (e.g., the Sternberg task for subject \#6), G-SICAMM+VI obtained a similar result.

| Method | Kappa | BER (\%) |
| :---: | :---: | :---: |
| ICAMM | 0.115 | 44.13 |
| SICAMM | 0.360 | 29.16 |
| SICAMM+BW | 0.475 | 22.48 |
| SICAMM+VI | 0.515 | 20.76 |
| G-SICAMM | 0.383 | 27.75 |
| G-SICAMM+BW | 0.521 | 19.80 |
| G-SICAMM+VI | 0.562 | 18.12 |
| BNT | 0.070 | 46.41 |
| DBN | 0.205 | 38.31 |
| DBN2 | 0.095 | 44.81 |

Table 6.9. Average BER and Cohen's kappa for each method during two-class classification.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 30.13 | 38.88 | 40.26 | 18.45 | 35.03 | 27.89 |
| TAVEC | 17.02 | 26.60 | 20.18 | 27.04 | 19.25 | 21.40 |
| WMS-R: Visual Paired Associates | 5.76 | 10.52 | 9.34 | 8.90 | 5.04 | 20.60 |
| WMS-R: Figural Memory | 27.26 | 3.74 | 12.11 | 8.47 | 9.73 | 2.50 |
| WAIS-III: Verbal Paired Associates | 2.70 | 35.94 | 14.48 | 6.24 | 15.42 | 10.45 |
| WAIS-III: Visual Reproduction | 5.82 | 14.77 | 12.89 | 17.38 | 7.52 | 6.18 |
| WAIS-III: Mental Control | 14.75 | 14.22 | 14.86 | 12.78 | 25.50 | 32.67 |
| WAIS-III: Digit Span | 21.38 | 31.85 | 27.33 | 22.42 | 10.14 | 48.73 |
| Verbal Fluency | 7.67 | 23.96 | 19.11 | 30.67 | 19.97 | 8.64 |
| TB: Visual Memory | 12.28 | 21.77 | 27.44 | 7.92 | 20.25 | 14.76 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.395 | 0.220 | 0.190 | 0.630 | 0.276 | 0.455 |
| TAVEC | 0.688 | 0.470 | 0.573 | 0.554 | 0.625 | 0.588 |
| WMS-R: Visual Paired Associates | 0.762 | 0.694 | 0.701 | 0.866 | 0.812 | 0.569 |
| WMS-R: Figural Memory | 0.314 | 0.871 | 0.555 | 0.799 | 0.637 | 0.967 |
| WAIS-III: Verbal Paired Associates | 0.870 | 0.319 | 0.534 | 0.713 | 0.731 | 0.686 |
| WAIS-III: Visual Reproduction | 0.612 | 0.408 | 0.296 | 0.444 | 0.475 | 0.604 |
| WAIS-III: Mental Control | 0.706 | 0.716 | 0.767 | 0.752 | 0.436 | 0.347 |
| WAIS-III: Digit Span | 0.423 | 0.277 | 0.354 | 0.559 | 0.795 | 0.321 |
| Verbal Fluency | 0.650 | 0.423 | 0.447 | 0.351 | 0.365 | 0.545 |
| TB: Visual Memory | 0.701 | 0.499 | 0.397 | 0.778 | 0.531 | 0.682 |

Table 6.10. Results of the two-class classification of EEG data from neuropsychological tests using the GSICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 42.85 | 44.19 | 46.43 | 28.74 | 42.87 | 24.61 |
| TAVEC | 16.97 | 46.10 | 39.17 | 40.39 | 52.52 | 22.10 |
| WMS-R: Visual Paired Associates | 46.59 | 41.46 | 39.07 | 15.63 | 33.77 | 12.46 |
| WMS-R: Figural Memory | 50.30 | 38.18 | 52.71 | 50.00 | 36.11 | 10.00 |
| WAIS-III: Verbal Paired Associates | 50.00 | 65.66 | 22.90 | 12.60 | 32.90 | 33.65 |
| WAIS-III: Visual Reproduction | 34.56 | 41.14 | 50.00 | 37.51 | 50.00 | 29.04 |
| WAIS-III: Mental Control | 40.66 | 30.94 | 50.00 | 38.98 | 47.95 | 44.34 |
| WAIS-III: Digit Span | 38.55 | 44.72 | 50.81 | 34.64 | 36.24 | 61.48 |
| Verbal Fluency | 19.51 | 40.90 | 47.02 | 30.20 | 50.00 | 21.18 |
| TB: Visual Memory | 47.27 | 37.13 | 50.00 | 21.05 | 50.00 | 28.00 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.136 | 0.127 | 0.064 | 0.426 | 0.129 | 0.487 |
| TAVEC | 0.680 | 0.087 | 0.186 | 0.118 | 0.031 | 0.556 |
| WMS-R: Visual Paired Associates | 0.065 | 0.147 | 0.142 | 0.600 | 0.189 | 0.730 |
| WMS-R: Figural Memory | 0.010 | 0.155 | 0.044 | 0.000 | 0.215 | 0.653 |
| WAIS-III: Verbal Paired Associates | 0.000 | 0.347 | 0.417 | 0.612 | 0.411 | 0.246 |
| WAIS-III: Visual Reproduction | 0.077 | 0.059 | 0.000 | 0.187 | 0.000 | 0.218 |
| WAIS-III: Mental Control | 0.187 | 0.381 | 0.000 | 0.230 | 0.049 | 0.114 |
| WAIS-III: Digit Span | 0.185 | 0.096 | 0.017 | 0.310 | 0.276 | 0.110 |
| Verbal Fluency | 0.472 | 0.213 | 0.091 | 0.367 | 0.000 | 0.380 |
| TB: Visual Memory | 0.072 | 0.217 | 0.000 | 0.510 | 0.000 | 0.364 |

Table 6.11. Results of the two-class classification of EEG data from neuropsychological tests using the DBN method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

Figure 6.21 shows an example of the classification of each of the proposed methods for the several tests and subjects. Results for other combinations of test and subjects are similar. It can be seen that the results of the non-dynamic methods (BNT, ICAMM) tended to oscillate very fast or to remain "locked" at a particular class, thus explaining the worse performance yielded by those methods. The single-chain dynamic Bayesian network achieved a good result in several cases (e.g., Figure 6.21.c), but a bad result in other cases (e.g., Figure 6.21.a), with an overall average result. On the other hand, the dynamic ICAMM-based methods yielded a consistently good result in most cases. The base SICAMM and G-SICAMM showed some of the oscillating behavior of ICAMM, while the Baum-Welch and Viterbi variants showed very few rapid changes and yielded a very smooth classification, particularly for the latter. This behavior produced a better average performance for those variants (SICAMM+BW, SICAMM+VI, G-SICAMM+BW, G-SICAMM+VI), although it led in some cases in to a loss of some rapid changes in the data (see the last class change in Figure 6.21.b). This is also supported by the high values of kappa, which seems to indicate a high concordance between the true classes and the classification obtained by ICAMM-based methods with the Baum-Welch and Viterbi variants.

Let us define an "event" as the time period that the test stays in the same class, i.e., the time between two consecutive class transitions. Figure 6.21 illustrates that most of the BER incurred in by SICAMM, G-SICAMM and the proposed variants, particularly SICAMM+VI and GSICAMM+VI, was caused by errors in the timing of each event rather than by missed events. That is to say, the dynamic ICAMM-based methods correctly detected the events but sometimes failed to pinpoint the start and end samples. The other considered methods did not detect these events with such precision, nor did they correctly detect their start and end samples.


Figure 6.21. Sample results for the two-class classification experiment of data from neuropsychological tests: a) Figural Memory test for subject \#4; b) TAVEC test for subject \#5; c) Verbal Paired Associates test for subject \#5; d) TAVEC test for subject \#6. In all cases, "high" represents the user response class and "low" represents the stimuli class.

### 6.3.3.b. Three-class classification

The classification experiment can be extended beyond two-class classification for several of the considered neuropsychological experiments. For instance, most visual working memory tests could be split in three stages or classes: stimulus presentation, retention, and user response. During the retention stage, the subject must retain the stimuli shown before in memory for a few seconds before proceeding to the user response stage. The tests that could be examined in this way were: Sternberg, Visual Paired Associates (WMS-R), Figural Memory (WMS-R), Visual Reproduction (WAIS-III), and Visual Memory (TB).

The proposed methods were trained as explained in Section 6.3.3.a, but with an increased number of classes $(K=3)$. The average performance indicators are shown in Table 6.12. The performance of all methods decreased with respect to the case of two-class classification (see Table 6.9), owing to the increased number of classes. Nevertheless, the conclusions obtained for two-class classification still held true for three-class classification, briefly: (i) dynamic methods performed better than non-dynamic ones; (ii) ICAMM-based methods yielded better results than the considered Bayesian networks; and (iii) G-SICAMM performed better than SICAMM and the best result was obtained by G-SICAMM combined with the Viterbi algorithm.

The tables with the BER and $\kappa$ values yielded by each method for each test and subject are shown in Appendix 1. Table 6.13 and Table 6.14 show the results of G-SICAMM+VI and DBN (respectively) for comparison with the values for two-class classification in Table 6.10 and Table 6.11. The values for three-class classification behave similarly to those for two-class classification, albeit with reduced performance. The performance of G-SICAMM+VI was better than that of DBN in all cases, and the difference is very high in most cases.

| Method | Kappa | BER (\%) |
| :---: | :---: | :---: |
| ICAMM | 0.108 | 60.35 |
| SICAMM | 0.303 | 47.81 |
| SICAMM+BW | 0.408 | 38.93 |
| SICAMM+VI | 0.391 | 39.81 |
| G-SICAMM | 0.320 | 46.70 |
| G-SICAMM+BW | 0.403 | 37.62 |
| G-SICAMM+VI | 0.442 | 36.10 |
| BNT | 0.049 | 64.15 |
| DBN | 0.153 | 56.61 |
| DBN2 | 0.134 | 58.93 |

Table 6.12. Average BER and Cohen's kappa for each method during three-class classification.

| Test |  | Subject \#: <br> a) BER (\%) |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Sternberg | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| WMS-R: Visual Paired Associates | 43.34 | 35.30 | 39.83 | 51.75 | 35.03 | 55.83 | 48.72 |
| WMS-R: Figural Memory | 51.11 | 33.23 | 48.08 | 46.08 | 22.95 | 47.94 |  |
| WAIS-III: Visual Reproduction | 37.24 | 45.24 | 31.80 | 31.82 | 15.18 | 10.13 | 15.20 |
| TB: Visual Memory | 24.07 | 41.68 | 39.84 | 24.63 | 36.22 | 22.69 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.401 | 0.128 | 0.199 | 0.509 | 0.170 | 0.302 |  |
| WMS-R: Visual Paired Associates | 0.771 | 0.444 | 0.770 | 0.225 | 0.543 | 0.488 |  |
| WMS-R: Figural Memory | 0.294 | 0.224 | 0.352 | 0.578 | 0.690 | 0.606 |  |
| WAIS-III: Visual Reproduction | 0.566 | 0.479 | 0.174 | 0.474 | 0.319 | 0.458 |  |
| TB: Visual Memory | 0.557 | 0.351 | 0.453 | 0.661 | 0.488 | 0.576 |  |

Table 6.13. Results of the three-class classification of EEG data from neuropsychological tests using the GSICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test |  | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| Sternberg | 65.56 | 66.67 | 63.40 | 63.83 | 63.77 | 66.67 |  |
| WMS-R: Visual Paired Associates | 69.63 | 58.29 | 62.45 | 65.81 | 66.67 | 58.13 |  |
| WMS-R: Figural Memory | 66.67 | 67.41 | 66.67 | 62.57 | 45.89 | 48.61 |  |
| WAIS-III: Visual Reproduction | 67.56 | 65.79 | 67.27 | 69.33 | 18.08 | 72.06 |  |
| TB: Visual Memory | 27.97 | 60.94 | 65.58 | 31.71 | 66.67 | 26.32 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.009 | 0.000 | 0.020 | 0.061 | 0.067 | 0.000 |  |
| WMS-R: Visual Paired Associates | 0.047 | 0.084 | 0.070 | 0.016 | 0.020 | 0.241 |  |
| WMS-R: Figural Memory | 0.000 | 0.030 | 0.022 | 0.127 | 0.616 | 0.462 |  |
| WAIS-III: Visual Reproduction | 0.030 | 0.008 | 0.025 | 0.069 | 0.235 | 0.121 |  |
| TB: Visual Memory | 0.479 | 0.047 | 0.026 | 0.502 | 0.000 | 0.573 |  |

Table 6.14. Results of the three-class classification of EEG data from neuropsychological tests using the DBN2 method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

Figure 6.22 shows an example of the classification of each of the proposed methods for the several tests and subjects. Figures for other combinations of test and subjects are similar. The results show the reduced performance obtained in the three-class classification when compared with two-class classification (see Figure 6.21). Furthermore, G-SICAMM and its variants yielded a classification that changed more rapidly than that of SICAMM. This led to some classification errors in some cases (see the last twenty seconds in Figure 6.22.d), but overall resulted in more accurate classifications (see Figure 6.22.c and most of Figure 6.22.d).


Figure 6.22. Sample results for the three-class classification experiment of data from neuropsychological tests: a) Figural Memory test for subject \#4; b) Visual Reproduction test for subject \#6; c) Visual Memory test for subject \#3; d) Visual Paired Associates test for subject \#2. In all cases, "low" corresponds to the stimulus class, "middle" to the retention class, and "high" to the user response class.

### 6.3.4. Exploratory results

The parameters of G-SICAMM can be used to model the dynamics of EEG signals, including the spatial projection of the sources on the scalp, in the same way that the parameter of ICAMM [190]. This approach considers the mixing matrices as sets of spatial patterns ("scalp maps") whose temporal activations are regulated by their corresponding sources. Thus, the $m$-th source of a given G-SICAMM can be expressed by its temporal activation, $s_{k, m}(n)$, and its corresponding scalp map, $\mathbf{a}_{k, m}$; where $\mathbf{a}_{k, m}$ is the $m$-th column of the mixing matrix of class $k$, $\mathbf{A}_{k}$. The study of these parameters can determine the connectivity of brain regions during the stages of the experiment and shed new light on the EEG data [162]. This sub-section explores several representative results of the parameters learned from the EEG data from subjects performing neuropsychological experiments.

The sources extracted for each subject and test are not limited to actual EEG activity, but also to several types of artifacts, such as eye blinks or muscle noise. The nature of the source separation method is such that artifacts are usually located within a limited number of sources that can be separated from the EEG contributions. This is the basis of ICA-based artifact removal [127]. In the following, artifacted sources were removed from the analysis. The basis for this selection was the spectral density of the particular source, since the most common artifacts have easilydistinguishable spectra or scalp maps. The remaining (non-artifacted) sources were scaled in order of decreasing activity in the alpha band.

In order to test the similarity of the model between events of the same class, a different class was fitted to every event (as defined in Section 6.3.3.a, an event is the time period that the test stays in the same class). In this way, one can search for repeating patterns across events of the
same class that are not repeated in events of the other class. Since the selection is partially based on the spectra of the sources, and to avoid reducing the sampling frequency of the data, no feature extraction was performed.

Figure 6.23 shows the spatial and temporal parameters for the first two sets of stimulus/response for the TAVEC test for subject \#4. It can be seen that the parameters for both events of the stimulus class are more similar to one another than they are to the parameters of the response class. This similarity can be seen in the kurtoses of the sources and the similar scalp maps. The maps for the stimulus class show higher responses on the left hemisphere, particularly on the temporal area. This suggests the activation of Wernicke's speech area on the dominant (left) cerebral hemisphere [185], which is in concordance with the fact that the TAVEC is a verbal test. The activation of the occipital cortex might suggest visual activity on the part of the subject. On the other hand, the activity during the response class is more centered and more oriented towards the front area of the brain. This suggests a suppression of the visual input during the responses, which fits the style of the test. The excitation of the left frontal temporal area suggests the activation of Broca's speech area, which is usually related with the production of speech [185]; again, this is in concordance with the verbal nature of the test.

The results of a verbal test are different from those of a visual test, Figural Memory (part of the WMS-R), as can be seen in Figure 6.24. For one, the sources are more varied, as indicated by their kurtoses and the shape of the time activations. Note that the time of each event is shorter in Figure 6.24 than it was in Figure 6.23, due to the different conditions of the test. It can be seen that there are differences between events of the stimulus class and events of the response class, while sources of the same class are similar. The scalp maps of all events show the activation of two regions related to the visual experiment. The first one is the excitation of the occipital region of the head, which is related to visual input and processing. Thus, its presence is in concordance with the test. The other common source is distributed on the frontal-central region of the head. This region has been found to be related with the processing of information during working memory, as seen in [189]. Since the experiment is based on working memory, it is indeed consistent that such an area would appear consistently across experiments. Finally, the third interesting source found in the response events, which seems to be more noisy than the other two, might be caused by electromyographic noise due to the movement required during the response (mouse movement and clicking).
 G-SICAMM. For each source, both the amplitude values (line plot) and the histogram (bar plot) are shown, as well as its kurtosis value.


Figure 6.24. Spatial and temporal parameters of three sources of the model for the Figural Memory test for subject \#4 using G-SICAMM. For each source, both the amplitude values (line plot) and the histogram (bar plot) are shown, as well as its kurtosis value.

### 6.4. Conclusions

In this chapter, the proposed G-SICAMM methods and variants of the Sequential ICAMM method have been applied to automatic classification of data from real-life problems. These methods, which were introduced in Chapter 4, use non-Gaussian models that include sequential dependence in the classes in order to better model dynamic, non-stationary data. The proposed methods were tested on biomedical (most commonly electroencephalographic) data from three different applications.

In the first application, the proposed extensions to SICAMM were tested on a set of polysomnograms, sets of biomedical data (EEG, ECG...) taken from sleeping subjects that are usually used for sleep staging. ICAMM, SICAMM and the proposed extensions were used to perform automatic sleep staging on data from six subjects. This staging was limited to two classes (awakening/sleep) in order to detect short periods of awakening, also known as microarousals. The detection of microarousals can help in the differential diagnosis of sleep disorders, such as sleep apnea. The classification problem is further compounded by the large difference in prior probability for each class, since microarousals are usually rare, even in ill subjects. The results of the proposed methods were compared with those of a Bayesian network (implementing a mixture of Gaussians) and a dynamic Bayesian network (a HMM with a GMM modeling the emissions of each state). Performance was measured using the balanced error rate and Cohen's kappa. These indicators are robust with respect to the number of samples in each class. Results show that dynamic methods performed better than non-dynamic methods, both for Bayesian networks and for ICAMM-based methods, with a minimum average improvement of 0.05 for both error indicators. SICAMM largely over-performed both types of Bayesian networks, particularly with respect to Cohen's kappa. Finally, the proposed extensions to SICAMM using the Baum-Welch and Viterbi algorithms achieved an even better result than the base method, particularly when using the Viterbi algorithm. These results demonstrate the potential of (G-)SICAMM and its variants for the automatic detection of microarousals, a vital part in the differential diagnosis of sleep apnea. Additionally, we performed a sensitivity analysis on the data. This analysis estimated the SICAMM parameters at several time instants, using a sliding window, and then compared the models. These comparisons considered the Amari distance between de-mixing matrices, the signal-to-noise ratio between sources, and the distance between probability densities. Results suggest a relation between the variations in the models (the sources in particular) and microarousals.

The second application tested the extension of SICAMM to multiple models, called Generalized SICAMM, on real EEG data from subjects performing Sternberg's task. These data were not classified by an expert. Instead, the EEG data of each subject were captured and pre-processed, and then several features were extracted from every epoch in the data. These features were used to label every epoch according to the state of activity of each brain hemisphere (high or low). The proposed methods were used for automatic classification of the brain activity of each hemisphere. To this effect, the data were split by hemisphere. G-SICAMM was applied to the problem directly, but some pre-processing was necessary to work with SICAMM and ICAMM. The proposed methods were compared against a Bayesian network (a GMM), a dynamic Bayesian network (implementing a HMM with GMM emission probabilities), and a dynamic Bayesian network similar in structure to G-SICAMM (a CHMM with GMM emissions). Classification performance was measured with the balanced error rate. Dynamical methods achieved higher classification performances than non-dynamic methods, particularly in the case of models with a different model for each hemisphere (G-SICAMM and the CHMM Bayesian network). ICA-based methods performed better overall than Bayesian networks, and GSICAMM yielded the best result in most cases. The proposed variants to G-SICAMM and SICAMM over-performed the base method in most cases. The SICAMM and G-SICAMM parameters were also shown to be different depending on the stage of the system. This implies that there is a significant statistical difference between EEG data depending on the level of neuronal activity, and that this difference can be modeled by G-SICAMM. Finally, we performed a sensitivity analysis of the data. This analysis estimated the G-SICAMM parameters at several time instants and then compared the models. These comparisons considered the Amari distance between de-mixing matrices, the signal-to-noise ratio between sources, and the distance between probability densities. Results suggest a relation between the variations in the models and the brain activity of the subjects (as indicated by the automatic labels). Among the indicators, the Amari distance was the most closely related to the ground truth.

The third application studied EEG data from six epileptic patients performing neuropsychological tests. For this purpose, we implemented a battery of neuropsychological tests that are used in the clinical environment: TAVEC, Wechsler Memory Scale, Wechsler Adult Intelligence Scale, Barcelona Neuropsychological Test, Stroop Color Word Test, Trail Making Test, Boston Naming Test, Verbal Fluency Test, and Sternberg Test. The tests were implemented in a computer with a large touch screen in order to make them user. The EEG and the stages of each test were recorded while the patients performed the tests. G-SICAMM, SICAMM and their proposed variants were then used to classify the data and perform automatic staging of the EEG data. In the case of G-SICAMM, the data were split into two sets by splitting the data from each hemisphere. Two types of classification were considered: two-class classification (stimulus/response) and three-class classification (stimulus/retention/response). The proposed methods were compared against a Bayesian network (a GMM), a dynamic Bayesian network (implementing a HMM with a GMM for the emission probabilities of each state), and a dynamic Bayesian network similar in structure to G-SICAMM (a CHMM with GMM emissions). Classification performance was measured by the balanced error rate and Cohen's kappa coefficient. Dynamic methods outperformed non-dynamic ones, and ICAMMbased methods performed better than Bayesian networks. SICAMM performed better than all Bayesian networks, and G-SICAMM performed better than SICAMM. Finally, the proposed variants that consider the Baum-Welch and Viterbi algorithms performed better than the base methods, with G-SICAMM+VI yielding the overall best classification result for both two- and three-class classification. The G-SICAMM parameters themselves were also studied to search for interesting sources that were related to the layout of the tests. Differences were found between the parameters for each class (stimulus/response), as well as between the parameters for different kind of tests (visual/verbal). Furthermore, several sources were found that correspond to activations of the brain during verbal tasks and during working memory tests. These findings show the promise of the method for the analysis of brain dynamics on electroencephalographic data.

Conclusions and future work

## Chapter 7 - Conclusions and future work

The general objective of this thesis was to further the knowledge on non-Gaussian mixtures and explore new possibilities for mixture models of independent component analyzers. The proposed contributions extend non-Gaussian mixtures for use in estimation problems and allow us to model complex probability densities that present some degree of sequential dependence in the feature record. In order to test the potential of the proposed methods, several applications on real data were considered. Thus, the applicability of the proposed methods to real-world problems was demonstrated.

This chapter summarizes the contributions and conclusions that can be drawn from this thesis. Section 7.1 summarizes the conclusions that can be drawn from the results of this thesis, and the level of completion of each of the objectives of the thesis. Section 7.2 enumerates the contributions of this thesis to knowledge, both from the theoretical and applied points of view. Section 7.3 explores possible future lines of research that branch off from this work. The chapter ends with a list of the publications produced by the research presented in this thesis.

### 7.1. Summary

The first two chapters of this thesis presented the motivation, methods and techniques that were to be explored therein. These procedures focused on signal estimation and classification problems using non-Gaussian mixtures. In particular, independent component analysis and its extension to mixture models (ICAMM) were considered. This work presented two novel methods for data estimation based on ICAMM, each optimizing a different criterion, and a new framework for generalized sequential ICA mixtures. This framework considers multiple dependence chains, non-parametric modeling of the ICA sources, and semi-supervised or unsupervised training. These methods were evaluated in diverse application to test their behavior on real-world problems.

ICA and ICAMM have established a framework for non-linear processing of data with complex non-Gaussian distributions. This complexity is modeled as a linear mixture of local ICA projections, which are used to model class-conditional probability densities. The mixture model relaxes the base assumptions of ICA, further increasing its capabilities. Existing extensions to ICAMM further expand the model to consider: a) sequential dependences in the feature observation record (SICAMM, [230]); b) relaxed independence assumptions, the use of any

ICA algorithm (e.g., JADE), and non-parametric estimation of the source densities (MIXCA, [231]). However, existing methods presented some unresolved or unexplored issues that were researched in this work: data estimation by means of mixtures of ICA models by one or more criteria; extension of the sequential dependence to multiple chains of dependence; and support for different types of learning of the sequential dependence. The formulation of these advances is a challenging task, particularly in the context of real-world applications were a priori information on the data is scarce and incomplete.

Chapter 3 presented two novel data estimation methods based on ICA mixture models. Both procedures interpolate missing data in the feature observation record using known data and the ICAMM parameters. The first method, called PREDICAMM, interpolates missing data by optimizing the maximum likelihood criterion, i.e., obtaining the set of data that maximizes the joint probability of known data, unknown data, and the model. PREDICAMM uses a gradient algorithm for optimization, and therefore, its convergence depends heavily on the gradient algorithm itself and the starting value of the solution. Several experiments were performed to select the optimal combination for this work. The second novel method is E-ICAMM, which optimizes the least mean squared error of the estimation by calculating the conditional expectation of missing data with respect to known data and the model. The solution can be written in a closed form, thus avoiding the convergence problems of gradient methods. Furthermore, the estimation error of E-ICAMM can be estimated from the data as well. The capabilities of the proposed methods were tested by Monte Carlo experiments on an extensive set of linear and non-linear simulated data. Their performances were compared with those of the following predictors: a classical linear predictor, Ordinary Kriging; a nonlinear predictor, Wiener structures; a matrix completion algorithm based of SRF; and thin-plate splines. In all cases, the performance of the proposed methods exceeded that of the methods selected for comparison. SRF obtained similar results to E-ICAMM and PREDICAMM, but only for cases with a single class, and its performance dropped in cases with multiple classes. The performance of all the methods decreased as the number of classes or the number of missing data increased. The proposed methods, however, experienced a smaller decrease in performance than the other methods; as a matter of fact, this decrease was almost non-existent for low amounts of missing data. The performance of the two proposed methods is similar in most cases, with PREDICAMM obtaining probabilities more similar to those of the true data and E-ICAMM yielding lower estimation error.

Chapter 4 has generalized the existing Sequential ICAMM method ( [230]) to consider multiple chains of sequential dependence in the feature record. This extension has been named Generalized SICAMM. It can be used to work simultaneously with several datasets in parallel, with multimodal data, or after splitting the data into disjoint sub-sets. This chapter also considered the application of the classical Baum-Welch and Viterbi algorithms for the classification of data using the G-SICAMM parameters. Furthermore, an algorithm for semisupervised or unsupervised learning of SICAMM and G-SICAMM parameters, which we have named UG-SICAMM, was presented. This method allows estimating the SICAMM and GSICAMM parameters even if the training data are unlabeled, and it can use labeled data to improve estimation. The performance of UG-SICAMM was tested by assessing the distance between the estimated model and the true model during a Monte Carlo experiment. Results showed the good behavior of the UG-SICAMM procedure and verified that performance increased with the number of known labels. Further experiments studied the performance of GSICAMM by performing classification on several sets of simulated data with varying degrees of sequential dependence. In these tests, the proposed methods are compared with Bayesian networks and dynamic Bayesian networks. Results show that non-dynamic methods were not affected by sequential dependence, yet dynamic methods obtained better performance as dependence increased. G-SICAMM obtained the best result in all these tests, and G-SICAMM extended by the Baum-Welch and Viterbi algorithms yielded better performances than the base method. A final Monte Carlo experiment tested the behavior of G-SICAMM when the assumptions of the model did not hold; in this work, this departure from the assumptions was
done through non-stationary sources. In this case, all the proposed methods decreased in performance as the number of non-stationary sources. Again, G-SICAMM (expanded with the Baum-Welch and Viterbi algorithms) obtained the best performance.

The proposed methods are general-purpose and can be used in many signal processing fields, such as time series forecast, image reconstruction, biomedical signal processing, etc. In Chapter 5 and Chapter 6 we showed several applications of the proposed methods in the field of data estimation and pattern recognition (respectively) on data from real-world problems. The problems were very varied: ground-penetrating radar surveys, seismic exploration studies, and several types of biomedical signals: electroencephalographic, electrocardiographic and electromyographic. Chapter 5 applied E-ICAMM and PREDICAMM to the reconstruction of missing traces from ground-penetrating radar surveys, seismic exploration studies, and the recovery of missing or artifacted EEG data. Chapter 6 explored the use of G-SICAMM and UGSICAMM for: (i) automatic detection of small awakening periods (microarousals) in apnea patients; (ii) staging of brain activity on subjects performing a memory task; and (iii) stage detection and source exploration of EEG/ECG data from epileptic patients that were performing several neuropsychological tests.

### 7.2. Contributions to knowledge

This section lists the contributions that this thesis makes to the field of non-Gaussian mixtures.

* Section 3.1 introduced a new method for data estimation based on ICAMM, which we call PREDICAMM. This method performs maximum likelihood by a gradient algorithm. The experiments show the high performance of the method, which can obtain good results even when the number of missing data is large. PREDICAMM can obtain good results even if some of its base assumptions do not hold, particularly, when the base model is not an ICAMM.
* A second novel method for data estimation based on ICAMM, named E-ICAMM, has been presented in Section 3.2. This algorithm seeks the optimum for the least mean squared error criterion, i.e., the conditional expectation of missing data w.r.t. known data. E-ICAMM obtains a closed-form solution to this expectation, and it can also predict the mean squared estimation error (Section 3.2.1), thus estimating the goodness of the solution. Furthermore, E-ICAMM can also be used to obtain the initial value for the gradient algorithm in PREDICAMM.
* The sequential dependence in the SICAMM procedure has been extended to multiple chains of sequential dependence in Section 4.2, in a method which we have named GSICAMM. G-SICAMM considers multiple parallel sets of data or "chains" in a model akin to a coupled HMM. The multiple-chain model can be used to model the joint probability density of multimodal data (e.g., EEG and ECG) or to work with disjoint partitions of the same set of data. Therefore, G-SICAMM is a flexible and powerful model that can model complex non-Gaussian probability densities. The performance of G-SICAMM was very good in all experiments, even on data with no dependence, and its performance increased with dependence. It was shown that the distance between the parameters of two G-SICAMM could be used to determine differences in the underlying probability (e.g., due to non-stationarity) in the data.
* Section 4.3 has presented a procedure for ML estimation of the G-SICAMM parameters, which we have named UG-SICAMM. The selected optimization technique was the natural gradient, which simplifies the learning rule and speeds up convergence. UG-SICAMM can estimate the G-SICAMM parameters from unsupervised or semisupervised data, and it can also be used to estimate SICAMM parameters. Performance
increased with the number of labeled data; however, UG-SICAMM was able to obtain a working model even with fully unlabeled data.
* Sections 4.1.2 and 4.2.3 have proposed the use of two classical methods, the BaumWelch and Viterbi algorithms, to improve the classification performance of SICAMM and G-SICAMM. Both methods were able to markedly increase the classification performance of SICAMM and G-SICAMM.
* E-ICAMM and PREDICAMM have been introduced for the reconstruction of missing data from non-destructive testing techniques in Sections 5.1, 5.2 and 5.3. Two different applications were considered: ground penetrating radar evaluation of historical walls, including both simulated and real data, and seismic exploration of underwater terrain. In both cases, obtaining estimated B-Scans that are almost undistinguishable from the true ones.
* E-ICAMM and PREDICAMM were introduced in Section 5.4 for the reconstruction of of missing EEG data. Both proposed methods over-performed splines for this task, and were less hampered by the number of channels to reconstruct.
* Chapter 6 explored the use G-SICAMM and its proposed variants for the automatic staging of biomedical data from three applications: (i) detection of short periods of awakening (microarousals) in apnea patients; (ii) automatic detection of brain activity in subjects performing a memory task; and (iii) automatic staging of data from epileptic patients performing neuropsychological tests. In all cases, the necessary SICAMM and G-SICAMM parameters were calculated using the UG-SICAMM procedure. The sequential dependence considered by G-SICAMM obtained the most accurate classification in all cases. Furthermore, it was shown that the parameters of GSICAMM are different depending on the stages of the experiment. These parameters can be explained as a combination of spatial distributions (through the mixing matrices) and temporal activations (the sources). The estimated G-SICAMM parameters showed the activations of brain regions consistent with those that could be expected from the experiments. These results show the potential impact of G-SICAMM in clinical applications with EEG data.


### 7.3. Future work

There are several open lines of research that can improve the methods proposed in this thesis, such as:

Data estimation methods

* Research on strategies to improve parameter initialization for PREDICAMM. This is an important issue because the convergence of the algorithm depends on the starting point. Regularization and penalization techniques can be applied to avoid local maxima, as well as estimating the initial value for the gradient. Another option would be converting (or approximating) the likelihood function to a concave function, thus ensuring the convergence of the gradient to the global maxima.
* Adaptation of E-ICAMM and PREDICAMM to work with sequential dependence models like SICAMM and G-SICAMM. Both methods consider the probability density of the data, but ignore any kind of sequential dependence in the data. Thus, it stands to reason that the adaptation of E-ICAMM and PREDICAMM to consider sequential dependence would improve the estimation of data that show sequential dependences.
* Combination of data estimation and parameter learning. E-ICAMM could be joined with a procedure to learn the parameters of the ICA mixture model, such as MIXCA. This combination would create a method that estimates missing data without the need of prior knowledge of the model and/or training data; and vice versa, learn the ICAMM parameters from partial data. This process could work like an expectation-maximization algorithm, where E-ICAMM would perform the expectation step and the parameterlearning procedure would perform the maximization step.


## Dynamic modeling methods

* Research on strategies to improve convergence in UG-SICAMM. This is an important issue because the convergence of the algorithm depends on the starting point of the procedure. Regularization and penalization techniques can be applied to avoid local minima, as well as determining the optimal starting value for the gradient. The estimation of parameters such as the stopping criterion should be improved, since at the moment it is set in an empirical fashion. Moreover, the UG-SICAMM procedure could be extended to include the Baum-Welch algorithm for parameter estimation as well, instead of using it only for classification, as it is currently.
* Development of a distance measure between ICAMM models. To the best of our knowledge, there is no measure of the distance between two mixtures of ICA models. The calculation of such a distance could help in tasks such as parameter estimation (e.g., by setting the stopping criterion in iterative algorithms) and model comparison. Furthermore, this distance should be extended to G-SICAMM models.
* Incorporation of online estimation of the G-SICAMM parameters. The online learning processing would perform simultaneous structure and parameter identification. This kind of processing allows long processes to be monitored online, which would help towards the implementation of the proposed methods in a clinical environment.

Other applications

* The methods proposed in this thesis could be applied to a myriad of applications, such as: time series prediction; recovery of missing data from images; study the event-related dynamics of the brain during sensorimotor processes; study brain connectivity during cognitive tasks, in mental disorders, or during neuropsychological tests; biometric access control by EEG or multimodal access control considering EEG and ECG using fusion techniques (continuing the work shown in [217] and [250,249], respectively); detection of credit card fraud (continuing the work shown in [214,228]); and so on.


### 7.4. List of publications

Refereed JCR journals

- G. Safont, A. Salazar, A. Rodriguez, and L. Vergara, "New Prediction Methods Based on Independent Component Analyzers Mixture Models," submitted to Signal Processing, 2015.
- G. Safont, A. Salazar and L. Vergara, "Probabilistic Distance between Independent Component Analyzers Mixture Models," submitted to IEEE Transactions on Signal Processing, 2015.
- J. Igual, A. Salazar, G. Safont, and L. Vergara, "Semi-Supervised Bayesian Classification of Materials with Impact-Echo Signals," Sensors, vol. 15(5), pp. 1152811550, 2015.
- G. Safont, A. Salazar and L. Vergara, "On Recovering Missing GPR Traces by Statistical Interpolation Method," Remote Sensing, vol. 6, pp. 7546-7565, 2014.


## Book chapters

- G. Safont, A. Salazar, A. Rodriguez and L. Vergara, "An Experimental Sensitivity Analysis of Gaussian and Non-Gaussian Based Methods for Dynamic Modeling in Brain Signal Processing," in Encyclopedia of Information Science and Technology, 3rd ed., Herhsey, PA, USA, IGI Global, 2014, pp. 4028-4041.

Peer-reviewed non-JCR journals

- G. Safont, A. Salazar, A. Rodriguez and L. Vergara, "Combinación de Múltiples Detectores para Identificación/Autenticación Biométrica Basada en Electroencefalogramas," Mundo Eléctrico, vol. 95, pp. 84-91, 2014.
- G. Safont, A. Salazar, A. Rodriguez and L. Vergara, "Extensions of Independent Component Analysis Mixture Models for classificacion and prediction of EEG signals," Waves, vol. 5, pp. 59-68, 2013.
- A. Salazar, J. Gosalbez, G. Safont and L. Vergara, "Data fusion of ultrasound and GPR signals for analysis of historic walls," IOP Conference Series: Materials Science and Engineering, vol. 42, pp. 1-4, 2012.
- A. Salazar, A. Rodriguez, G. Safont and L. Vergara, "Prospective of the Application of Ultrasounds in Archaeology," IOP Conference Series: Materials Science and Engineering, vol. 42, pp. 1-5, 2012.
- J. Gosalbez, A. Salazar, S. G., I. Bosch, R. Miralles, L. Vergara and V. Albert, "Application of non-destructive evaluation and signal processing for diagnosis of historic heritage buildings," Waves, vol. 3, p. 107-116, 2011.
- G. Safont, A. Salazar, J. Gosalbez and L. Vergara, "Aplicación de señales VHF y UHF para la evaluación de muros históricos," Mundo Eléctrico, vol. 82, pp. 54-58, 2011.
- C. Gosalbez, G. Safont and A. Salazar, "Caracterización del estado tensional de sistemas constructivos complejos como muros históricos mediante ensayos no destructivos y quasi-no destructivos," Boletín de la Asociación Española de Ensayos No Destructivos, vol. 1, pp. 6-13, 2011.

International conferences

- A. Salazar, G. Safont and L. Vergara, "Surrogate techniques for testing fraud detection algorithms in credit card operations," in 48th International Carnahan Conference on Security Technology (ICCST2014), Rome, Italy, 2014.
- G. Safont, A. Salazar, L. Vergara, E. Gomez and V. Villanueva, "Mixtures of Independent Component Analyzers for Microarousal Detection," in International Conference on Biomedical and Health Informatics (BHI2014), Valencia, Spain, 2014.
- A. Salazar, G. Safont, A. Rodriguez and L. Vergara, "Estimation of consolidation profiles for archaeological ceramics using ultrasonic signature," in IEEE International Ultrasonic Symposium (IUS2014), pp. 365-368, Chicago, IL, USA, 2014.
- G. Safont, A. Salazar, L. Vergara and A. Rodriguez, "New Applications of Sequential ICA Mixture Models Compared with Dynamic Bayesian Networks for EEG Signal Processing," in Fifth International Conference on Computational Intelligence, Communication Systems and Networks, Madrid, Spain, 2013.
- G. Safont, A. Salazar, A. Soriano and L. Vergara, "Combination of Multiple Detectors for EEG based Biometric Identification/Authentication," in 46th IEEE International Carnahan Conference on Security Technology (ICCST2012), Boston, MA, USA, 2012.
- G. Safont, A. Salazar, A. Rodriguez and L. Vergara, "Automatic Credit Card Detection based on Non-linear Signal Processing," in 46th IEEE International Carnahan Conference on Security Technology (ICCST2012), Boston, MA, USA, 2012.
- A. Soriano, L. Vergara, G. Safont and A. Salazar, "On Comparing Hard and Soft Fusion of Dependent Detectors," in 22nd IEEE International Workshop on Machine Learning for Signal Processing, Santander, Spain, 2012.
- A. Salazar, G. Safont and L. Vergara, "Application of Independent Component Analysis for Evaluation of Ashlar Masonry Walls," in 11th International Work-Conference on Artificial Neural Networks (IWANN2011), Torremolinos-Málaga, Spain, 2011.
- G. Safont, A. Salazar and L. Vergara, "Nonlinear Prediction based on Independent Component Analysis Mixture Modeling," in 11th International Work-Conference on Artificial Neural Networks (IWANN2011), Torremolinos-Málaga, Spain, 2011.
- G. Safont, A. Salazar, L. Vergara, R. Llinares and J. Igual, "Wiener System for Reconstruction of Missing Seismic Traces," in International Joint Conference on Neural Networks, San José, CA, USA, 2011.
- G. Safont, A. Salazar, J. Gosalbez and L. Vergara, "Intelligent System for NonDestructive Evaluation of Historic Walls using Ground-Penetrating Radar," in 9th International Conference on Cybernetic Intelligent Systems, Reading, UK, 2010.
- G. Safont, A. Salazar and L. Vergara, "Detection of Imperfections within Historic Walls Using Ground-Penetrating Radar," in 10th International Conference on Computational and Mathematical Methods in Science and Engineering, Almería, Spain, 2010.
- G. Safont, A. Salazar, J. Gosalbez and L. Vergara, "Estimation of Missing Seismic Data based on Non-linear Systems," in 10th International Conference on Computational and Mathematical Methods in Science and Engineering (CMMSE2010), Almería, Spain, 2010.

National (Spanish) conferences

- G. Safont, A. Salazar, A. Soriano and L. Vergara, "Análisis de Componentes Independientes aplicado a la recuperación de señales GPR," in XXVII Simposio Nacional de la Unión Científica Internacional de Radio (URSI2012), Elche, Spain, 2012.
- A. Soriano, L. Vergara, A. Salazar and G. Safont, "Hard versus soft fusion of dependent data," in XXVII Simposio Nacional de la Unión Científica Internacional de Radio (URSI2012), Elche, Spain, 2012.
- J. Gosalbez, G. Safont and A. Salazar, "Experimentación en laboratorio de reproducciones a escala de muros históricos mediante monitorización END y QEND," in 3 a Edición Jornadas Internacionales REHABEND, Bilbao, Spain, 2009.


## Apendices

## Appendix 1 - Classification results for the neuropsychological

 experimentThis Appendix includes the tables of results of all the methods considered for the classification experiment on EEG data from neuropsychological tests in Section 6.3.3. Each of the tables contained herein presents the balanced error rate and Cohen's kappa ( [58]) of the classification with two or three classes obtained using one of the considered methods.

## Two-class classification

| Test |  | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| Sternberg | 41.92 | 44.15 | 49.49 | 27.23 | 46.44 | 40.20 |  |
| TAVEC | 46.93 | 47.66 | 46.19 | 44.59 | 46.78 | 44.33 |  |
| WMS-R: Visual Paired Associates | 50.90 | 43.32 | 45.64 | 45.36 | 45.65 | 42.44 |  |
| WMS-R: Figural Memory | 48.41 | 47.63 | 53.67 | 41.13 | 49.42 | 36.63 |  |
| WAIS-III: Verbal Paired Associates | 37.48 | 48.26 | 50.12 | 48.98 | 47.54 | 45.81 |  |
| WAIS-III: Visual Reproduction | 50.08 | 50.53 | 48.57 | 41.82 | 22.03 | 48.58 |  |
| WAIS-III: Mental Control | 49.65 | 47.54 | 43.51 | 35.63 | 34.94 | 48.06 |  |
| WAIS-III: Digit Span | 41.74 | 43.75 | 47.94 | 44.85 | 42.68 | 62.68 |  |
| Verbal Fluency | 45.59 | 45.07 | 44.39 | 44.22 | 44.69 | 34.95 |  |
| TB: Visual Memory | 37.32 | 42.82 | 43.83 | 32.30 | 37.90 | 35.56 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.157 | 0.118 | 0.010 | 0.454 | 0.070 | 0.199 |  |
| TAVEC | 0.068 | 0.045 | 0.076 | 0.094 | 0.068 | 0.124 |  |
| WMS-R: Visual Paired Associates | 0.027 | 0.100 | 0.094 | 0.067 | 0.102 | 0.158 |  |
| WMS-R: Figural Memory | 0.049 | 0.052 | 0.069 | 0.190 | 0.017 | 0.254 |  |
| WAIS-III: Verbal Paired Associates | 0.175 | 0.037 | 0.002 | 0.014 | 0.062 | 0.049 |  |
| WAIS-III: Visual Reproduction | 0.003 | 0.010 | 0.025 | 0.133 | 0.321 | 0.042 |  |
| WAIS-III: Mental Control | 0.007 | 0.049 | 0.065 | 0.294 | 0.282 | 0.039 |  |
| WAIS-III: Digit Span | 0.101 | 0.106 | 0.032 | 0.103 | 0.146 | 0.118 |  |
| Verbal Fluency | 0.126 | 0.075 | 0.172 | 0.142 | 0.097 | 0.306 |  |
| TB: Visual Memory | 0.263 | 0.145 | 0.119 | 0.344 | 0.225 | 0.252 |  |

Table A1.1. Results of the two-class classification of EEG data from neuropsychological tests using the (nondynamic) ICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: <br> a) BER (\%) |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Sternberg | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |  |  |  |  |  |
| TAVEC | 26.40 | 42.56 | 50.74 | 20.98 | 41.52 | 34.26 |  |  |  |  |  |  |
| WMS-R: Visual Paired Associates | 14.52 | 30.53 | 36.86 | 41.05 | 27.88 | 29.01 |  |  |  |  |  |  |
| WMS-R: Figural Memory | 38.72 | 41.65 | 39.31 | 30.75 | 22.36 | 17.28 |  |  |  |  |  |  |
| WAIS-III: Verbal Paired Associates | 23.44 | 39.68 | 39.18 | 11.38 | 18.60 | 32.24 |  |  |  |  |  |  |
| WAIS-III: Visual Reproduction | 5.82 | 19.80 | 28.76 | 11.88 | 16.98 |  |  |  |  |  |  |  |
| WAIS-III: Mental Control | 35.25 | 43.50 | 30.16 | 32.89 | 30.55 | 22.79 |  |  |  |  |  |  |
| WAIS-III: Digit Span | 33.77 | 30.07 | 32.09 | 37.40 | 27.21 | 48.93 |  |  |  |  |  |  |
| Verbal Fluency | 8.43 | 37.86 | 30.58 | 32.83 | 34.01 | 19.39 |  |  |  |  |  |  |
| TB: Visual Memory | 22.34 | 32.35 | 42.57 | 14.84 | 26.73 | 22.18 |  |  |  |  |  |  |
| b) Kappa |  |  |  |  |  |  |  |  |  |  |  |  |
| Sternberg | 0.475 | 0.149 | 0.014 | 0.579 | 0.157 | 0.321 |  |  |  |  |  |  |
| TAVEC | 0.583 | 0.398 | 0.269 | 0.160 | 0.406 | 0.433 |  |  |  |  |  |  |
| WMS-R: Visual Paired Associates | 0.512 | 0.280 | 0.162 | 0.330 | 0.473 | 0.648 |  |  |  |  |  |  |
| WMS-R: Figural Memory | 0.298 | 0.132 | 0.027 | 0.656 | 0.513 | 0.632 |  |  |  |  |  |  |
| WAIS-III: Verbal Paired Associates | 0.373 | 0.219 | 0.188 | 0.478 | 0.408 | 0.504 |  |  |  |  |  |  |
| WAIS-III: Visual Reproduction | 0.703 | 0.330 | 0.231 | 0.550 | 0.464 | 0.406 |  |  |  |  |  |  |
| WAIS-III: Mental Control | 0.295 | 0.130 | 0.245 | 0.353 | 0.387 | 0.151 |  |  |  |  |  |  |
| WAIS-III: Digit Span | 0.214 | 0.342 | 0.226 | 0.254 | 0.457 | 0.256 |  |  |  |  |  |  |
| Verbal Fluency | 0.670 | 0.194 | 0.376 | 0.386 | 0.217 | 0.521 |  |  |  |  |  |  |
| TB: Visual Memory | 0.553 | 0.299 | 0.124 | 0.643 | 0.431 | 0.470 |  |  |  |  |  |  |

Table A1.2. Results of the two-class classification of EEG data from neuropsychological tests using the basic SICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 31.03 | 35.45 | 45.61 | 21.33 | 35.86 | 28.75 |
| TAVEC | 16.54 | 20.87 | 29.22 | 31.32 | 22.66 | 22.55 |
| WMS-R: Visual Paired Associates | 11.69 | 18.82 | 25.51 | 11.79 | 9.65 | 15.17 |
| WMS-R: Figural Memory | 37.50 | 18.07 | 36.77 | 13.34 | 9.06 | 5.38 |
| WAIS-III: Verbal Paired Associates | 19.93 | 45.53 | 36.10 | 11.01 | 25.14 | 12.33 |
| WAIS-III: Visual Reproduction | 7.88 | 20.25 | 6.99 | 16.82 | 9.64 | 15.60 |
| WAIS-III: Mental Control | 21.72 | 30.05 | 25.67 | 23.84 | 25.05 | 36.50 |
| WAIS-III: Digit Span | 24.76 | 23.68 | 25.30 | 33.23 | 11.13 | 32.10 |
| Verbal Fluency | 8.71 | 41.40 | 19.65 | 18.38 | 19.11 | 5.60 |
| TB: Visual Memory | 14.01 | 27.36 | 35.16 | 9.76 | 20.84 | 20.37 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.382 | 0.291 | 0.082 | 0.571 | 0.261 | 0.435 |
| TAVEC | 0.687 | 0.639 | 0.433 | 0.341 | 0.511 | 0.565 |
| WMS-R: Visual Paired Associates | 0.577 | 0.491 | 0.341 | 0.744 | 0.670 | 0.685 |
| WMS-R: Figural Memory | 0.373 | 0.501 | 0.195 | 0.644 | 0.657 | 0.796 |
| WAIS-III: Verbal Paired Associates | 0.439 | 0.095 | 0.269 | 0.661 | 0.570 | 0.638 |
| WAIS-III: Visual Reproduction | 0.438 | 0.298 | 0.473 | 0.461 | 0.432 | 0.440 |
| WAIS-III: Mental Control | 0.566 | 0.399 | 0.334 | 0.537 | 0.483 | 0.269 |
| WAIS-III: Digit Span | 0.330 | 0.470 | 0.323 | 0.338 | 0.779 | 0.295 |
| Verbal Fluency | 0.697 | 0.139 | 0.614 | 0.647 | 0.411 | 0.690 |
| TB: Visual Memory | 0.682 | 0.379 | 0.247 | 0.728 | 0.580 | 0.503 |

Table A1.3. Results of the two-class classification of EEG data from neuropsychological tests using the SICAMM+BW method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg |  |  |  |  |  |  |
| TAVEC | 16.51 | 35.47 | 42.58 | 21.95 | 38.95 | 28.20 |
| WMS-R: Visual Paired Associates | 9.89 | 29.26 | 25.97 | 29.97 | 21.75 | 19.25 |
| WMS-R: Figural Memory | 35.30 | 29.91 | 23.74 | 9.96 | 6.80 | 12.02 |
| WAIS-III: Verbal Paired Associates | 19.05 | 37.15 | 12.15 | 5.70 | 6.38 | 4.62 |
| WAIS-III: Visual Reproduction | 2.90 | 12.87 | 6.40 | 17.01 | 9.86 | 7.50 |
| WAIS-III: Mental Control | 29.41 | 30.27 | 11.10 | 16.61 | 23.92 | 25.58 |
| WAIS-III: Digit Span | 24.67 | 26.20 | 38.27 | 28.09 | 7.89 | 44.15 |
| Verbal Fluency | 18.50 | 25.56 | 22.00 | 13.01 | 19.87 | 5.01 |
| TB: Visual Memory | 14.36 | 24.86 | 32.58 | 8.38 | 24.61 | 17.13 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.207 | 0.293 | 0.139 | 0.558 | 0.203 | 0.442 |
| TAVEC | 0.688 | 0.474 | 0.502 | 0.370 | 0.614 | 0.643 |
| WMS-R: Visual Paired Associates | 0.628 | 0.467 | 0.373 | 0.820 | 0.755 | 0.757 |
| WMS-R: Figural Memory | 0.411 | 0.268 | 0.385 | 0.679 | 0.743 | 0.822 |
| WAIS-III: Verbal Paired Associates | 0.467 | 0.260 | 0.637 | 0.761 | 0.569 | 0.601 |
| WAIS-III: Visual Reproduction | 0.669 | 0.455 | 0.499 | 0.455 | 0.425 | 0.539 |
| WAIS-III: Mental Control | 0.412 | 0.394 | 0.529 | 0.678 | 0.506 | 0.488 |
| WAIS-III: Digit Span | 0.366 | 0.419 | 0.201 | 0.444 | 0.843 | 0.312 |
| Verbal Fluency | 0.602 | 0.546 | 0.586 | 0.717 | 0.379 | 0.693 |
| TB: Visual Memory | 0.671 | 0.419 | 0.290 | 0.765 | 0.486 | 0.561 |

Table A1.4. Results of the two-class classification of EEG data from neuropsychological tests using the SICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 29.13 | 43.80 | 39.89 | 22.80 | 40.38 | 32.53 |
| TAVEC | 24.41 | 36.87 | 29.31 | 33.99 | 27.09 | 30.82 |
| WMS-R: Visual Paired Associates | 16.45 | 23.76 | 36.10 | 29.40 | 20.36 | 29.75 |
| WMS-R: Figural Memory | 36.16 | 33.54 | 19.32 | 13.03 | 23.48 | 17.88 |
| WAIS-III: Verbal Paired Associates | 19.35 | 49.14 | 30.93 | 17.16 | 24.63 | 29.98 |
| WAIS-III: Visual Reproduction | 16.81 | 32.74 | 32.00 | 15.73 | 8.61 | 13.92 |
| WAIS-III: Mental Control | 28.05 | 32.27 | 25.77 | 23.98 | 28.70 | 38.08 |
| WAIS-III: Digit Span | 32.34 | 38.07 | 28.64 | 28.63 | 20.73 | 58.45 |
| Verbal Fluency | 21.25 | 29.15 | 32.31 | 32.81 | 30.16 | 17.06 |
| TB: Visual Memory | 18.53 | 27.18 | 23.45 | 16.92 | 26.08 | 25.40 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.412 | 0.123 | 0.197 | 0.543 | 0.181 | 0.358 |
| TAVEC | 0.523 | 0.256 | 0.388 | 0.381 | 0.420 | 0.382 |
| WMS-R: Visual Paired Associates | 0.529 | 0.463 | 0.238 | 0.363 | 0.518 | 0.393 |
| WMS-R: Figural Memory | 0.200 | 0.277 | 0.509 | 0.669 | 0.455 | 0.621 |
| WAIS-III: Verbal Paired Associates | 0.578 | 0.017 | 0.274 | 0.502 | 0.550 | 0.337 |
| WAIS-III: Visual Reproduction | 0.445 | 0.190 | 0.134 | 0.473 | 0.435 | 0.513 |
| WAIS-III: Mental Control | 0.439 | 0.355 | 0.358 | 0.527 | 0.399 | 0.238 |
| WAIS-III: Digit Span | 0.255 | 0.197 | 0.317 | 0.433 | 0.586 | 0.121 |
| Verbal Fluency | 0.445 | 0.295 | 0.192 | 0.310 | 0.226 | 0.438 |
| TB: Visual Memory | 0.609 | 0.405 | 0.477 | 0.612 | 0.423 | 0.482 |

Table A1.5. Results of the two-class classification of EEG data from neuropsychological tests using the G-SICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 26.94 | 39.78 | 41.07 | 18.89 | 35.37 | 24.43 |
| TAVEC | 17.07 | 30.96 | 24.40 | 33.07 | 18.86 | 28.43 |
| WMS-R: Visual Paired Associates | 10.62 | 7.02 | 19.30 | 16.57 | 7.46 | 21.70 |
| WMS-R: Figural Memory | 30.10 | 10.28 | 11.80 | 8.47 | 9.73 | 2.50 |
| WAIS-III: Verbal Paired Associates | 1.80 | 33.87 | 24.62 | 7.70 | 14.98 | 18.47 |
| WAIS-III: Visual Reproduction | 5.57 | 18.78 | 13.98 | 14.01 | 7.63 | 6.18 |
| WAIS-III: Mental Control | 22.18 | 25.54 | 21.71 | 17.97 | 23.35 | 31.05 |
| WAIS-III: Digit Span | 25.51 | 25.41 | 28.24 | 25.39 | 17.45 | 53.01 |
| Verbal Fluency | 9.98 | 15.89 | 15.79 | 31.24 | 21.91 | 9.33 |
| TB: Visual Memory | 11.92 | 24.48 | 21.67 | 11.26 | 19.54 | 15.91 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.456 | 0.202 | 0.176 | 0.621 | 0.272 | 0.524 |
| TAVEC | 0.687 | 0.378 | 0.483 | 0.429 | 0.575 | 0.433 |
| WMS-R: Visual Paired Associates | 0.669 | 0.781 | 0.518 | 0.643 | 0.735 | 0.548 |
| WMS-R: Figural Memory | 0.295 | 0.678 | 0.563 | 0.799 | 0.637 | 0.967 |
| WAIS-III: Verbal Paired Associates | 0.911 | 0.335 | 0.384 | 0.661 | 0.750 | 0.537 |
| WAIS-III: Visual Reproduction | 0.631 | 0.324 | 0.273 | 0.551 | 0.471 | 0.604 |
| WAIS-III: Mental Control | 0.556 | 0.490 | 0.430 | 0.653 | 0.499 | 0.378 |
| WAIS-III: Digit Span | 0.350 | 0.378 | 0.345 | 0.499 | 0.650 | 0.216 |
| Verbal Fluency | 0.614 | 0.532 | 0.426 | 0.332 | 0.334 | 0.522 |
| TB: Visual Memory | 0.713 | 0.461 | 0.493 | 0.701 | 0.549 | 0.648 |

Table A1.6. Results of the two-class classification of EEG data from neuropsychological tests using the GSICAMM+BW method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 30.13 | 38.88 | 40.26 | 18.45 | 35.03 | 27.89 |
| TAVEC | 17.02 | 26.60 | 20.18 | 27.04 | 19.25 | 21.40 |
| WMS-R: Visual Paired Associates | 5.76 | 10.52 | 9.34 | 8.90 | 5.04 | 20.60 |
| WMS-R: Figural Memory | 27.26 | 3.74 | 12.11 | 8.47 | 9.73 | 2.50 |
| WAIS-III: Verbal Paired Associates | 2.70 | 35.94 | 14.48 | 6.24 | 15.42 | 10.45 |
| WAIS-III: Visual Reproduction | 5.82 | 14.77 | 12.89 | 17.38 | 7.52 | 6.18 |
| WAIS-III: Mental Control | 14.75 | 14.22 | 14.86 | 12.78 | 25.50 | 32.67 |
| WAIS-III: Digit Span | 21.38 | 31.85 | 27.33 | 22.42 | 10.14 | 48.73 |
| Verbal Fluency | 7.67 | 23.96 | 19.11 | 30.67 | 19.97 | 8.64 |
| TB: Visual Memory | 12.28 | 21.77 | 27.44 | 7.92 | 20.25 | 14.76 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.395 | 0.220 | 0.190 | 0.630 | 0.276 | 0.455 |
| TAVEC | 0.688 | 0.470 | 0.573 | 0.554 | 0.625 | 0.588 |
| WMS-R: Visual Paired Associates | 0.762 | 0.694 | 0.701 | 0.866 | 0.812 | 0.569 |
| WMS-R: Figural Memory | 0.314 | 0.871 | 0.555 | 0.799 | 0.637 | 0.967 |
| WAIS-III: Verbal Paired Associates | 0.870 | 0.319 | 0.534 | 0.713 | 0.731 | 0.686 |
| WAIS-III: Visual Reproduction | 0.612 | 0.408 | 0.296 | 0.444 | 0.475 | 0.604 |
| WAIS-III: Mental Control | 0.706 | 0.716 | 0.767 | 0.752 | 0.436 | 0.347 |
| WAIS-III: Digit Span | 0.423 | 0.277 | 0.354 | 0.559 | 0.795 | 0.321 |
| Verbal Fluency | 0.650 | 0.423 | 0.447 | 0.351 | 0.365 | 0.545 |
| TB: Visual Memory | 0.701 | 0.499 | 0.397 | 0.778 | 0.531 | 0.682 |

Table A1.7. Results of the two-class classification of EEG data from neuropsychological tests using the GSICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 |
| a) BER (\%) |  |  |  |  |  |  |
| Sternberg | 42.84 | 48.01 | 49.47 | 31.09 | 47.53 | 40.42 |
| TAVEC | 49.80 | 50.59 | 48.09 | 47.86 | 50.00 | 44.43 |
| WMS-R: Visual Paired Associates | 46.65 | 44.04 | 45.88 | 47.63 | 43.33 | 43.71 |
| WMS-R: Figural Memory | 49.81 | 45.02 | 49.33 | 44.38 | 50.61 | 37.40 |
| WAIS-III: Verbal Paired Associates | 50.00 | 50.00 | 50.98 | 43.90 | 49.84 | 44.94 |
| WAIS-III: Visual Reproduction | 50.00 | 38.47 | 50.00 | 45.09 | 50.00 | 50.91 |
| WAIS-III: Mental Control | 50.51 | 46.64 | 41.67 | 39.59 | 51.09 | 49.29 |
| WAIS-III: Digit Span | 45.00 | 46.98 | 48.12 | 49.40 | 43.11 | 65.74 |
| Verbal Fluency | 41.88 | 50.00 | 44.68 | 43.47 | 50.00 | 41.51 |
| TB: Visual Memory | 43.99 | 46.57 | 50.00 | 32.51 | 55.22 | 35.74 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.133 | 0.044 | 0.010 | 0.379 | 0.051 | 0.197 |
| TAVEC | 0.005 | 0.015 | 0.043 | 0.045 | 0.000 | 0.120 |
| WMS-R: Visual Paired Associates | 0.055 | 0.088 | 0.058 | 0.031 | 0.088 | 0.136 |
| WMS-R: Figural Memory | 0.006 | 0.059 | 0.015 | 0.115 | 0.016 | 0.207 |
| WAIS-III: Verbal Paired Associates | 0.000 | 0.000 | 0.020 | 0.091 | 0.004 | 0.072 |
| WAIS-III: Visual Reproduction | 0.000 | 0.176 | 0.000 | 0.109 | 0.000 | 0.024 |
| WAIS-III: Mental Control | 0.010 | 0.067 | 0.088 | 0.224 | 0.021 | 0.015 |
| WAIS-III: Digit Span | 0.061 | 0.049 | 0.049 | 0.013 | 0.138 | 0.052 |
| Verbal Fluency | 0.177 | 0.000 | 0.155 | 0.123 | 0.000 | 0.155 |
| TB: Visual Memory | 0.118 | 0.072 | 0.000 | 0.327 | 0.113 | 0.225 |

Table A1.8. Results of the two-class classification of EEG data from neuropsychological tests using the (nondynamic) BNT method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 |
| a) BER (\%) |  |  |  |  |  |  |
| Sternberg | 42.85 | 44.19 | 46.43 | 28.74 | 42.87 | 24.61 |
| TAVEC | 16.97 | 46.10 | 39.17 | 40.39 | 52.52 | 22.10 |
| WMS-R: Visual Paired Associates | 46.59 | 41.46 | 39.07 | 15.63 | 33.77 | 12.46 |
| WMS-R: Figural Memory | 50.30 | 38.18 | 52.71 | 50.00 | 36.11 | 10.00 |
| WAIS-III: Verbal Paired Associates | 50.00 | 65.66 | 22.90 | 12.60 | 32.90 | 33.65 |
| WAIS-III: Visual Reproduction | 34.56 | 41.14 | 50.00 | 37.51 | 50.00 | 29.04 |
| WAIS-III: Mental Control | 40.66 | 30.94 | 50.00 | 38.98 | 47.95 | 44.34 |
| WAIS-III: Digit Span | 38.55 | 44.72 | 50.81 | 34.64 | 36.24 | 61.48 |
| Verbal Fluency | 19.51 | 40.90 | 47.02 | 30.20 | 50.00 | 21.18 |
| TB: Visual Memory | 47.27 | 37.13 | 50.00 | 21.05 | 50.00 | 28.00 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.136 | 0.127 | 0.064 | 0.426 | 0.129 | 0.487 |
| TAVEC | 0.680 | 0.087 | 0.186 | 0.118 | 0.031 | 0.556 |
| WMS-R: Visual Paired Associates | 0.065 | 0.147 | 0.142 | 0.600 | 0.189 | 0.730 |
| WMS-R: Figural Memory | 0.010 | 0.155 | 0.044 | 0.000 | 0.215 | 0.653 |
| WAIS-III: Verbal Paired Associates | 0.000 | 0.347 | 0.417 | 0.612 | 0.411 | 0.246 |
| WAIS-III: Visual Reproduction | 0.077 | 0.059 | 0.000 | 0.187 | 0.000 | 0.218 |
| WAIS-III: Mental Control | 0.187 | 0.381 | 0.000 | 0.230 | 0.049 | 0.114 |
| WAIS-III: Digit Span | 0.185 | 0.096 | 0.017 | 0.310 | 0.276 | 0.110 |
| Verbal Fluency | 0.472 | 0.213 | 0.091 | 0.367 | 0.000 | 0.380 |
| TB: Visual Memory | 0.072 | 0.217 | 0.000 | 0.510 | 0.000 | 0.364 |

Table A1.9. Results of the two-class classification of EEG data from neuropsychological tests using the DBN method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test |  | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| Sternberg | 43.99 | 50.00 | 50.02 | 50.00 | 50.00 | 44.16 |  |
| TAVEC | 34.21 | 50.00 | 49.88 | 50.00 | 52.13 | 43.29 |  |
| WMS-R: Visual Paired Associates | 23.07 | 50.16 | 50.76 | 23.26 | 50.00 | 22.19 |  |
| WMS-R: Figural Memory | 50.00 | 43.46 | 52.48 | 35.29 | 51.68 | 39.13 |  |
| WAIS-III: Verbal Paired Associates | 16.22 | 48.23 | 50.00 | 6.68 | 50.00 | 50.21 |  |
| WAIS-III: Visual Reproduction | 50.25 | 50.00 | 50.00 | 53.11 | 50.00 | 50.12 |  |
| WAIS-III: Mental Control | 62.26 | 50.00 | 50.00 | 52.40 | 43.00 | 40.55 |  |
| WAIS-III: Digit Span | 47.61 | 50.00 | 43.95 | 44.54 | 36.25 | 74.88 |  |
| Verbal Fluency | 14.53 | 45.26 | 34.76 | 53.41 | 50.00 | 40.77 |  |
| TB: Visual Memory | 51.06 | 52.48 | 49.16 | 21.92 | 50.00 | 45.58 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.108 | 0.000 | 0.000 | 0.000 | 0.000 | 0.112 |  |
| TAVEC | 0.303 | 0.000 | 0.002 | 0.000 | 0.024 | 0.120 |  |
| WMS-R: Visual Paired Associates | 0.377 | 0.004 | 0.022 | 0.407 | 0.000 | 0.516 |  |
| WMS-R: Figural Memory | 0.000 | 0.076 | 0.071 | 0.385 | 0.049 | 0.294 |  |
| WAIS-III: Verbal Paired Associates | 0.443 | 0.026 | 0.000 | 0.787 | 0.000 | 0.006 |  |
| WAIS-III: Visual Reproduction | 0.009 | 0.000 | 0.000 | 0.068 | 0.000 | 0.004 |  |
| WAIS-III: Mental Control | 0.245 | 0.000 | 0.000 | 0.054 | 0.192 | 0.193 |  |
| WAIS-III: Digit Span | 0.065 | 0.000 | 0.136 | 0.112 | 0.270 | 0.000 |  |
| Verbal Fluency | 0.510 | 0.144 | 0.087 | 0.050 | 0.000 | 0.054 |  |
| TB: Visual Memory | 0.031 | 0.067 | 0.023 | 0.555 | 0.000 | 0.098 |  |

Table A1.10. Results of the two-class classification of EEG data from neuropsychological tests using the DBN2 method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

## Three-class classification

| Test | Subject \#: |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 60.46 | 64.70 | 66.22 | 46.96 | 64.79 | 60.49 |
| WMS-R: Visual Paired Associates | 63.55 | 63.98 | 66.78 | 58.44 | 65.40 | 61.20 |
| WMS-R: Figural Memory | 68.86 | 61.49 | 67.01 | 63.29 | 50.36 | 61.13 |
| WAIS-III: Visual Reproduction | 66.00 | 65.11 | 65.30 | 62.18 | 33.32 | 67.30 |
| TB: Visual Memory | 59.38 | 67.59 | 61.76 | 50.70 | 51.89 | 44.73 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.118 | 0.035 | 0.017 | 0.374 | 0.047 | 0.133 |
| WMS-R: Visual Paired Associates | 0.095 | 0.053 | 0.002 | 0.170 | 0.033 | 0.153 |
| WMS-R: Figural Memory | 0.064 | 0.150 | 0.010 | 0.091 | 0.329 | 0.126 |
| WAIS-III: Visual Reproduction | 0.030 | 0.036 | 0.044 | 0.086 | 0.297 | 0.026 |
| TB: Visual Memory | 0.077 | 0.014 | 0.076 | 0.250 | 0.259 | 0.323 |

Table A1.11. Results of the three-class classification of EEG data from neuropsychological tests using the (nondynamic) ICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| a) BER (\%) |  |  |  |  |  |  |  |
| Sternberg | 46.52 | 62.93 | 63.26 | 44.91 | 58.18 | 55.24 |  |
| WMS-R: Visual Paired Associates | 42.86 | 42.18 | 52.29 | 60.91 | 39.79 | 44.32 |  |
| WMS-R: Figural Memory | 78.46 | 58.56 | 48.82 | 38.06 | 37.89 | 28.52 |  |
| WAIS-III: Visual Reproduction | 37.48 | 55.17 | 61.40 | 53.90 | 24.45 | 37.65 |  |
| TB: Visual Memory | 45.79 | 53.57 | 54.81 | 33.05 | 43.21 | 30.24 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.312 | 0.074 | 0.028 | 0.404 | 0.204 | 0.232 |  |
| WMS-R: Visual Paired Associates | 0.544 | 0.563 | 0.285 | 0.185 | 0.315 | 0.596 |  |
| WMS-R: Figural Memory | 0.184 | 0.240 | 0.315 | 0.592 | 0.377 | 0.224 |  |
| WAIS-III: Visual Reproduction | 0.462 | 0.143 | 0.099 | 0.218 | 0.394 | 0.383 |  |
| TB: Visual Memory | 0.253 | 0.184 | 0.204 | 0.533 | 0.419 | 0.504 |  |

Table A1.12. Results of the three-class classification of EEG data from neuropsychological tests using the basic SICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | $\mathbf{7}$ | Subject \#: |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 48.17 | 57.99 | 58.02 | 33.92 | 56.64 | 47.02 |
| WMS-R: Visual Paired Associates | 40.90 | 47.06 | 42.67 | 36.38 | 24.32 | 35.46 |
| WMS-R: Figural Memory | 66.15 | 32.55 | 64.97 | 31.32 | 32.18 | 34.73 |
| WAIS-III: Visual Reproduction | 26.85 | 38.36 | 50.27 | 36.40 | 5.79 | 10.29 |
| TB: Visual Memory | 35.81 | 45.65 | 38.55 | 25.01 | 39.28 | 25.28 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.298 | 0.177 | 0.143 | 0.528 | 0.211 | 0.358 |
| WMS-R: Visual Paired Associates | 0.661 | 0.480 | 0.529 | 0.412 | 0.496 | 0.742 |
| WMS-R: Figural Memory | 0.021 | 0.677 | 0.053 | 0.600 | 0.529 | 0.157 |
| WAIS-III: Visual Reproduction | 0.654 | 0.171 | 0.208 | 0.335 | 0.530 | 0.483 |
| TB: Visual Memory | 0.408 | 0.269 | 0.425 | 0.644 | 0.470 | 0.556 |

Table A1.13. Results of the three-class classification of EEG data from neuropsychological tests using the SICAMM+BW method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | $\mathbf{y y y y y y}$ | Subject \#: |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 48.88 | 56.69 | 61.35 | 36.92 | 58.99 | 54.23 |
| WMS-R: Visual Paired Associates | 29.99 | 59.39 | 42.67 | 34.42 | 23.41 | 34.71 |
| WMS-R: Figural Memory | 48.62 | 45.77 | 64.97 | 28.12 | 19.43 | 39.46 |
| WAIS-III: Visual Reproduction | 31.02 | 36.32 | 28.70 | 34.04 | 5.05 | 14.71 |
| TB: Visual Memory | 30.88 | 66.67 | 44.70 | 23.74 | 60.10 | 30.45 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.286 | 0.198 | 0.076 | 0.487 | 0.155 | 0.244 |
| WMS-R: Visual Paired Associates | 0.912 | 0.192 | 0.529 | 0.420 | 0.524 | 0.762 |
| WMS-R: Figural Memory | 0.478 | 0.461 | 0.053 | 0.713 | 0.595 | 0.049 |
| WAIS-III: Visual Reproduction | 0.643 | 0.205 | 0.344 | 0.361 | 0.573 | 0.464 |
| TB: Visual Memory | 0.462 | 0.000 | 0.318 | 0.655 | 0.087 | 0.481 |

Table A1.14. Results of the three-class classification of EEG data from neuropsychological tests using the SICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| a) BER (\%) |  |  |  |  |  |  |  |
| Sternberg | 48.28 | 60.37 | 56.04 | 45.40 | 56.80 | 52.93 |  |
| WMS-R: Visual Paired Associates | 54.29 | 44.42 | 54.45 | 54.22 | 39.80 | 53.18 |  |
| WMS-R: Figural Memory | 60.42 | 48.88 | 53.26 | 47.34 | 44.68 | 40.05 |  |
| WAIS-III: Visual Reproduction | 40.47 | 56.25 | 51.67 | 36.94 | 19.12 | 31.96 |  |
| TB: Visual Memory | 38.32 | 56.50 | 43.75 | 37.78 | 39.80 | 33.48 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.342 | 0.124 | 0.132 | 0.393 | 0.212 | 0.241 |  |
| WMS-R: Visual Paired Associates | 0.298 | 0.452 | 0.307 | 0.193 | 0.345 | 0.357 |  |
| WMS-R: Figural Memory | 0.121 | 0.192 | 0.332 | 0.346 | 0.476 | 0.463 |  |
| WAIS-III: Visual Reproduction | 0.471 | 0.169 | 0.150 | 0.522 | 0.285 | 0.395 |  |
| TB: Visual Memory | 0.381 | 0.135 | 0.369 | 0.469 | 0.452 | 0.487 |  |

Table A1.15. Results of the three-class classification of EEG data from neuropsychological tests using the GSICAMM method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| Sternberg | 48.33 | 59.05 | 52.30 | 38.36 | 54.74 | 51.16 |  |
| WMS-R: Visual Paired Associates | 45.27 | 42.31 | 48.24 | 45.87 | 24.02 | 47.33 |  |
| WMS-R: Figural Memory | 52.28 | 33.59 | 45.27 | 38.01 | 16.39 | 19.07 |  |
| WAIS-III: Visual Reproduction | 36.90 | 50.48 | 32.70 | 33.64 | 10.20 | 11.54 |  |
| TB: Visual Memory | 28.99 | 39.32 | 38.83 | 22.15 | 37.89 | 24.38 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.363 | 0.140 | 0.184 | 0.466 | 0.176 | 0.274 |  |
| WMS-R: Visual Paired Associates | 0.509 | 0.415 | 0.442 | 0.230 | 0.507 | 0.506 |  |
| WMS-R: Figural Memory | 0.258 | 0.216 | 0.439 | 0.422 | 0.658 | 0.529 |  |
| WAIS-III: Visual Reproduction | 0.601 | 0.276 | 0.162 | 0.476 | 0.317 | 0.458 |  |
| TB: Visual Memory | 0.477 | 0.384 | 0.469 | 0.692 | 0.472 | 0.583 |  |

Table A1.16. Results of the three-class classification of EEG data from neuropsychological tests using the GSICAMM+BW method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | $\mathbf{y y y y y y}$ | Subject \#: |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 43.34 | 59.83 | 51.75 | 35.03 | 55.83 | 48.72 |
| WMS-R: Visual Paired Associates | 36.30 | 39.20 | 36.08 | 46.08 | 22.95 | 47.94 |
| WMS-R: Figural Memory | 51.11 | 33.23 | 48.36 | 33.88 | 15.18 | 17.20 |
| WAIS-III: Visual Reproduction | 37.24 | 45.24 | 31.80 | 31.82 | 10.13 | 15.54 |
| TB: Visual Memory | 24.07 | 41.68 | 39.84 | 24.63 | 36.22 | 22.69 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.401 | 0.128 | 0.199 | 0.509 | 0.170 | 0.302 |
| WMS-R: Visual Paired Associates | 0.771 | 0.444 | 0.770 | 0.225 | 0.543 | 0.488 |
| WMS-R: Figural Memory | 0.294 | 0.224 | 0.352 | 0.578 | 0.690 | 0.606 |
| WAIS-III: Visual Reproduction | 0.566 | 0.479 | 0.174 | 0.474 | 0.319 | 0.458 |
| TB: Visual Memory | 0.557 | 0.351 | 0.453 | 0.661 | 0.488 | 0.576 |

Table A1.17. Results of the three-class classification of EEG data from neuropsychological tests using the GSICAMM+VI method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| a) BER (\%) |  |  |  |  |  |  |  |
| Sternberg | 63.23 | 66.81 | 68.37 | 53.39 | 62.58 | 61.70 |  |
| WMS-R: Visual Paired Associates | 61.65 | 65.57 | 68.56 | 66.67 | 64.28 | 62.57 |  |
| WMS-R: Figural Memory | 66.26 | 67.80 | 68.94 | 64.63 | 67.11 | 66.67 |  |
| WAIS-III: Visual Reproduction | 66.67 | 62.80 | 64.83 | 65.41 | 66.67 | 65.82 |  |
| TB: Visual Memory | 58.92 | 65.74 | 68.37 | 49.29 | 73.39 | 49.91 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.051 | 0.003 | 0.041 | 0.301 | 0.095 | 0.112 |  |
| WMS-R: Visual Paired Associates | 0.132 | 0.017 | 0.038 | 0.000 | 0.044 | 0.118 |  |
| WMS-R: Figural Memory | 0.016 | 0.004 | 0.067 | 0.064 | 0.002 | 0.000 |  |
| WAIS-III: Visual Reproduction | 0.000 | 0.048 | 0.066 | 0.035 | 0.000 | 0.029 |  |
| TB: Visual Memory | 0.083 | 0.017 | 0.028 | 0.279 | 0.128 | 0.286 |  |

Table A1.18. Results of the three-class classification of EEG data from neuropsychological tests using the (nondynamic) BNT method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | Subject \#: |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |  |
| Sternberg | 57.50 | 61.49 | 56.27 | 48.41 | 60.69 | 50.16 |  |
| WMS-R: Visual Paired Associates | 46.73 | 73.21 | 65.92 | 66.67 | 45.67 | 38.49 |  |
| WMS-R: Figural Memory | 68.84 | 61.74 | 74.22 | 66.67 | 68.19 | 66.67 |  |
| WAIS-III: Visual Reproduction | 54.03 | 60.96 | 53.93 | 65.29 | 66.67 | 22.43 |  |
| TB: Visual Memory | 45.00 | 62.54 | 62.78 | 33.72 | 66.67 | 26.65 |  |
| b) Kappa |  |  |  |  |  |  |  |
| Sternberg | 0.190 | 0.109 | 0.134 | 0.410 | 0.139 | 0.300 |  |
| WMS-R: Visual Paired Associates | 0.493 | 0.134 | 0.011 | 0.000 | 0.085 | 0.750 |  |
| WMS-R: Figural Memory | 0.016 | 0.090 | 0.155 | 0.000 | 0.021 | 0.000 |  |
| WAIS-III: Visual Reproduction | 0.073 | 0.037 | 0.303 | 0.044 | 0.000 | 0.388 |  |
| TB: Visual Memory | 0.185 | 0.084 | 0.067 | 0.455 | 0.000 | 0.556 |  |

Table A1.19. Results of the three-class classification of EEG data from neuropsychological tests using the DBN method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

| Test | $\mathbf{7}$ | Subject \#: |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| a) BER (\%) | $\mathbf{1}$ | $\mathbf{2}$ | $\mathbf{3}$ | $\mathbf{4}$ | $\mathbf{5}$ | $\mathbf{6}$ |
| Sternberg | 65.56 | 66.67 | 63.40 | 63.83 | 63.77 | 66.67 |
| WMS-R: Visual Paired Associates | 69.63 | 58.29 | 62.45 | 65.81 | 66.67 | 58.13 |
| WMS-R: Figural Memory | 66.67 | 67.41 | 66.67 | 62.57 | 45.89 | 48.61 |
| WAIS-III: Visual Reproduction | 67.56 | 65.79 | 67.27 | 69.33 | 18.08 | 72.06 |
| TB: Visual Memory | 27.97 | 60.94 | 65.58 | 31.71 | 66.67 | 26.32 |
| b) Kappa |  |  |  |  |  |  |
| Sternberg | 0.009 | 0.000 | 0.020 | 0.061 | 0.067 | 0.000 |
| WMS-R: Visual Paired Associates | 0.047 | 0.084 | 0.070 | 0.016 | 0.020 | 0.241 |
| WMS-R: Figural Memory | 0.000 | 0.030 | 0.022 | 0.127 | 0.616 | 0.462 |
| WAIS-III: Visual Reproduction | 0.030 | 0.008 | 0.025 | 0.069 | 0.235 | 0.121 |
| TB: Visual Memory | 0.479 | 0.047 | 0.026 | 0.502 | 0.000 | 0.573 |

Table A1.20. Results of the three-class classification of EEG data from neuropsychological tests using the DBN2 method: a) balanced error rate (\%); b) Cohen's kappa coefficient.

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[^0]:    - ¿Cuándo empiezas, Johnny?
    -No sé. Hoy, creo, ¿eh, Dé?
    -No, pasado mañana.

[^1]:    Table 6.1. Estimated transition probabilities for the studied subjects.

