UNIVERSITAT POLITÈCNICA DE VALÈNCIA

DEPARTAMENTO DE INGENIERÍA HIDRÁULICA Y MEDIO AMBIENTE

TESIS DOCTORAL

ANÁLISIS DE LA DEPENDENCIA ESPACIO-TEMPORAL DE LA APORTACIÓN EN RÍOS MEDIANTE MODELIZACIÓN CAUSAL

Doctorando

Santiago Zazo del Dedo

Directores

Manuel Augusto	José Luis	Héctor
Pulido Velázquez	Molina González	Macián Sorribes

Valencia, julio 2025

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ANÁLISIS DE LA DEPENDENCIA ESPACIO-TEMPORAL DE LA APORTACIÓN EN RÍOS MEDIANTE MODELIZACIÓN CAUSAL

Tesis Doctoral, por compendio de artículos, para la obtención del Grado de Doctor por la Universitat Politènica de València

Programa de Doctorado en Ingeniería del Agua y Medioambiental

Doctorando

Santiago Zazo del Dedo

Directores

Dr. Manuel Augusto Pulido Velázquez	**Dr. José Luis Molina González**	**Dr. Héctor Macián Sorribes**

Valencia, julio 2025

“La Naturaleza nos es hostil porque no la conocemos…”

“…Escuchar sus latidos íntimos con el fervor de apasionada curiosidad, equivale a descifrar sus secretos…”.

Santiago Ramón y Cajal

Dedicado a:

Mari Cruz mi pareja, mis padres y herman@s.

Agradecimientos

No hay mejor frase para resumir el porqué de esta Tesis Doctoral que "*yo soy yo y mis circunstancias*[1]", ya lo fue en el año 2017 y lo vuelve a ser 8 años después.

Todo el que se enfrenta, o se ha enfrentado al desafío de una Tesis, conoce muy bien lo que supone y exige llegar hasta este punto. Sin lugar a duda, la determinación y la fuerza de voluntad son cualidades personales a las que debo agradecer encontrarme en esta situación, por segunda vez. Una situación que, no siendo nueva, me vuelve a generar las mismas sensaciones y emociones vividas. Sin embargo, por mucho empeño personal que uno tenga, alcanzar este reto es la consecuencia de una empresa colectiva.

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En segundo lugar, a mi familia por su comprensión del tiempo no dedicado. Agradecer, a mis padres Basi y Santiago los principios inculcados y la importancia del esfuerzo en la vida. A mi hermano Jorge Juan por su apoyo. Y en especial, a mi pareja Mari Cruz. Tú mejor que nadie sabes lo que esta Tesis ha supuesto. Gracias por estar a mi lado en los momentos difíciles, que los ha habido, por tu apoyo, por entender las motivaciones para pasar, otra vez, por todo lo que implica una Tesis, por sufrir mis ausencias en cuerpo y sobre todo en alma, por hacer fácil lo difícil; en definitiva, por ser mi mitad.

A todos, gracias por volver a hacer realidad lo que un día fue un sueño.

Santiago Zazo del Dedo

[1] José Ortega y Gasset. Meditaciones del Quijote, 1914.

ÍNDICE GENERAL

ÍNDICE DETALLADO

ÍNDICE DE FIGURAS[2]

[2] Los Capítulos II, III y IV reproducen prácticamente íntegras las versiones de autor de los artículos científicos que componen esta Tesis Doctoral, razón por la que el texto de las Figuras de esos capítulos está en idioma inglés.

ÍNDICE DE TABLAS[3]

[3] Los Capítulos II, III y IV reproducen prácticamente íntegras las versiones de autor de los artículos científicos que componen esta Tesis Doctoral, razón por la que el texto de las Tablas de esos capítulos está en idioma inglés.

TIPO DE TESIS

TÍTULO / *TÍTOL* / <u>*TITLE*</u>

Análisis de la dependencia espacio-temporal de la aportación en ríos mediante modelización causal.

Anàlisi de la dependència espaciotemporal de l'aportació en rius mitjançant modelització causal.

<u>*Spatial-temporal dependence analysis of rivers´ runoff through causal modelling.*</u>

MODALIDAD / *MODALITAT* / <u>*FORMAT*</u>

Tesis Doctoral por compendio de artículos.

Tesi Doctoral per compendi d'articles.

<u>*Doctoral Thesis through compentidum of articles/publications.*</u>

PROGRAMA DE DOCTORADO / *PROGRAMA DE DOCTORAT* / <u>*Ph.D. PROGRAM*</u>

Programa de Doctorado en Ingeniería del Agua y Medio Ambiente, según R.D. 99/2011, propuesto por la Universidad Politécnica de Valencia, España.

Programa de Doctorat en Enginyeria de l'Aigua i Medi Ambient, segons RD 99/2011, proposat per la Universitat Politècnica de València, Espanya.

<u>*Ph.D. Programme in Water and Environmental Engineering, according to R.D. 99/2011, proposed by the Universitat Politècnica de València, Spain.*</u>

Esta Tesis Doctoral, redactada en la modalidad de compendio de artículos, está compuesta por tres artículos de investigación, previamente aceptados y publicados en prestigiosas revistas científicas[4] internacionales de impacto (sujetas a evaluación crítica mediante revisiones anónimas, por pares expertos internacionales, de reconocida trayectoria), en el ámbito de la Hidrología y la Gestión de Recursos Hídricos; siendo todas ellas indexadas en las bases de datos Journal Citation Report (JCR) y SCImago Journal Rank (SJR), en el primer cuartil (Q1):

1. **Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling**

   Macian-Sorribes, H., Molina, J.L., Zazo, S., Pulido-Velázquez, M. 2020. Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling. *Journal of Hydrology*, 597, 125722. https://doi.org/10.1016/j.jhydrol.2020.125722.

2. **Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework**

   Zazo, S., Martín, A. M., Molina, J.L., Macian-Sorribes, H., Pulido-Velázquez, M. 2022. Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework. *Journal of Hydrology*, 610, 127832. https://doi.org/10.1016/j.jhydrol.2022.127832.

3. **Assessment of the predictability of inflow to reservoirs through Bayesian causality**

   Zazo, S., Molina, J.L., Macian-Sorribes, H., Pulido-Velazquez, M. 2023. Assessment of the predictability of inflow to reservoirs through Bayesian Causality. *Hydrological Sciences Journal*, 68:10, 1323-1337. https://doi.org/10.1080/02626667.2023.2200143.

[4] Journal of Hydrology, publicación indexada en el primer cuartil (Q1) primer decil, categoría: *Water Resources* según *Journal Citation Reports*, categoría: *Water Resources*, años 2021 y 2022.

Hydrological Sciences Journal, publicación indexada en el primer cuartil (Q1), categoría: *Water Science and Technology* según *SCImago Journal Rank*, y en el segundo cuartil (Q2) según *Journal Citation Reports*, categoría: *Water Resources,* año 2023.

Ver Apéndice II "Índices de calidad de las revistas científicas".

Por otro lado, las investigaciones desarrolladas en esta Tesis Doctoral han dado lugar a cuatro contribuciones presentadas en Congresos Internacionales; una en el ámbito de la Ingeniería de modelización y validación (ICEUBI2019), y tres en el de la Estadística e Hidrología (ICSH STAHY 2021). Todas ellas, también, previamente evaluadas mediante revisiones anónimas, por expertos internacionales:

- **Qualitative approach for assessing runoff temporal dependence through geometrical symmetry**

  Presentación oral: Santiago Zazo

  Zazo, S., Macian-Sorribes, H., Sena-Fael, C.M., Martín-Casado, A.M., Molina, J.L. and Pulido-Velazquez, M. 2019. Qualitative approach for assessing runoff temporal dependence through geometrical symmetry. (Contributed Paper). Proceedings Internacional Congress on Engineering. Engineering for Evolution (ICEUBI2019). 27 - 29 November 2019, Covilhã, Portugal.

- **Innovative spatio temporal time series analysis through Causal Reasoning**

  Presentación oral: Santiago Zazo.

  Zazo, S., Molina, J.L., Macian-Sorribes, H. and Pulido-Velazquez, M. 2021. Innovative spatio temporal time series analysis through Causal Reasoning. (Contributed Paper). Workshop ICSH STAHY 2021. International Association of Hydrological Sciences (IAHS) and the Research Institute of Water and Environmental Engineering (IIAMA) of the Universitat Politècnica de València. 16 - 17 September 2021, Valencia, Spain.

- **Analysis of predictability of uncertain inflows to reservoirs**

  Presentación oral: Santiago Zazo.

  Zazo, S., Molina, J.L., Macian-Sorribes, H. and Pulido-Velazquez, M. 2021. Analysis of predictability of uncertain inflows to reservoirs. (Contributed Paper). Workshop ICSH STAHY 2021. International Association of Hydrological Sciences (IAHS) and the Research Institute of Water and Environmental Engineering (IIAMA) of the Universitat Politècnica de València. 16 - 17 September 2021, Valencia, Spain.

- **Advances in the analysis of the spatio-temporal properties of multivariate hydrological time series based on Information Theory**

  Presentación oral (corta): Santiago Zazo.

  Zazo, S., Molina, J.L., Macian-Sorribes, H. and Pulido-Velazquez, M. 2021. Advances in the analysis of the spatio-temporal properties of multivariate hydrological time series based on Information Theory. (Contributed Paper). Workshop ICSH STAHY 2021. International Association of Hydrological Sciences (IAHS) and the Research Institute of Water and Environmental Engineering (IIAMA) of the Universitat Politècnica de València. 16 - 17 September 2021, Valencia, Spain.

RESUMEN

Es evidente como la alteración de los patrones espacio-temporales de los eventos meteorológicos y climáticos influye en los procesos hidrológicos; incrementando su incertidumbre, dificultando su predicción, y provocando una mayor presión sobre los recursos hídricos. A su vez, esta realidad supone un escenario complejo para la sostenibilidad y disponibilidad de los recursos hídricos, y en especial de los superficiales. Sin embargo, ofrece un reto científico para el desarrollo de nuevos enfoques que permitan aumentar la resiliencia hídrica de un territorio, basados en el conocimiento.

Por otro lado, la aplicación del paradigma de la Inteligencia Artificial al ámbito hidrológico ha supuesto un punto de inflexión a la hora de abordar el análisis "profundo" de la información (datos, interrelaciones, etc.), dando lugar a avances significativos en la causalidad, la inferencia causal a partir de datos observacionales y la cuantificación de la incertidumbre. En las últimas décadas, son reseñables las innovaciones en este campo sobre modelos gráficos, lo que ha provocado que éstos hayan ganado notoriedad entre la comunidad científica. Esto se debe a su formalismo intuitivo, que permite modelar estructuras de datos mediante un conjunto de nodos y aristas que definen una red. De entre estos modelos, destacan las redes neuronales, con un amplio y diverso espectro de enfoques metodológicos, y las redes bayesianas. Sin embargo, éstas últimas han recibido mucha menor atención, especialmente en su aplicación al descubrimiento de estructuras causales en series temporales; si bien, presentan características de interés para abordar este desafío. Principalmente, las redes bayesianas destacan por su capacidad para abordar problemas de razonamiento en condiciones de incertidumbre (razonamiento plausible); la posibilidad de incorporar el conocimiento experto en el proceso, además de la inferencia y el razonamiento omnidireccional (dinamismo) ante cualquier evidencia sobre la red, total o parcial.

Las características distintivas de las redes bayesianas, junto con el reto de descubrir estructuras causales en series temporales hidrológicas, han inspirado esta Tesis Doctoral desde la perspectiva de la modelización causal (Causalidad Bayesiana). Esta novedosa área de investigación hidrológica, implementada mediante redes bayesianas, se basa en el Razonamiento Causal como metodología de análisis centrada en la causa, y cuyo objetivo es predecir su efecto o consecuencia. Para este fin, se ha diseñado un innovador marco metodológico que ha permitido evaluar su potencial para mejorar el conocimiento espacio-temporal de los recursos hídricos superficiales, y su aplicación a la predicción hidrológica. A su vez, este marco ha permitido descubrir la estructura lógica causal temporal, y/o espacio-temporal que caracteriza la respuesta hidrológica de una o varias cuencas. Dicha estructura, latente en los registros temporales hidrológicos, define el comportamiento de los recursos hídricos superficiales, y hasta ahora no había sido investigada suficientemente, a pesar del potencial que este enfoque supone.

Asimismo, la modelización causal bayesiana ha permitido identificar interacciones espacio-temporales claves a partir de la señal de dependencia presente en los registros históricos hidrológicos. Interacciones, incluso débiles, que se han podido poner de manifiesto en el caso de cuencas con un comportamiento temporal esencialmente independiente, y un limitado número de registros; condiciones éstas bajo las que también se ha evaluado su capacidad de predicción. Asimismo, ha sido posible optimizar los factores claves implicados en el proceso de aprendizaje-entrenamiento de los modelos causales bayesianos, como son el número de series sintéticas y los intervalos de las distribuciones discretas de probabilidad de los datos sintéticos.

En resumen, la modelización causal (Causalidad Bayesiana), a partir de los registros temporales de aportaciones, ha demostrado ser un enfoque eficiente y robusto para su aplicación al análisis y predicción de procesos naturales complejos como los hidrológicos.

RESUM

És evident com l'alteració dels patrons espaciotemporals dels esdeveniments meteorològics i climàtics influïx en els processos hidrològics; incrementant la seua incertesa, dificultant la seua predicció, i provocant una major pressió sobre els recursos hídrics. Al seu torn, esta realitat suposa un escenari complex per a la sostenibilitat i disponibilitat dels recursos hídrics, i especialment dels superficials. No obstant això, oferix un repte científic per al desenrotllament de nous enfocaments que permeten augmentar la resiliència hídrica d'un territori, basats en el coneixement.

D'altra banda, l'aplicació del paradigma de la Intel·ligència Artificial a l'àmbit hidrològic ha suposat un punt d'inflexió a l'hora d'abordar l'anàlisi "profunda" de la informació (dades, interrelacions, etc), donant lloc a avanços significatius en la causalitat, la inferència causal a partir de dades observacionals i la quantificació de la incertesa. En les últimes dècades, són ressenyables les innovacions en este camp sobre models gràfics, la qual cosa ha provocat que estos hagen guanyat notorietat entre la comunitat científica. Això es deu al seu formalisme intuïtiu, que permet modelar estructures de dades mitjançant un conjunt de nodes i arestes que definixen una xarxa. D'entre estos models, destaquen les xarxes neuronals, amb un ampli i divers espectre d'enfocaments metodològics, i les xarxes bayesianes. No obstant això, estes últimes han rebut molta menor atenció, especialment en la seua aplicació al descobriment d'estructures causals en sèries temporals; si bé, presenten característiques d'interés per a abordar este desafiament. Principalment, les xarxes bayesianes destaquen per la seua capacitat per a abordar problemes de raonament en condicions d'incertesa (raonament plausible); la possibilitat d'incorporar el coneixement expert en el procés, a més de la inferència i el raonament omnidireccional (dinamisme) davant qualsevol evidència sobre la xarxa, total o parcial.

Les característiques distintives de les xarxes bayesianes, juntament amb el repte de descobrir estructures causals en sèries temporals hidrològiques, han inspirat esta Tesi Doctoral des de la perspectiva de la modelització causal (Causalitat Bayesiana). Esta nova àrea d'investigació hidrològica, implementada mitjançant xarxes bayesianes, es basa en el Raonament Causal com a metodologia d'anàlisi centrada en la causa, i l'objectiu de la qual és predir el seu efecte o conseqüència. Per a este fi, s'ha dissenyat un innovador marc metodològic que ha permés avaluar el seu potencial per a millorar el coneixement espaciotemporal dels recursos hídrics superficials, i la seua aplicació a la predicció hidrològica. Al seu torn, este marc ha permés descobrir l'estructura lògica causal temporal, i/o espaciotemporal que caracteritza la resposta hidrològica d'una o diverses conques. Esta estructura, latent en els registres temporals hidrològics, definix el comportament dels recursos hídrics superficials, i fins ara no havia sigut investigada suficientment, malgrat el potencial que este enfocament suposa.

Així mateix, la modelització causal bayesiana ha permés identificar interaccions espaciotemporals claus a partir del senyal de dependència present en els registres històrics hidrològics. Interaccions, fins i tot febles, que s'han pogut posar de manifest en el cas de conques amb un comportament temporal essencialment independent, i un limitat nombre de registres; condicions estes sota les quals també s'ha avaluat la seua capacitat de predicció. Així mateix, ha sigut possible optimitzar els factors claus implicats en el procés d'aprenentatge-entrenament dels models causals bayesians, com són el nombre de sèries sintètiques i els intervals de les distribucions discretes de probabilitat de les dades sintètiques.

En resum, la modelització causal (Causalitat Bayesiana), a partir dels registres temporals d'aportacions, ha demostrat ser un enfocament eficient i robust per a la seua aplicació a l'anàlisi i predicció de processos naturals complexos com els hidrològics.

SUMMARY

It is evident how the alteration of the spatiotemporal patterns of meteorological and climatic events influences hydrological processes, increasing their uncertainty, making their prediction more difficult, and causing higher pressure on water resources. In turn, this reality represents a complex scenario for the sustainability and availability of water resources, especially surface ones. However, it offers a scientific challenge for the development of new approaches to increase the water resilience of a territory, based on knowledge.

On the other hand, the application of the Artificial Intelligence paradigm to the hydrological field has been a turning point in the approach to the "deep" analysis of information (data, interrelationships, etc.), leading to significant advances in causality, causal inference from observational data and uncertainty quantification. In the last decades, the innovations in this field on graphical models have been remarkable, which have gained notoriety among the scientific community. This is due to their intuitive formalism, which allows data structures to be modelled by means of a set of nodes and edges that define a network. Among these models, neural networks, with a wide and diverse spectrum of methodological approaches, and Bayesian networks stand out. However, the latter have received much less attention, especially in their application to the discovery of causal structures in the time series, although they present interesting features to address this challenge. Mainly, Bayesian networks stand out for their ability to address reasoning problems under conditions of uncertainty (plausible reasoning); the possibility of incorporating expert knowledge in the process, in addition to omnidirectional inference and reasoning (dynamism) in the face of any evidence on the network, total or partial.

The distinctive features of Bayesian networks, together with the challenge of discovering causal structures in hydrological time series, have inspired this Doctoral Thesis from the perspective of causal modeling (Bayesian Causality). This novel area of hydrological research, implemented by means of Bayesian networks, is based on Causal Reasoning as an analysis methodology focused on the cause, and whose objective is to predict its effect or consequence. For this purpose, an innovative methodological framework has been designed to evaluate its potential for improving spatio-temporal knowledge of surface water resources and its application to hydrological forecasting. In turn, this framework has made it possible to discover the temporal and/or spatio-temporal causal logical structure that characterizes the hydrological response of one or several basins. This structure, latent in the hydrological temporal records, defines the behavior of surface water resources, and until now has not been sufficiently investigated, despite the potential of this approach.

Likewise, Bayesian causal modeling has made it possible to identify key spatio-temporal interactions from the dependence signal present in the historical hydrological records. These interactions, even weak, have been revealed in the case of basins with an essentially independent temporal behavior and a limited number of records; conditions under which their predictive capacity has also been evaluated. Likewise, it has been possible to optimize the key factors involved in the learning-training process of Bayesian causal models, such as the number of synthetic series and the intervals of the discrete probability distributions of the synthetic data.

In summary, causal modeling (Bayesian causality), from temporal runoff time series, has proven to be an efficient and robust approach for its application to the analysis and prediction of complex natural processes such as hydrological ones.

CAPÍTULO I

Introducción

I.1 MOTIVACIÓN

Las ideas fundamentales que inspiran esta Tesis Doctoral son el Agua como principio de todas las cosas según Tales de Mileto[5] (*"arche"* filosófico griego clásico), junto con el deseo humano por el conocimiento[6] y una visión causa-efecto de hostilidad hacia la Naturaleza por su desconocimiento[7].

Las tres premisas anteriores han sido la "*piedra angular*" de esta investigación, basada en modelos causales sobre datos observacionales desde una perspectiva bayesiana, como metodología para reducir la incertidumbre sobre una realidad hidrológica, parcialmente conocida, que se aspira a conocer para su predicción.

I.2 INTERÉS DE LA INVESTIGACIÓN

Es evidente que los patrones espacio-temporales de los eventos meteorológicos y climáticos están experimentando cambios significativos a nivel local y global (Molina y Zazo, 2018; Rubio-Martin et al., 2023), induciendo modificaciones evidentes en los procesos hidrológicos. Entre los factores que explican este cambio destaca el cambio climático (IPCC, 2023; Marotzke et al., 2017; O'Gorman 2015; Suárez-Almiñana, 2021). Esta realidad es la causa de eventos extremos cada vez más recurrentes y de mayor intensidad (IPCC 2023; Rubio-Martin et al., 2023; Sanchez-Matos et al., 2023), lo que incrementa su inherente aleatoriedad e incertidumbre (Ochoa-Rivera et al., 2007; Ochoa-Rivera, 2008; Zazo, 2017); y deriva en una mayor presión sobre los recursos hídricos (Ali et al., 2022; Battistelli et al., 2023; Zazo et al., 2020).

Por su parte, según CEDEX (2017) y UNFCCC (2021) las proyecciones regionalizadas de impactos y riesgos del Cambio Climático sobre el ciclo hidrológico en España pronostican una disminución de las precipitaciones medias anuales y una reducción generalizada de los caudales de los ríos. Todo ello unido, además, a una disminución de la recarga de los acuíferos; un incremento de las sequías cada vez más frecuentes y de mayor duración, y un incremento de eventos extremos de inundaciones y precipitaciones torrenciales. Además, estos riesgos se prevén más acusados conforme

[5] Al no disponerse de texto escritos por Tales, se recurre como fuente a "*Metafísica*" de Aristóteles, donde se define a Tales de Mileto como "*archegós*" o iniciador en griego clásico, y se describe su teoría sobre el agua como principio de la Naturaleza. Véase Solana Dueso (2009), página 12.

[6] Aristóteles. Metafísica. "Todos los hombres desean por naturaleza saber".

[7] Santiago Ramón y Cajal. Recuerdos de mi vida. Segunda parte. Historia de mi labor científica. Capítulo XXVII 1917.

avance el siglo XXI y para los escenarios de mayores emisiones de gases de efecto invernadero. Recientes estudios cuantifican estos impactos con una reducción de las precipitaciones superior a 50 mm/°C y una probable disminución de la disponibilidad hídrica de entre un 2 y 15% por cada 2°C de calentamiento (Lionello y Scarascia, 2018; Solans et al., 2023).

Esta situación plantea un escenario complejo para la sostenibilidad y disponibilidad de los recursos hídricos. Sin embargo, a su vez ofrece un reto para el desarrollo de enfoques innovadores capaces de abordar la incertidumbre en la predicción, y que permitan capturar la estructura lógica característica de la respuesta hidrológica de una cuenca (implícitamente latente en los registros hidrológicos; Zazo et al., 2020), y que explica el comportamiento de sus recursos hídricos (Macian-Sorribes et al., 2020; Molina et al., 2019; Zazo et al., 2023). Respuesta que se enmarca en un contexto de causa-efecto, típico de las cuestiones hidrometeorológicas (Ombadi et al., 2020).

Por tanto, para aumentar la resiliencia hídrica de un territorio, es esencial descubrir ese "conocimiento oculto", siendo clave el desarrollo de marcos metodológicos novedosos, fiables y robustos de modelización y predicción espacio-temporal, y donde la Causalidad[8] tiene mucho que aportar. En este sentido, estudios como Runge et al., (2019) y Reichstein et al., (2019) han puesto ya de manifiesto cómo el descubrimiento causal es capaz de mejorar la representatividad de los sistemas físicos, generando modelos más interpretables y parsimoniosos.

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[8] La Causalidad se aborda en esta Tesis, conceptualmente, como una relación entre variables, de acuerdo con Pearl et al., (2016), donde se considera que una variable $\boldsymbol{X}$ es la causa de otra variable $\boldsymbol{Y}$ si el valor de $\boldsymbol{Y}$ depende o está influido por $\boldsymbol{X}$ en cualquier circunstancia; de esta forma el estado o valor de una variable (efecto) dependen del estado de la otra (causa).

El término "Causalidad" ha evolucionado a lo largo del tiempo, desde las definiciones filosóficas propuestas por David Hume en 1739 y 1748, empíricas fundamentadas en la contigüidad, sucesión en el tiempo y conjunción constante (Álvarez, 1992), la actualización de éstas mediante las Condiciones INUS (*Insufficient but Necessary part of an Unnecessary but Sufficient condition*; Mackie, 1965), donde se define la causa "*como una condición que quizá sea insuficiente por sí misma para producir el efecto, pero que forma parte no redundante de un conjunto de condiciones que pueden ser innecesarias pero suficientes*", pasando por el concepto de Causalidad Probabilística basado en la idea de que la causa incrementa la probabilidad del efecto (Suppes, 1970), la Causalidad de Granger (aplicada al análisis de series temporales; Granger, 1969) cuyo objetivo es averiguar si una variable es indicativa de otra, hasta la definición propuesta en Pearl y Mackenzie (2018) para ciencias empíricas, en términos de causas y efectos para entender la realidad, desde el novedoso enfoque de la "Escalera de causalidad (Ladder of causation)", estructurada en un modelo de tres niveles, basado en "ver", "hacer" e "imaginar" (Nivel 1: Observación; Nivel 2: Intervención y Nivel 3: Contrafactuales o razonamiento sobre escenarios hipotéticos; Stone, 2020).

En la Causalidad y los métodos de descubrimiento causal destacan, por su impacto científico, las investigaciones llevadas a cabo por Granger[9] y Pearl[10]. El primero, por su pionero trabajo (Granger, 1969), donde se proponía un método para evaluar la causalidad entre dos conjuntos de variables basado en la predicción, la direccionalidad (dirección de causalidad entre las variables) y la hipótesis (aparentemente trivial e intuitiva[11]) de que la causa precede al efecto en el tiempo. El segundo, por su parte, introdujo los modelos probabilísticos gráficos (principalmente las redes bayesianas) y los diagramas causales en los problemas de razonamiento causal, con trabajos como Pearl (1988, 1995, 2009).

A su vez, en el campo de la inferencia causal a partir de datos observados se han continuado produciendo avances (Ombadi et al., 2020), abarcando un espectro heterogéneo de temáticas. De entre éstas, destacan el estudio de los factores generadores de la circulación invernal en el Ártico (Kretschmer et al., 2016), la relación entre la humedad del suelo y la precipitación en las regiones de latitudes bajas y medias del hemisferio norte (Wang et al., 2018), el análisis de las relaciones causales para descubrir los factores impulsores de la evapotranspiración estival e invernal (Ombadi et al., 2020), o la conectividad hidrológica en áreas de deltas fluviales (Sendrowski y Passalacqua, 2017).

Asimismo, en los últimos años, los modelos gráficos han ido ganando notoriedad entre la comunidad científica, principalmente debido a ser intuitivos y a la vez capaces de modelar estructuras de datos provenientes de sistema complejos. Estos modelos emplean un conjunto de nodos y aristas, que definen las relaciones de (in)dependencia del conjunto de variables que definen el modelo (Gutiérrez et al., 2009). De esta forma es posible, por ejemplo desarrollar análisis dinámicos espacio-temporales de sequías, basados en el análisis de Zonas Contiguas de Sequías y el Índice de Precipitación Evapotranspiración Estandarizada (Diaz et al., 2020); explorar las firmas (huellas) hidrológicas de los patrones espaciales y temporales para mejorar la predicción de caudales mediante Redes Neuronales Gráficas (Sun et al., 2021); comparar el rendimiento entre distintos enfoques

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[9] Premio Nobel de Economía, año 2003, compartido por F. Engle y Clive W.J. Granger, por sus aportaciones en el campo de las series temporales permitiendo la incorporación de la influencia de elementos no previsibles. De acuerdo con Ombadi et al., (2020) la Causalidad de Granger "*quizá sea el primer método práctico para comprobar la causalidad*".

[10] Premio Turing, año 2011, por sus contribuciones a la Inteligencia Artificial a través del desarrollo del cálculo de probabilidad y el razonamiento causal.

[11] Ombadi et al., (2020) pone de manifiesto como debilidad del método propuesto por Granger (1969), su incapacidad para detectar la causalidad simultánea, ya que la Causalidad se interpreta en función del orden temporal de los acontecimientos.

de redes neuronales, como las de Memoria a Largo-Corto plazo y las Wavelet, para la predicción espacio-temporal de tendencias en series temporales de precipitación y escorrentía a partir de registros meteorológicos satelitales (Ouma et al., 2021); modelizar, basado en series temporales, las dependencias espaciotemporales entre estaciones de una red fluvial mediante un gráfico de correlación parcial (Venna et al., 2021); estimar la correlación espacio-temporal entre series temporales de escorrentía de dos embalses a través de Redes Generativas Adversativas (Ma et al., 2022); o mediante una red neuronal de grafos heterogéneos espaciotemporales modelar la heterogeneidad espacial y la correlación de las variables hidrometeorológicas para predecir inundaciones (Luo et al., 2024).

Una de las metodologías más prometedoras dentro de los modelos gráficos son las redes bayesianas. Vogel et al., (2014) enumera sus principales características a través de seis propiedades: Propiedad-1: su estructura proporciona información sobre los procesos que en ella subyacen y en el modo en el que las variables se relacionan y comparten información, conforme ésta se propaga por la red; Propiedad-2: su interpretación intuitiva permite su definición a partir de conocimientos previos (conocimiento experto), el aprendizaje a partir de datos, o una combinación de ambos; Propiedad-3: identifican las variables relevantes; Propiedad-4: puede propagar la incertidumbre fácilmente entre cualquier nodo, estimando distribuciones de probabilidad en lugar de valores puntuales; Propiedad-5: posibilitan la inferencia y el razonamiento omnidireccional; y Propiedad-6: las observaciones incompletas de datos no son un problema ya que afectan exclusivamente a la incertidumbre global. Asimismo, hay que reseñar la capacidad que las redes bayesianas tienen para definir un único modelo sobre el que se propagan las evidencias, frente a la necesidad de usar modelos específicos para cada conjunto de variables evidenciales en el caso de las redes neuronales (Ancell Trueba, 2009), además de su idoneidad para el aprendizaje estructural no supervisado (Molina y Zazo, 2017).

Por contra, las redes neuronales presentan dos debilidades frente a las redes bayesianas; no permiten considerar la incertidumbre, y no son capaces de incorporar el conocimiento experto en el proceso (Rodríguez y Dolado, 2007)[12].

En el contexto de los recursos hídricos, las redes bayesianas se han aplicado con éxito a la gestión de embalses (Mediero et al., 2007), la evaluación del impacto ambiental de grandes presas (Ahmadi et al., 2015), el análisis y predicción de daños por inundaciones (Schroeter et al., 2014; Zhang et al., 2023), la sostenibilidad de cuencas bajo escenarios de cambio climático (Chanapathi y Thatikonda, 2020), la predicción de niveles de acuíferos (Moghaddam et al., 2019) y su gestión (Molina y García-Aróstegui, 2023), así como la resolución de problemas de demanda de servicios ecosistémicos (Pham et al., 2021). Sin embargo, aún no se ha investigado a fondo su aplicación al descubrimiento de estructuras causales en series temporales de registros hidrológicos (Macian-Sorribes et al., 2020; Zazo et al., 2022, 2023).

Por las razones anteriores, esta Tesis Doctoral aborda el descubrimiento de las relaciones espacio-temporales en cuencas hidrográficas mediante Causalidad Bayesiana. Esta novedosa área de investigación hidrológica se basa en el Razonamiento Causal implementado a través de Redes Bayesianas (Pearl, 2009). Este enfoque se ha demostrado eficiente y robusto a la hora de identificar interacciones espacio-temporales (dependencias condicionales), a partir de una mínima señal de dependencia presente en los registros históricos hidrológicos, e incluso en cuencas con un comportamiento temporal esencialmente independiente.

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[12] Véase "Técnicas cuantitativas para la gestión en la ingeniería del software", Capítulo 10: "Redes bayesianas en la ingeniería del software" página 220:

> De acuerdo con Rodríguez y Dolado (2007), *"...las redes neuronales producen muy buenos resultados en bases de datos con muchas instancias. Sin embargo, a diferencia de las redes Bayesianas, las redes neuronales no consideran la incertidumbre. Además, las redes neuronales actúan como una caja negra en el sentido de que no es posible saber cómo se ha llegado a los resultados obtenidos, ni los nodos intermedios pueden ser interpretados. En las redes Bayesianas todos los nodos y las tablas de probabilidad pueden ser interpretados con respecto al dominio. Otra desventaja de las redes neuronales con respecto a las Bayesianas, es que no pueden incorporar conocimiento de los expertos del dominio, solo pueden ser generadas mediante entrenamiento usando bases de datos y si se incrementa el número de registros en la base de datos hay que entrenar de nuevo a la red"*.

I.3 OBJETIVOS DE LA INVESTIGACIÓN

El Objetivo General de esta Tesis Doctoral es evaluar el potencial de la modelización causal bayesiana para la mejora del conocimiento espacio-temporal de los recursos hídricos superficiales, y su aplicación en la predicción hidrológica. Esto supone el desarrollo de un marco metodológico que permita el descubrimiento de la estructura lógica de interdependencia espacio-temporal de los recursos hídricos superficiales, tanto en cuencas adyacentes como individuales, y que definen su comportamiento.

Para la consecución de este objetivo se han definido los siguientes Objetivos Específicos (OE):

- OE-1: Avanzar en el descubrimiento de estructuras causales temporales y espacio-temporales, en cuencas hidrográficas en régimen natural.
- OE-2: Proponer un marco metodológico para optimizar los factores claves implicados en el proceso de aprendizaje-entrenamiento de los modelos causales bayesianos.
- OE-3: Proponer un nuevo indicador dinámico del comportamiento temporal de las series hidrológicas de aportaciones, a través de la propagación de la fuerza de dependencia temporal en el tiempo, inicialmente a escala anual.
- OE-4: Validar el marco metodológico desarrollado y el nuevo indicador dinámico de comportamiento temporal propuesto, comparando con metodologías estadísticas y/o la Teoría de la Información.

I.4 HIPÓTESIS DE TRABAJO

Esta investigación se fundamenta en la aplicación de nuevas estrategias y metodologías de análisis, modelado y predicción sobre series temporales hidrológicas de aportaciones. En el contexto anterior se han planteado las siguientes hipótesis:

- La capacidad de análisis omnidireccional que los modelos causales bayesianos ofrecen puede permitir detectar y cuantificar las relaciones espacio-temporales claves entre las variables que simulan las aportaciones de una o varias cuencas.
- El hecho de que las series temporales hidrológicas sean un conjunto ordenado de datos puede dar lugar a la presencia de una señal de dependencia, que podría poner de manifiesto la existencia de una estructura lógica subyacente en la serie.

- El descubrimiento de una estructura lógica causal permite conocer más en detalle el comportamiento espacio-temporal de los recursos hídricos superficiales, y servir de base para la generación de modelos predictivos.

I.5 CASOS DE ESTUDIO

El objetivo general de esta Tesis implica la elección de zonas de estudio relevantes y adecuadas. En primer lugar, por el comportamiento de sus recursos hídricos superficiales, por las posibles interacciones espaciales entre cuencas, y por su (in)dependencia temporal individual. Y, en segundo lugar, por factores como su morfológica, geología, hidrogeología y actividades antropogénicas, que condicionan el caudal de un río (Madsen et al., 2014). Igualmente, es preciso considerar también la irregular distribución de las precipitaciones en la España peninsular (MITECO, 2024), que condiciona y caracteriza la extrema variabilidad de los recursos hídricos superficiales (Garrote et al., 2007), con un "norte húmedo" y un "sur seco". Esta particularidad presenta un marcado gradiente positivo respecto de la latitud y una asimetría meridional que aumenta con la altitud (Martín Vide, 1994), y que en las zonas áridas y semiáridas mediterráneas puede llegar a ser crítica debida al impacto del cambio climático (Rubio-Martin et al., 2023).

Con las premisas anteriores, los casos de estudio se han localizado en las Demarcaciones Hidrográficas del Júcar (DHJ) y del Duero (DHD), con dos categorías diferenciadas: los de carácter aplicativo y los de índole metodológica. Los primeros se han localizado en la DHJ, habiendo sido seleccionadas las subcuencas altas de los ríos Júcar y Cabriel que alimentan a los embalses de Alarcón y Contreras (ver Capítulo II), y Guadalaviar-Turia (Embalse de Arquillo de San Blas) y Alfambra. Asimismo, se consideran las cabeceras de las subcuencas de los ríos Cabriel y Mijares (de forma aislada) por su comportamiento temporal. Los segundos, ubicados en la DHD, se han seleccionan exclusivamente atendiendo a su casuística distintiva individual temporal. En este caso se han escogido las cabeceras de las subcuencas de los ríos Porma, en el norte de la DHD, perteneciente al subsistema "Esla-Valderaduey" y caracterizada por un comportamiento dependiente; y los ríos Voltoya, Adaja y Chico, en el sur, integrados en el subsistema Cega-Eresma-Adaja, con un comportamiento esencialmente independiente (ver Capítulos III y IV). En total diez han sido los casos de estudio considerados (Figura I.1), cuatro de carácter aplicativo, otros cuatro metodológicos y dos en ambas categorías, siendo estos últimos los casos de los ríos Porma y Adaja. La evaluación preliminar de las dependencias espacio-temporales y temporales de cada uno de los casos de estudio considerados se llevó a cabo mediante correlogramas (Figuras I.2 y I.3).

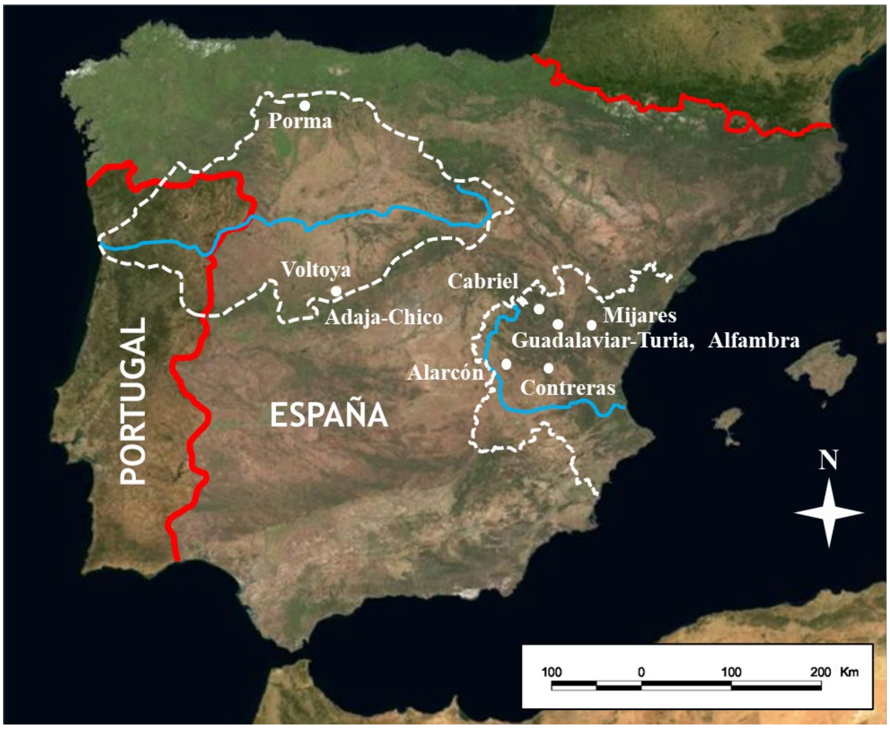

Figura I.1: Localización de los casos de estudio considerados. Fuente: IDEE (2023).

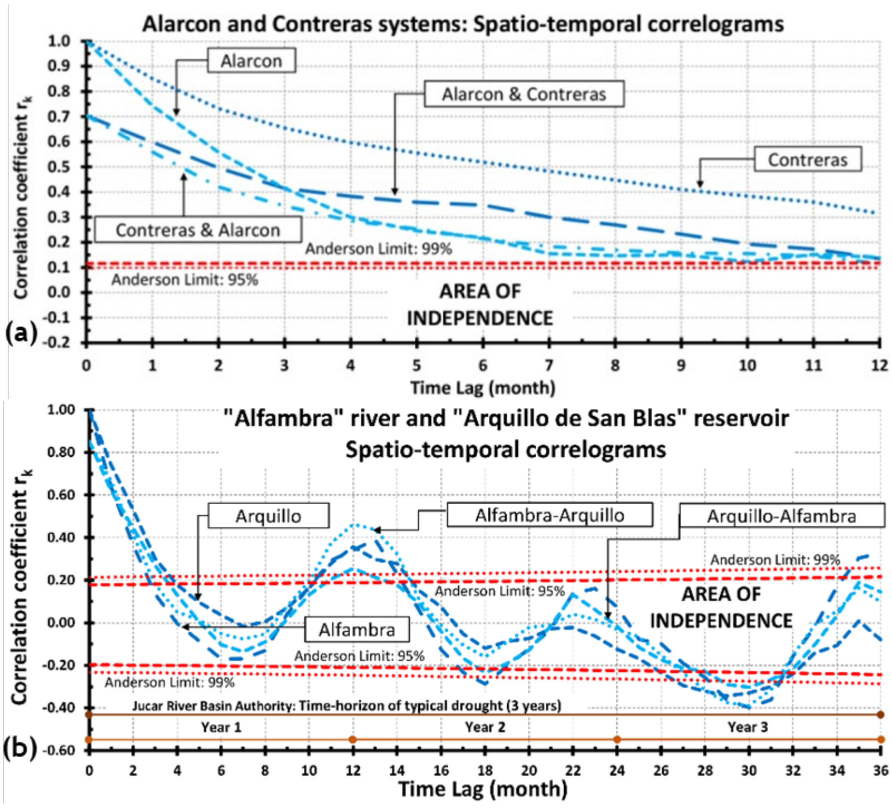

Figura I.2: Correlogramas espacio-temporales. (a) Embalses de Alarcón, río Júcar y Contreras ríos Cabriel y Guadazaón (Macian-Sorribes et al., 2020). (b) Embalse de Arquillo de San Blas, río Guadalaviar-Turia y río Alfambra estación de aforo 8027 (Zazo et al., 2021b).

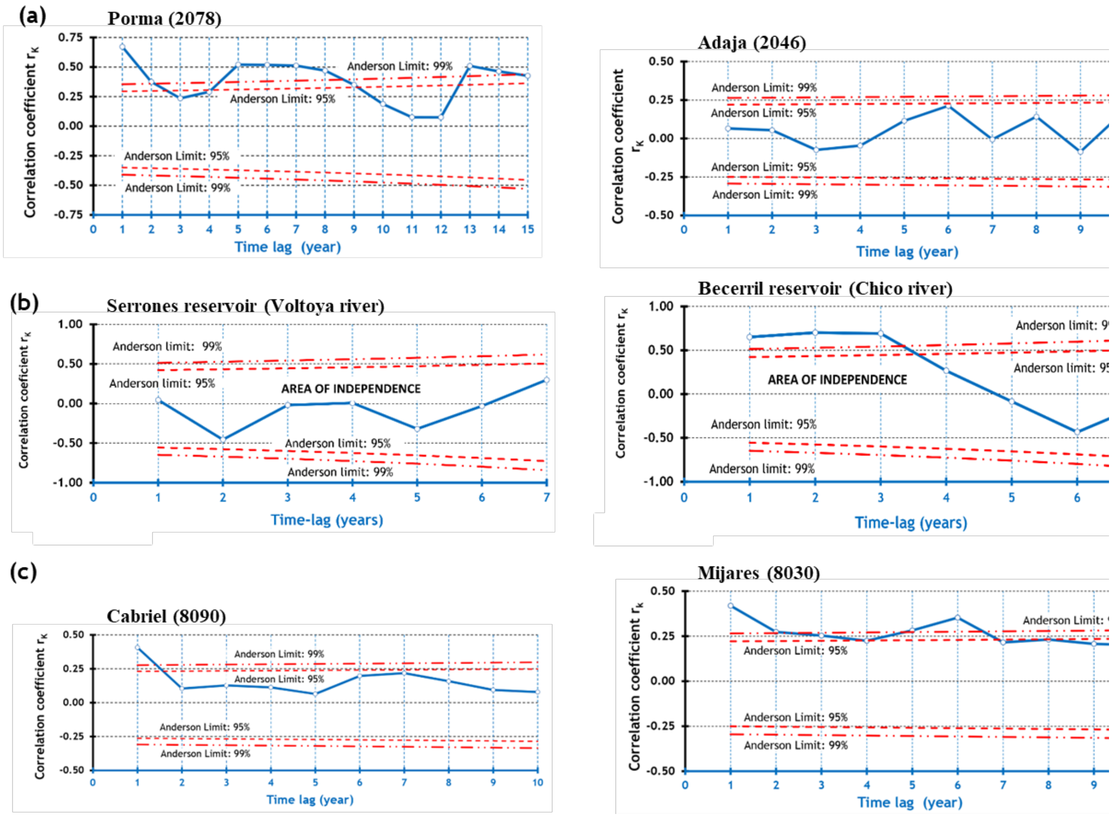

Figura I.3: Casos de estudio. Correlogramas temporales: (a) ríos Porma y Adaja, (b) embalses de Serones, río Voltoya y Becerril, río Chico y (c) ríos Cabriel y Mijares (Zazo et al., 2019,2021a,2023). Nota: Entre paréntesis se indica el código de las estaciones de aforo consideradas.

I.6 EVOLUCIÓN DEL ANÁLISIS DE LA DEPENDENCIA EN LOS PROCESOS HIDROLÓGICOS

La complejidad de los sistemas naturales no lineales, como los hidrológicos, y el conocimiento parcial de las relaciones físicas que en ellos subyacen (Aqil et al., 2007; Giupponi y Sgobbi, 2013; Liu et al., 2015; Zazo, 2017) implica considerar un enfoque holístico (Macian-Sorribes, 2017; Molina, 2009; Pulido-Velazquez, 2004; Zazo, 2017), si se aspira a una gestión sostenible y segura de este tipo de sistemas naturales. Esto, necesariamente, supone analizar la evolución y dependencias de las variables[13] hidrológicas (Croitoru y Minea, 2015; Romano et al., 2013); razón por la que la dependencia en los procesos hidrológicos ha sido objeto de estudio recurrente en la hidrología estocástica (Bras y Rodriguez-Iturbe, 1985; Hipel y McLeod, 1994; Macian-Sorribes et al., 2020; Rodriguez-Iturbe et al., 1972; Salas et al., 1980, 2000). Al mismo tiempo, las características intrínsecas y diferenciadoras de cada cuenca y/o de los registros

[13] Véase González Casimiro, (2009), página 1:

> *"La mayoría de los métodos estadísticos elementales suponen que las observaciones individuales que forman un conjunto de datos son realizaciones de variables aleatorias mutuamente independientes…"*

hidrometeorológicos, conjuntamente con su cada vez más reconocida no estacionariedad (Macian-Sorribes y Pulido-Velazquez, 2020; Mediero et al., 2014; Molina y Zazo, 2018) han dado lugar a la aplicación de diferentes perspectivas y enfoques para abordar este reto (Ilich y Despotovic, 2008; Hao y Singh 2016; Srivastav et al., 2011).

El estudio de la dependencia en hidrología se ha abordado tradicionalmente desde el punto de vista de la estadística descriptiva mediante análisis de correlación. De acuerdo con Helsel y Hirsch (2002), este tipo de análisis mide la fuerza de asociación entre dos variables continuas, mediante la covariación observada, siendo de interés conocer sus patrones de variación conjunta. Sin embargo, es preciso resaltar que está asociación no implica necesariamente una relación causal entre las variables. De hecho, la correlación exclusivamente muestra que las variables comparten información (variabilidad), y que ésta puede deberse a múltiples factores, por ejemplo, a que comparten una causa común.

De entre las métricas empleadas en evaluar la correlación, el coeficiente de Pearson, basado en una distribución normal (Pearson, 1896), ha sido el enfoque paramétrico más ampliamente utilizado (Helsel y Hirsch, 2002). Este coeficiente se ha empleado habitualmente en hidrología para estimar el grado de dependencia lineal de una variable respecto a otra (Barber et al., 2020).

Para superar las limitaciones de aplicación en contextos de dependencia no lineal, planteamientos no paramétricos como las correlaciones de Spearman (Spearman, 1904) y Kendall (Kendall, 1955) son alternativas habitualmente empleadas (Nelsen 2006). Ambos coeficientes muestran el grado de "asociación" entre variables (Nelsen 2006) basado en rangos, es decir, operan con los rangos de los datos y no con los propios datos (Barber et al., 2020; Helsel y Hirsch, 2002). De hecho, el coeficiente de correlación de Spearman se corresponde con el coeficiente de correlación de Pearson una vez transformados los datos en rangos (Barber et al., 2020).

Otros enfoques con alto impacto y profusamente empleados en el estudio de las dependencias han sido el coeficiente de Hurst (Hurst 1951) y los estadísticos de almacenamiento y sequía (Salas et al., 1980). El primero es entendido como una medida de la memoria a largo plazo (interdependencia) de las series temporales basado en el concepto estadístico de "persistencia", como propiedad de las series temporales. Los segundos se definen en un contexto de modelado de series temporales hidrológicas (Salas et al., 1980). Igualmente, son reseñables, a partir de los modelos genéricos ARIMA (AutoRegresive Integrated Moving Average) propuestos por Box y Jenkins (1976), y desde la asunción de la hipótesis de normalidad en los datos, la caracterización de la dependencia lineal entre variables aleatorias multivariantes mediante modelos autorregresivos (AR) o modelos autorregresivos de medias móviles (ARMA) (Chenoweth et al., 2000; Mohammadi et al., 2006; Salas et al., 1980). Además, en este ámbito de series temporales lineales es preciso resaltar las funciones de correlación simple y parcial como medidas de la dependencia general. Éstas permiten la modelización de procesos y una representación sencilla a través de correlogramas fácilmente interpretables (Bermejo Mancera, 2011). Este enfoque gráfico se ha demostrado eficiente no solo a la hora de evaluar, preliminarmente, la dependencia espacial, temporal y espacio-temporal en series temporales hidrológicas multivariantes; sino también como fuente de validación de nuevos desarrollos (Macian-Sorribes et al., 2020; Molina et al., 2016; Zazo, 2017).

Otra área reciente de investigación es la construcción de una distribución multivariante para la modelización de diferentes estructuras de dependencia (Sarabia-Alzaga y Gómez-Déniz 2008). Este planteamiento se ha aplicado al análisis de frecuencias, técnicas de regionalización o reescalado (downscaling), simulación de caudales o precipitaciones, o la interpolación geoestadística entre otras (Molina y Zazo, 2018). En esta última área, es reseñable la aplicación de variogramas de desplazamiento temporal para caracterizar la estructura de dependencia temporal de caudales fluviales (Chiverton et al., 2014). También merecen atención métodos como la distribución paramétrica multivariante (Balakrishnan y Lai 2009) y la cópula a la hora de estudiar distribuciones multivariantes a partir de distribuciones marginales dadas (Nelsen 2006).

Desde finales del siglo XX, los avances en la informática han sido el catalizador de la revolución científico-técnica experimentada (Zazo, 2017), y a la que los estudios sobre sistemas hidrológicos y gestión de los recursos hídricos no ha resultado ajena (Jayakrishnan et al., 2005). Asimismo, la creciente demanda global de recursos hídricos (Koutroumanidis et al., 2009; Macian-Sorribes y Pulido-Velazquez, 2020), junto con la necesidad de predicciones fiables (Jain y Kumar, 2007) y las perspectivas negativas sobre disponibilidad de recursos hídricos (Versini et al., 2016; Zhang et al., 2019) han favorecido, de la mano de la Inteligencia Artificial, la aparición de estrategias innovadoras para el análisis de las “dependencias” (Macian-Sorribes y Pulido-Velazquez, 2020; Molina y Zazo, 2017; Zazo, 2017).

La aplicación de la Inteligencia Artificial en estos procesos de análisis ofrece ventajas distintivas como: i) permitir utilizar los datos en bruto (raw data) directamente (Tripathy y Mishra, 2024; Zounemat-Kermani y Teshnehlab, 2008); ii) no requerir un conocimiento previo (He et al., 2024; Nourani et al., 2011) ni explícito de las características físicas del proceso en estudio (Shiau y Hsu, 2016; Singh et al., 2012); iii) gestionar una gran cantidad de información procedente de sistemas no lineales dinámicos (Aqil et al., 2007; Fang et al., 2024); iv) ser capaz de definir relaciones no triviales en sistemas naturales complejos (Eythorsson y Martyn, 2025; Molina et al., 2013; Zazo et al., 2020); y v) posibilitar el descubrimiento de estructuras causales en datos estadísticos brutos (Spirtes, 2010).

En este nuevo paradigma de análisis de las dependencias destacan las metodologías/técnicas de aprendizaje automático o “machine learning”. De acuerdo con Jimeno Saez (2018) estos métodos, mediante algoritmos, estiman la dependencia, inicialmente desconocida, entre las entradas y salidas de un sistema en base a los datos existentes; siendo posible, a partir de la relación de dependencia, predecir resultados de acuerdo con valores de entrada conocidos. Esta capacidad de descubrimiento de las (in)dependencias, lineales y no lineales, (Madsen et al., 2003; Steck, 2001; Ochoa-Rivera et al., 2007; Ochoa-Rivera, 2008; Macian-Sorribes et al., 2020; Zazo et al., 2023) ha dado lugar a avances significativos en causalidad, inferencia causal a partir de datos puramente observacionales (Ombadi et al., 2020), y cuantificación de la incertidumbre (Rolnick et al., 2022). En el ámbito hidrológico destacan técnicas como Redes Neuronales Artificiales (Artificial Neural Networks), Sistemas Adaptativos de Inferencia Neuro-Difusa (Adaptative Network based in Fuzzy Inference Systems), Máquina de Aprendizaje Extremo (Extreme Learning Machine), Redes Neuronales Wavelet (Wavelet Artificial Neural Network), Máquinas de Vector Soporte (Support Vector Machines), Lógica Difusa (Fuzzy Logic), Algoritmos Genéticos (Genetic Algorithms), Redes Bayesiana (Bayesian Networks) y Redes Bayesianas Dinámicas (Dynamic Bayesian Networks) entre otras (Jimeno Saez, 2018; Macian-Sorribes, 2017, Molina, 2009; Ochoa-Rivera, 2002; Zazo, 2017).

Teniendo en cuenta el número de aplicaciones, del conjunto de técnicas anteriores, las más populares son las redes neuronales y las redes bayesianas (redes probabilísticas; Gutiérrez et al., 2004). Las primeras, inspiradas en el cerebro humano, "aprenden" tratando de reproducir la realidad codificada en un conjunto de datos (Gutiérrez et al., 2004). Por su parte, las segundas, son adecuadas para el tratamiento de problemas con incertidumbre (Chang et al., 2023) en sistemas basados en el conocimiento (Molina et al., 2016) y con elevado número de variables (Pearl, 1988). Otra ventaja de éstas es que permiten definir un modelo único sobre el que se propaga cualquier evidencia, frente a los modelos específicos para cada conjunto de variables evidenciales en el caso de las redes neuronales. Además, las redes probabilísticas presentan la capacidad de codificar las (in)dependencias considerando tanto las dependencias marginales como las condicionadas entre el conjunto de variables a estudio (Ancell Trueba, 2009).

Charniak (1991) define las Redes Bayesianas (RB) como "*… técnica de modelado que reproduce las características esenciales del razonamiento plausible (razonamiento en condiciones de incertidumbre) de una manera consistente, eficiente y matemáticamente correcta*". Conceptualmente, pueden considerarse como relaciones causa-efecto, donde se modela y representa explícitamente la incertidumbre (Cain, 2001), a partir de la combinación de las teorías de grafos (representación de las relaciones de independencia-dependencia del conjunto de variables) y probabilidad (cuantificaciones de las relaciones; Gutiérrez et al., 2009; Vogel et al., 2014,2018). Así es posible realizar tanto el aprendizaje automático como la inferencia a partir de la evidencia disponible (Gutiérrez et al., 2004). Por su parte, desde la perspectiva de la teoría de grafos, un grafo dirigido describe las relaciones causales entre las variables del sistema, representadas por nodos, siendo las aristas dirigidas entre nodos las que expresan las influencias casuales directas (Dechter, 2013). Si el grafo codifica información probabilística entonces se denomina RB (Darwiche, 2009; Pearl, 1988).

Más en detalle, las RBs son una clase de modelo probabilístico gráfico (Pearl, 1988) definido sobre un conjunto de variables aleatorias donde cada una describe alguna cantidad de interés (Scutari et al., 2019), basada en el concepto de probabilidad condicionada (Molina, 2009), mediante la implementación del Teorema de Bayes (Bayes, 1763) y la actualización de las probabilidades ante nuevas evidencias (McGrayne, 2011). Molina (2009) caracteriza su estructura en tres elementos: el "conjunto de variables" que definen el sistema y que muestran distintos estados en forma de valor de probabilidad; los "enlaces" entre las variables; y las "tablas de probabilidad condicionada" asociadas a cada variable, que son utilizadas para calcular la probabilidad de sus estados. Las variables, representadas por "nodos", se interconectan en una estructura acíclica dirigida que relaciona las dependencias probabilísticas entre las variables (Koller y Friedman, 2009; Molina, 2009). Los dos primeros elementos representan la componente cualitativa, y el tercero la cuantitativa, que mide las relaciones causa-efecto (Chang et al., 2023).

Además, las RBs permiten por cada nodo determinar una distribución de probabilidad independiente del resto (distribución marginal), y una representación compacta de la distribución de probabilidad conjunta sobre el conjunto de variables (Ancell Trueba, 2009). Esto posibilita la propagación de la probabilidad condicionada[14] "omnidireccionalmente" (Molina et al., 2013,2016,2021). Así, ante una evidencia (observación) sobre cualquier nodo o subconjuntos de nodos de la red es posible obtener las probabilidades *a posteriori* de todos los demás, independientemente de su situación en la red (Cain, 2001; Molina, 2009). De este modo, la información pasada proporcionará un conocimiento previo sobre el futuro (Molina et al., 2010; Zazo, 2017) y se cuantifica la fuerza de la relación entre las variables aleatorias (Castelletti y Soncini-Sessa, 2007).

Por otro lado, el potencial que las RBs ofrecen para detectar estructuras causales temporales en datos estadísticos en bruto (raw data; Spirtes, 2010) ha comenzado a aplicarse al descubrimiento y caracterización de la estructura lógica y no trivial de interdependencia espacio-temporal, que subyace inherentemente en los registros históricos (Macian-Sorribes et al., 2020; Molina et al., 2019; Molina y Zazo, 2018; Zazo et al., 2023).

Por último, este marco general de análisis de la dependencia pone, más si cabe, de manifiesto el interés que los estudios de dependencia espacio-temporal suscitan aplicados a los sistemas hídricos (Holmström et al., 2015). En este sentido, el modo característico de analizar las dependencias que las RBs ofrecen es lo que ha inspirado esta Tesis, a la hora de aplicar y evaluar la capacidad que la Causalidad Bayesiana tiene para descubrir la estructura lógica que define el comportamiento espacio-temporal de los recursos hídricos superficiales en cuencas adyacentes o individuales.

I.7 MARCO METODOLÓGICO GENERAL

En primer lugar, es preciso definir un marco general que permita evaluar la capacidad de modelado y predicción de la Causalidad Bayesiana en un contexto de dependencia espacio-temporal o exclusivamente temporal. Dicho marco será adaptado de acuerdo con el propósito de cada una de las investigaciones a desarrollar (ver Capítulo II, III y IV). Este planteamiento permitirá analizar la idoneidad de la Causalidad Bayesiana aplicada a la investigación hidrológica bajo distintos escenarios y escalas espacio-

[14] Según Ancell Trueba (2009), el concepto de probabilidad condicionada proporciona la forma de definir la dependencia estadística de dos conjuntos de variables aleatorias.

temporales. El marco general propuesto incluirá tres fases claves en cada una de las investigaciones (Figura I.4).

En primer lugar, existirá una fase inicial de *Datos de entrada*, que comprenderá la adquisición, tratamiento y análisis de los datos. En esta fase los datos se adaptarán para alimentar y entrenar los modelos bayesianos causales. Esta adaptación, en el caso de conjuntos de datos de una longitud insuficiente para el entrenamiento de los modelos, implicará la generación de series sintéticas equiprobables; proceso que se llevará a cabo mediante modelos paramétricos según el marco metodológico expuesto en Salas et al., (1980).

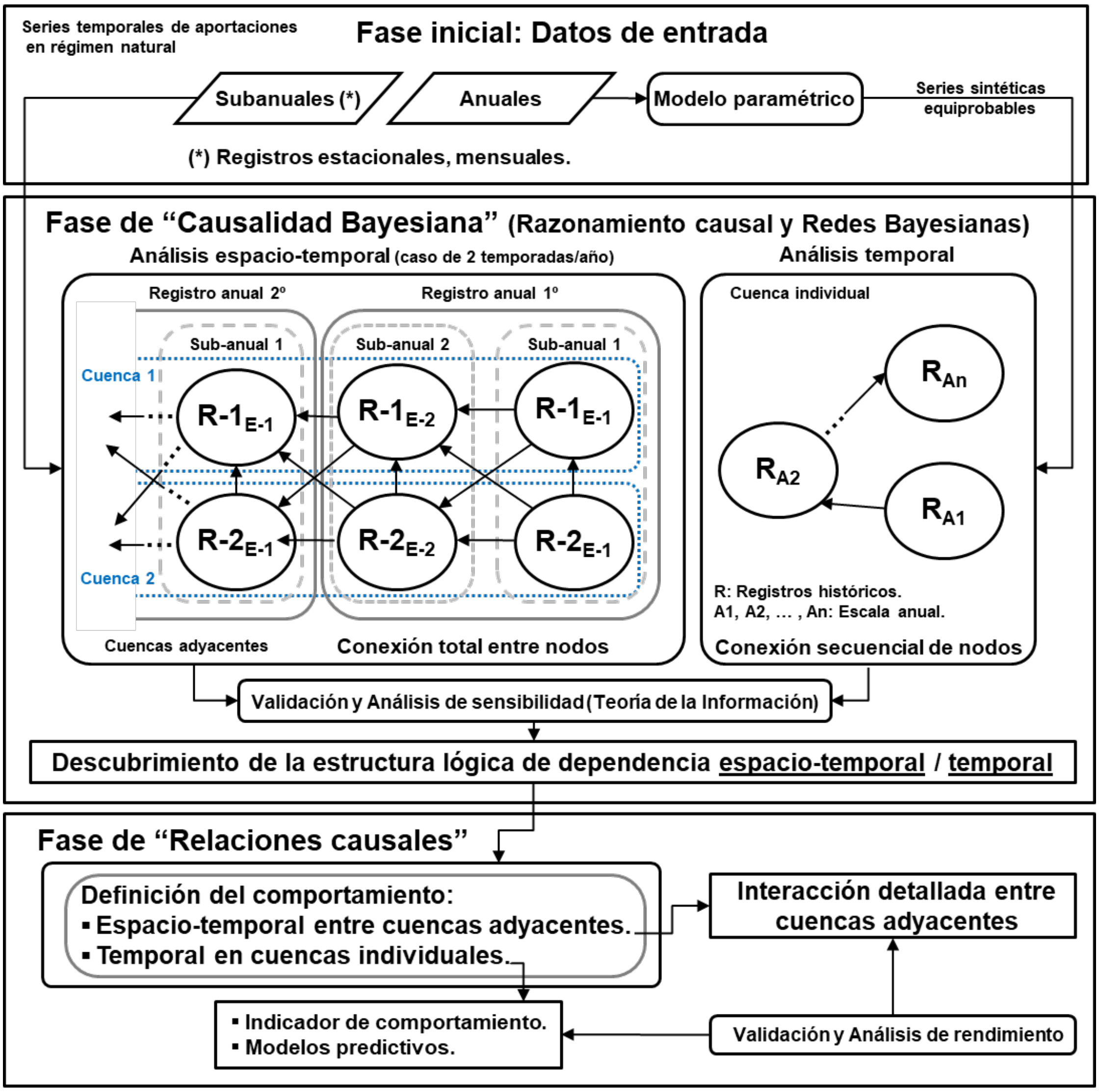

Figura I.4: Marco metodológico general.

La siguiente fase comprenderá los pasos requeridos por el análisis de la *Causalidad Bayesiana*. En ella se definirán los modelos causales, espacio-temporales o temporales, mediante un proceso de diseño, alimentación, entrenamiento y validación; esto último mediante un enfoque basado en la Teoría de la Información. Esta fase será clave ya que permitirá descubrir, extraer y cuantificar la estructura lógica interna, trivial (relaciones consecutivas) y no trivial (relaciones con desfase temporal > 1), de dependencias inducidas y difusas (Hao y Singh 2016; Wang et al., 2009), que subyace inherentemente en las series hidrológicas; y que definirá la respuesta hidrometeorológica de cada cuenca (Macian-Sorribes et al., 2020). El hecho de abordar el análisis de las dependencias en forma de consultas de probabilidad condicionada posibilita considerar la influencia (condicionalidad) que sucesos pasados puedan tener en otros futuros, y no necesariamente de forma trivial (consecutiva).

Por último, habrá una fase de *Relaciones causales* dedicada al cálculo y análisis de las relaciones de causalidad detectadas. A partir de ellas se obtendrán las interacciones entre cuencas adyacentes, el desarrollo de indicadores individuales de comportamiento temporal y modelos predictivos (Molina et al., 2019; Zazo et al., 2023). Todos estos resultados serán sometidos a un proceso de validación y análisis de rendimiento (evaluación de la capacidad de modelado y predicción).

I.7.1 Esquema conceptual para la modelización causal espacio-temporal[15]

Metodológicamente, esta investigación se articulará bajo el diseño general expuesto, basado en tres fases principales.

La Fase-1 implica el tratamiento, análisis y adaptación de los datos brutos de las aportaciones a las subcuencas de los embalses de Alarcón y Contreras (ambas adyacentes; escala espacial), y que alimentarán y entrenarán los modelos causales. La escala temporal será estacional (temporada de riego y no riego por año). Se plantea un doble análisis; general y de periodos secos, en este último caso en la sequía sufrida por el Júcar entre 2005 y 2008 (3 años hidrológicos)

En la Fase-2 se procederá a la construcción de los modelos causales bayesianos para el análisis espacio-temporal. Para captar la dependencia de las aportaciones espacial y temporalmente se diseñará una red con sus nodos completamente conectados (ver Figura

[15] Ver Capítulo II apartado II.4, donde se describe en detalle la metodología específica diseñada.

I.4, Fase de "Causalidad Bayesiana"), donde cada uno interactuará (relación causal) con los tres restantes para cada año de análisis.

La Fase-3, mediante el análisis de las relaciones causales, permitirá descubrir la estructura lógica de dependencia espacio-temporal que definirá el comportamiento entre las dos subcuencas. La validación de los modelos causales se abordará desde la perspectiva de la Teoría de la Información, basada en la Entropía Condicional y la Información Mutua entre las variables implicadas.

I.7.2 Marco general para la optimización de los factores del proceso de aprendizaje-entrenamiento de los modelos temporales causales[16]

Esta investigación evaluará la estabilidad de la modelización temporal causal bayesiana. Basada en el enfoque metodológico general previamente expuesto, la metodología diseñada comienza con la identificación de los dos factores claves que condicionan la modelización temporal causal bayesiana: número de series sintéticas (cantidad de datos; Factor 1) y número de intervalos de las distribuciones de probabilidad para los procesos de entrenamiento y aprendizaje de los modelos causales (Factor 2). A continuación, se analiza en detalle la influencia de ambos en el proceso de aprendizaje-entrenamiento de los modelos causales. El ámbito de estudio se centrará en las subcuencas altas de los ríos "Porma-Esla" y Adaja, ambas en la DHD; siendo la escala temporal de modelado anual.

La fase inicial comprenderá, en principio, la generación de series temporales equiprobables (datos sintéticos), a partir de los registros históricos mediante modelos paramétricos, de acuerdo con el marco metodológico expuesto en Salas et al., (1980).

A continuación, se desarrollará el diseño de la modelización de las Redes Bayesianas, bajo el esquema de: aprendizaje, preprocesamiento, restricciones y proceso de aprendizaje de estructuras. El carácter individual del análisis supone una conexión secuencial entre los nodos (variables) de la red (ver Figura I.4, Fase de "Causalidad Bayesiana"), sobre los que se procederá a la propagación de la fuerza de la (in)dependencia entre las variables que conforman la red. La propagación se basará en el análisis de las bandas de incertidumbre de los gráficos de mitigación de la dependencia.

[16] Ver Capítulo III apartado III.2, para una descripción detallada de la metodología específica diseñada.

Por último, se evaluará el rendimiento de los dos factores indicados sobre el modelado causal bayesiano. La novedad de la investigación implica, también, el diseño de un marco innovador de estabilidad. Se considerarán niveles de análisis diferentes para cada uno de los dos factores, además de la definición de dos novedosos índices, denominados "Índices de Similitud y Estabilidad", a partir de la combinación de ambos factores. La relación óptima de factores se determinará por medio de un enfoque recursivo bi-objetivo basado en los índices anteriores.

I.7.3 Esquema general para la predicción temporal mediante modelización causal[17]

El objetivo de esta investigación será estudiar la capacidad de predicción temporal de la causalidad bayesiana, aplicada al caso de las aportaciones a embalses en régimen natural, y en cuencas caracterizadas por un comportamiento temporal independiente de sus recursos superficiales y con un número limitado de registros históricos (16 años disponibles en este caso). En concreto, se considerarán los embalses actuales para abastecimiento de la ciudad de Ávila, pertenecientes al subsistema Cega-Eresma-Adaja de la DHD. La escala temporal de modelado será anual.

En primer lugar, y de acuerdo con el enfoque metodológico general (fase inicial: *Datos de entrada*), al disponer de limitados registros, será necesario generar un conjunto de datos temporales equiprobables a los registros históricos, basado en el mencionado enfoque de modelos paramétricos de Salas et al., (1980). Este conjunto sintético de datos posteriormente será empleado en el proceso de aprendizaje-entrenamiento de los modelos causales.

La siguiente fase supondrá el diseño de la Red Bayesiana. Al igual que en el caso anterior, siendo también un análisis temporal individual (cada embalse se analiza de forma independiente), se adoptará un esquema de relación secuencial entre variables (ver Figura I.4, Fase de “Causalidad Bayesiana”). De igual modo, se procederá a la propagación de la fuerza de la (in)dependencia entre las variables que integran la red.

A continuación, se identificarán y cuantificarán las fracciones temporalmente condicionadas que constituyen cualquier aportación (Molina y Zazo, 2018), puesta de manifiesto por el modelado causal en forma de una novel matriz de dependencias. Estas fracciones se denominan: aportación temporalmente condicionada (debida al tiempo;

[17] Ver Capítulo IV apartado IV.3, para la descripción de la metodología diseñada.

TCR por sus siglas en inglés) y aportación temporalmente no condicionada (no influida por el tiempo; TNCR en inglés).

Por último, a partir de la condicionalidad temporal oculta en los registros temporales, para cada una de las fracciones antes indicadas se implementarán sendos modelos predictivos. El horizonte de predicción de estos modelos será de un año, debido a la elevada variabilidad anual que caracteriza la disponibilidad de los recursos hídricos en España (CEDEX, 2017). La validación de resultados se llevará a cabo bajo una doble perspectiva, probabilística (de carácter general) y metrológica (detallada), debido a que la fracción TNCR puede considerarse una fuente de incertidumbre al no depender del tiempo.

I.8 ESTRUCTURA DEL DOCUMENTO

La organización se articula en cinco capítulos que siguen el orden lógico de la investigación, de acuerdo con el objetivo general y los específicos fijados en esta Tesis Doctoral, y tres Apéndices.

El Capítulo I "Introducción" proporciona una visión general de la Tesis y se justifica y motiva el interés que ésta tiene para la comunidad científica e ingenieril. Al mismo tiempo, se concreta el objetivo general y los específicos de las investigaciones, se exponen las hipótesis consideradas, así como se definen las zonas de estudio consideradas. Asimismo, se detalla el marco metodológico general diseñado para alcanzar los objetivos definidos, que se particularizará en cada una de las investigaciones desarrolladas conforme al propósito fundamental de cada una de ellas. Después, se expone una visión de la evolución del análisis de la dependencia en los procesos hidrológicos. Por último, se indica la estructura general del documento.

Los Capítulos II, III y IV constituyen el núcleo central de la Tesis. En ellos se presentan los desarrollos y resultados obtenidos en las investigaciones, a través de las tres publicaciones científicas indexadas en revistas científicas de alto impacto.

El Capítulo II, "*Dependencia espacio-temporal de las aportaciones mediante modelización causal*", está íntegramente dedicado a evaluar la capacidad de este enfoque metodológico para captar las relaciones espaciales, temporales y espacio-temporales entre dos cuencas adyacentes y paralelas. Se presentan los resultados de la investigación, adaptada al formato de la tesis, y publicados en el artículo científico:

> "*Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling*". Como novedad, esta investigación aborda la dimensión espacial de la modelización causal bayesiana en Hidrología mediante RBs. El enfoque realizado supone un avance frente a la aplicación de las RBs en un contexto temporal, permitiendo un triple análisis conjunto espacial, temporal y espacio-temporal. La validación se ha basado en parámetros de la Teoría de la Información como la entropía, la entropía condicionada y la información mutua. La capacidad de modelización y predicción puesta de manifiesto tiene importantes implicaciones en el ámbito de la planificación y la gestión de los recursos hídricos, así como para mejorar y optimizar las reglas de explotación de los embalses.

El Capítulo III, "*Optimización de la modelización causal bayesiana*", presenta la investigación llevada a cabo para optimizar los parámetros claves en la modelización temporal causal bayesiana:

> "*Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework*". La investigación propone un marco metodológico innovador para evaluar y mejorar el rendimiento de la modelización temporal bayesiana causal. Esto se debe a la reciente aplicación de las RBs para descubrir la estructura lógica de dependencias temporales latente en los registros históricos de aportaciones en régimen natural. Se propone un nuevo marco de estabilidad para evaluar el rendimiento de los "*Learning-Training Processes*" que optimiza los factores claves del proceso: número de series sintéticas que "alimentan y entrenan" los modelos causales y el número de intervalos definidos para las distribuciones discretas de probabilidad de los datos sintéticos. Esto ha implicado la definición de dos nuevos indicadores denominados "Índice de similitud" e "Índice de estabilidad", que permiten evaluar el rendimiento global del proceso de la optimización. Esta investigación permitirá avanzar en el desarrollo de nuevos indicadores de comportamiento temporal.

El Capítulo IV, "*Modelización causal bayesiana aplicada a la predicción de aportaciones*", muestra la capacidad de predicción y un nuevo índice para evaluar cuantitativamente la dependencia temporal en el artículo científico:

"*Assessment of the predictability of inflow to reservoirs through Bayesian causality*". Esta investigación evalúa la capacidad y rendimiento predictivo en cuencas con un comportamiento temporal independiente, a partir de una mínima señal de dependencia presente en los registros históricos. Por otra parte, propone un nuevo indicador cuantitativo, denominado "Índice de simetría", para evaluar el comportamiento temporal de los recursos hídricos superficiales de una cuenca. Los resultados alcanzados abren nuevas posibilidades para el desarrollo de modelos hidrológicos predictivos basados en el marco de modelización del razonamiento causal bayesiano y con longitudes de series temporales reducidas.

En el Capítulo V "*Discusión, conclusiones y líneas futuras de investigación*", se exponen las conclusiones finales y las principales aportaciones de esta Tesis de acuerdo con las realizadas en los distintos artículos científicos. Seguidamente, se proponen futuras líneas de investigación que permitan avanzar con las investigaciones iniciadas.

El Apéndice I detalla los fundamentos matemáticos de un nuevo indicador, denominado "índice de dependencia temporal (I-DT)", propuesto para evaluar, conjuntamente, la evolución de la dependencia temporal y la fuerza de esa relación en series temporales a escala anual. Este nuevo índice se basa en el "Índice de simetría" definido en el Capítulo IV.

Los Apéndices II y III, representan una medida externa y objetiva de la calidad de los artículos publicados. Resumen los principales índices de calidad de las revistas científicas donde han sido publicados los artículos de investigación, e indican el número de citas recibidas por los artículos desde su publicación hasta la fecha de redacción de esta Tesis.

Apéndice II: "*Índices de calidad de las revistas científicas*". Detalla las revistas científicas internacionales de prestigio, indexadas en las bases de datos Journal Citation Report (JCR) y SCImago Journal Rank (SJR), donde han sido publicados los artículos que constituyen esta Tesis. Se indica la clasificación por cuartiles en el área de conocimiento de las investigaciones llevadas a cabo, y se detallan sus factores de impacto e índices en las principales bases de datos bibliográficas.

Apéndice III: "*Repercusión de las investigaciones*". En él se recogen las citas recibidas de los artículos que componen esta Tesis Doctoral a nivel internacional.

CAPÍTULO II

Dependencia espacio-temporal de las aportaciones mediante modelización causal

Este Capítulo II reproduce la versión de autor, adaptada al formato tesis, del artículo científico "Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling", publicado en la revista científica *Journal of Hydrology* (ISSN: 0022-1694) el día 5 de noviembre de 2020.

La investigación que compone este capítulo evalúa, en detalle, la dependencia espacio-temporal de las aportaciones en dos cuencas adyacentes, paralelas, en diferentes pasos de tiempo, mediante la Causalidad Bayesiana. Para este fin se ha llevado a cabo una "prueba de concepto", abordada desde un novedoso enfoque metodológico basado en el Razonamiento Causal, aplicado a la cuenca alta del río Júcar (caracterizada por largas y severas condiciones de sequía), en concreto en los embalses de Alarcón y Contreras, los de mayor capacidad de toda la cuenca hidrográfica. El objetivo de la investigación es doble. En primer lugar, realizar un análisis global de la dependencia, y en segundo, otro específico sobre periodos secos centrado en el horizonte temporal de la sequía típica de la cuenca del Júcar (3 años). Estos retos comprenden el desarrollo de dos Redes Bayesianas completamente conectadas, una para cada objetivo, alimentadas y entrenadas a partir de registros históricos de caudales. Ambas redes se diseñaron a escala estacional considerando los periodos de riego y de no riego, de acuerdo con las prácticas operativas de la Demarcación Hidrográfica del Júcar.

Los resultados obtenidos mostraron que la Causalidad Bayesiana captó, satisfactoriamente, las dependencias espacio-temporales de ambos sistemas, poniendo de manifiesto, a su vez, cuestiones claves de interdependencias entre ambas subcuencas como la magnitud de las dependencias espaciales entre las series temporales, su condicionalidad temporal y la dependencia espacio-temporal. Aspectos todos ellos intrínsecamente presentes en las series temporales de aportaciones. Este enfoque podría ser muy valioso para la planificación y gestión de los recursos hídricos, debido a su capacidad de aplicación para predecir fenómenos extremos (por ejemplo, sequías), así como para mejorar y optimizar las reglas de explotación de embalses.

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[18] Macian-Sorribes, H., Molina, J. L., Zazo, S., Pulido-Velázquez, M. 2020. Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling. Journal of Hydrology, 597, 125722. https://doi.org/10.1016/j.jhydrol.2020.125722.
Se omiten los apartados: "CRediT authorship contribution statement", "Declaration of Competing Interest" y "Acknowledgements". La sección "References" se integra en la Bibliografía de esta Tesis.
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II.0 Abstract

This research aims to assess fully the spatio-temporal dependence dimensions of inflow across two adjacent and parallel basins and among different time steps through Causality. This is addressed from the perspective of Causal Reasoning, supported by Bayesian modelling, under a novel framework named Bayesian Causal Modelling (BCM). This is applied, through a "concept-proof", to the Jucar River Basin (the second largest basin of Eastern Spain, characterized by long and severe drought conditions). In this "concept-proof" a double goal is evaluated; first dedicated to a lumped analysis of dependence and second a specific one over dry periods focused on time-horizon of the Jucar basin typical drought (3 years). These challenges comprise the development of two fully connected Bayesian Networks (BNs), one for each challenge populated/trained from historical-inflow records. BNs were designed at a season-scale and consequently, time was upscaled and grouped into Irrigation and Non-Irrigation periods, according to Jucar River Basin Authority operational practices. Results achieved showed that BCM framework satisfactorily captured the spatio-temporal dependencies of systems. Furthermore, BCM is able to answer to some key questions over interdependencies between adjacent and parallel subbasins. Those questions may comprise, the amount of spatial dependences among time series, the temporarily conditionality among subbasins and the spatio-temporal dependence among basins. This provides a relevant insight on the intrinsic spatio-temporal dependence structure of inflow time series in complex basins systems. This approach could be very valuable for water resources planning and management, due to its application power for predicting extreme events (e.g. droughts) as well as improving and optimizing the reservoirs operation rules.

II.1 Introduction

The inherent nonlinear nature of hydrologic series and their associated processes is widely known (Wei et al., 2012; Molina et al., 2016; Peng et al., 2017). Furthermore, the nonstationarity of records (annual or even larger time scale) is rapidly growing worldwide over the last years due to modifications/alterations in the climatic patterns (Allan and Soden 2008; Trenberth 2011; Kalra et al., 2013; Chang et al., 2015; Wasko and Sharma, 2015; Donat et al., 2016;) as result of the influence of climate change into small-scale meteorological processes (Marotzke et al., 2017; Pfahl et al., 2017). This global situation is materialized in the increasing occurrence, intensity, and persistence of extreme events (Jyrkama and Sykes, 2007; Marcos-Garcia et al., 2017; Molina and Zazo, 2018) including droughts, which can produce significant economic losses (Gil et al., 2011; Kahil et al., 2015; Freire-González et al. 2017; Lopez-Nicolas et al., 2017). In order to reduce these negative impacts, it is necessary to better understand the internal structure of dependencies that inherently underlies in the runoff time series (Molina et al., 2019). The meteorological-hydrological basin response is captured by means of this internal structure (Wang et al., 2009; Hao and Singh 2016; Molina and Zazo, 2018; Zazo et al., 2019). Furthermore, the spatio-temporal changes in weather patterns are likely to further aggravate the appearance and persistence of drought events (Mishra and Singh, 2010).

Likewise, the dependence of hydrological processes is a traditional studied matter, given its importance to assess, model and forecast the behavior and availability of water resources, especially in a context of droughts (Mishra and Singh, 2011). Classic ways to evaluate these dependences are mainly related to statistical procedures, including regression (e.g. Hao and Singh, 2016), time series modeling (e.g. Salas et al., 1980; Hipel and McLeod, 1994; Mishra and Desai, 2005), recurrence analysis (e.g. Estrela et al., 2000), and principal component analysis (e.g. Vicente-Serrano et al., 2004; Vicente-Serrano and Cuadrat-Prats, 2007). For a deeper explication of these techniques, the reader is referred to the work Mishra and Singh (2011).

Regarding temporal dependence of hydrological time series, this has traditionally received a more attention by the scientific community, for example by means of Persistence (inherent statistical property of time series), which is strongly related to the measure of the time series long-term memory through Hurst coefficient (Hurst, 1951), or storage and drought statistics (Salas et al., 1980), which are currently benchmarks; or other ones such us Copula applications (De Michele and Salvadori, 2003), the usage of multivariate distributions in modeling different dependence structures (Sarabia-Alzaga and Gómez-Déniz, 2008), or novel analysis strategies based on Artificial Intelligence (AI), such as Artificial neural networks (ANNs; Ochoa-Rivera, 2008), Bayesian Networks (BN; Molina and Zazo, 2017; Zazo et al., 2019) or Dynamic Bayesian networks (DBNs; Molina et al., 2013). However, spatial and spatio-temporal dependence for hydrologic science and engineering is much poorer studied (Holmström et al., 2015) and even more through a Bayesian perspective (Wikle et al., 1998; Jona Lasinio et al., 2005). This is because of: (a) complexity of characterizing and differentiate water sub-systems, (b) scarcity of spatial data availability and (c) difficulties on the application of spatial statistical methods, among others.

On the other side, in the last years, the emergence of AI and Information Theory techniques have allowed tackling new ways of approaching, characterizing and quantifying dependences (Wang et al., 2009; Hejazi and Cai, 2011; Singh, 2011; Wu et al., 2015; Lima et al., 2016; Molina et al., 2016; Kousari et al., 2017; Yang et al., 2016, 2017a,b). These techniques are useful for exploring the evolution of meteorological and hydrological dynamics in order to find suitable drought predictors at different spatio-temporal scales (Molina et al., 2020).

On the other hand, Causality in hydrological records has not been deeply studied and it could be done by means of the joint use of different forms of reasoning patterns. These forms are Causal Reasoning (CR), Evidential Reasoning (ER) and Intercausal Reasoning (IR) (Koller and Friedman, 2009; Pearl, 2009). CR is used when the approach is done from top to bottom. In this sense, the analysis is focused on the cause and the objective comprises the prediction of the effect or consequence. Consequently, the queries in form of conditional probability, where the "downstream" effects of various factors are predicted, are instances of causal reasoning or prediction. Classical Stochastic Hydrology has been very focused along several decades on the characterization of temporal behavior for runoff or streamflow in different basins worldwide. In this sense, CR approach becomes especially useful when hydrological dependence analysis takes place because it is about an evaluation of the influence of past events on posterior hydrological processes. ER comprises bottom-up reasoning, so the analysis is focused on the consequence (effect) and the cause is inferred (Bayesian Inference). This approach would be appropriate to the analysis of catastrophic events such as flooding where the most important thing to be studied is the consequence. IR is probably the hardest concept to understand. It comprises the interaction of different causes for the same effect. This type of reasoning is very useful in hydrology, where a consequence can be generated or explained from several causes. This approach would be very appropriate for developing Decision Support Systems based on Causality and Causal Modelling (Molina et al., 2010) where there is a high heterogeneity of variables´ nature and high complexity of causal relationships. Furthermore, one of the most exciting prospects in recent years has been the possibility of using the theory of BNs to discover causal structures in raw data (historical runoff record) (Pearl, 2014). This is done in this research through the usage of historical inflow data to train and populate the BN model. Consequently, AI techniques such as CR and ER and/or IR provide new horizons for this type of studies.

Recently, the potential of BNs to find temporal causal structures into raw statistical data (Spirtes, 2010) has begun to be applied to discover and characterize the logical and non-trivial structure of dependencies that inherently underlies historical records (Zazo, 2017; Molina and Zazo, 2018; Molina et al., 2019, Zazo et al., 2019). Consequently, there is a general clear necessity of strengthen the spatio-temporal dependence studies on water systems (Holmström et al., 2015).

This study has been applied in Jucar River Basin (the second largest basin on Mediterranean side of Spain). This river basin is characterized by an irregular hydrology, with long drought episodes, an intense irrigation activity and the existence of large reservoirs able to provide carryover storage (Marcos et al., 2017). In order to achieve an efficient system operation, within a context of sustainable and safe management of water resources of a basin, it is necessary to adequately characterize, both in space and time, the hydrological discharge to its main reservoirs (Alarcon and Contreras) and their evolution, as well as deepening in the knowledge of their spatial-temporal behavior through the discovery and analysis of the non-trivial and logical structure of interdependence, which intrinsically underlies the historical records and that define of its behavior.

This research is mainly aimed to provide a new methodological approach, named Bayesian Causal Modelling (BCM). This is done by means of an innovative "concept-proof", focused on Causality, here addressed by Causal Reasoning and supported by Bayesian modelling. This provides not only temporal dependence behavior but also the spatial and spatio-temporal dependencies behavior of inflow across river basins. This knowledge is practically unexplored in the field of water engineering and science and that is what the novelty is about. In this sense, the application of BCM both to the prediction of droughts and to operation rules improvement of reservoirs, by means of this approach seems quite straightforward in the case of in parallel interconnected basins.

On the other side, this work, although addressed through a "concept-proof", is a further step in the research initiated with Molina et al., (2016) and Zazo (2017). This research activity is largely characterized by the application of BNs, in a dynamic and stochastically way, to increase knowledge over water resources behavior of basins.

II.2 Materials and methods

II.2.1 Bayesian networks

Bayesian Networks (BN), also known as Bayesian Belief Networks or Belief Networks, belong to the AI methods, such as artificial neural networks, fuzzy logic systems and decision trees (Molina et al., 2016). They are Probabilistic Graphical Models (PGM) in which a visual representation of a reasoning problem is performed to infer a new knowledge into an uncertainty context (Cabañas de Paz, 2017).

BNs combine probability theory with graph theory (Vogel et al., 2014). In this sense, they are based on: 1) a graphical representation comprising nodes and links, of a given set of random variables with their conditional interdependencies; and 2) a probabilistic model consisting of probabilistic expressions that describe the probability distributions/functions of the variables involved and the relationships between them depicted in the links (Cain, 2001; Castelletti and Soncini-Sessa, 2007; Sperotto et al., 2017). Furthermore, BNs aim to model the joint probability distribution of all considered variables. This is performed by means of propagation of (in)dependencies between the variables throughout the whole graphical structure, which can be seen as a general description of the behavior of a system (Vogel et al., 2018). In other words, PGMs offer a compact representation of the joint probability distribution over sets of random variables (Said, 2006; Castelletti and Soncini-Sessa, 2007).

On the other side, each node in the network represents a variable. The input variables to a BN are graphically represented through the parent nodes (nodes without arriving links) and the output variables are computed following the links between the root nodes and the leaf nodes (nodes without departing links, which represent the output variables in the network). For each link, the probabilistic expressions representing the relationship between the departing and arriving nodes are applied. The input variables can be provided as single values or as probability functions, while the output variables are obtained as probability functions. This probabilistic assessment is the main distinctive feature of a BN and enables the possibility of characterizing uncertainty, perform risk analyses and support decision-making processes (Castelletti and Soncini-Sessa, 2007; Vogel et al., 2013, 2012; Sperotto et al., 2017).

Formally, BN *N = (G, P)* consists of a Direct Acyclic Graph (DAG; (Lappenschaar et al., 2012)) denoted by *G = (V, E)* and a set of probability distributions P (Molina et al., 2013), therefore, a BN *N = (G, P)* defines a joint probability distribution over all the analyzed variables. The DAG is defined by a set of nodes (or variables) *V* and a set of links (or edges) *E*. The edges join the variables and are oriented, indicating the causal dependence between the connected variables ($A|B$ indicates *A* causes *B* or *B* is the effect of *A*) (Madsen et al., 2003). The set of probability distributions P includes "*a priori*" probabilities and a set of conditional probabilities (expressed in form of Conditional Probabilities Tables; CPTs). Theorem of Bayes is performed as updater of "a priori" probabilities adding the observed evidence and providing "*a posteriori*" probabilities, mathematically expressed as (Bayes, 1763):

$$P(B|A) = \frac{P(A|B) \cdot P(B)}{P(A)}$$

where $P(B|A)$ is the conditional probability of *B* for a given state of variable *A*; $P(B|A)$ the other-way-round conditional probability; $P(B)$ the probability of *B*; and $P(A)$ the probability of *A*.

Specifically applied to "concept-proof" over BCM of this research, the nodes in this case represent the hydrological space and time variables, which summarize the response of a basin to the hydrological cycle (Zazo, 2017) due to the fact that the inflow values intrinsically encompasses the influence of key factors such as rainfall-temperature variability, orography, fluvial morphodynamics, and anthropic factor (e.g. land-use change) as well as river-aquifer interaction that condition of the water flow in a point (Molina and Zazo, 2018), in this case inflow at a reservoir.

On the other hand, BNs present relevant advantages such as: 1) the explicit graphical representation, that lets any user see the variables and the relationships analyzed by them; and 2) the propagation of uncertainty, something very valuable in risk assessment and decision-making. They are also able to quantify the interdependencies existing between variables and they allow defining, in an easy and automatically way, relationships into complex systems (Molina et al., 2010) and proving more accurate results in the modeling of natural processes (See and Openshaw, 2000; Jain and Kumar, 2007). In contrast, their data requirements are big, their complexity grows are the systems and processes being modeled increase, and the fact that it is difficult to perform a quantitative validation on the results (Molina et al., 2010; Sperotto et al., 2017).

II.2.2 Spatio-temporal dependence analysis through causality

Spatio-temporal dependence analyses in hydrology are mainly related to the use of statistics and time series modeling procedures, which require them as a preliminary step (Salas et al., 1980; Hipel and McLeod, 1994). A crucial part of these approaches is the postulation of the stochastic model to be used (e.g. *AR 1*; *ARMA 1,1*; *AR 2*), and the choice of the statistical distribution followed by the variables considered by the model. Both decisions constrain the modeling of spatio-temporal dependences, since they assume that the analyzed variables are structured in a specific way and that this structure does not change over time, or that it changes following a specific pathway. In fact, the goal of these choices is to look for a spatio-temporal pattern close enough to the one shown by the available data records of the modeled variables. AI models, on the other hand, do not need to make assumptions on the data, as they are able to find out the properties and spatio-temporal patterns shown by it, even if they could not be identified before the analysis (Molina et al., 2016; Molina and Zazo, 2017). Although, AI approaches require large amount of data that not always is easy to obtain (Zazo, 2019; Molina et al., 2020).

At this point, it is worth highlighting that BNs are able to discover, extract and quantify the logical and non-trivial time-dependency relationships existing among variables by CR (Molina and Zazo, 2018; Molina et al., 2019). This research comprises an advance over the previous ones as it is able to discover and extract both spatial and spatio-temporal dependencies. Furthermore, once the BN is built, it possible to determine how strong are the strength of relationships between variables by modifying the probability distribution of one of them and seeing how it affects the probability distributions of the remaining ones (Molina et al., 2016). This modification may be successfully addressed by means of maximizing its highest interval, and its impact is measured quantifying the change in the expected value of the other variables (the average) found when the first one is maximized (Molina et al., 2016). Under this approach, small changes mean that the relationship is weak, while large modifications refer to strong bonds between the variables represented in those nodes. If the BN represents the values of a given variable for different locations and time stages, the relationships obtained from the analysis are spatial, temporal and spatio-temporal.

II.2.3 Potential applications of BN for spatio-temporal analysis

The use of BNs to perform spatio-temporal analyses shows a main advantage in comparison with classic statistics as the spatio-temporal dynamics of these relationships can be easily assessed. Their potential applications include:

1. Situations in which it is desired to explore if two or more variables show a causal relationship (e.g. between dry or wet cycles and climatic indicators such as the ENSO).
2. Situations in which the spatio-temporal pattern of the relationship cannot be not known in advance or cannot be adequately modelled with traditional statistics (because stochastic models able to fit the given pattern would be very complex and thus, less parsimonious).
3. Situations in which fitting a probability distribution to the variables cannot be reliably done (because no probability function is found adequate enough or the chosen one would be very complex).
4. Situations in which the spatio-temporal dependencies vary over time (e.g. river basins subject to changing climatic patterns).

II.3 Case study: the Jucar River Basin in Spain

II.3.1 Description

The case study is located at Jucar River Basin, a Mediterranean basin of 22,261 km² in Eastern Spain (Figure II.1). It flows through 497 Km between the Iberian Mountains and the Mediterranean Sea. Following a typical Mediterranean pattern (peaks in autumn and very little values during summer), the annual rainfall spans from 309 to 717 mm, with an average value of 473 mm. Its mean annual resource is 1,605 Mm³/year, in which 70% comes from groundwater outflow through springs and stream-aquifer interaction (CHJ, 2015). Its main reservoirs are Alarcon (1,088 Mm³ useful capacity), Contreras (429 Mm3), they are the most one's capacity of Jucar River Basin. Alarcón and Contreras are placed at the outlets of the upper basins of the Jucar and Cabriel rivers, while Tous is located at the limit of the Jucar floodplain, in which most urban and agricultural demands concentrate.

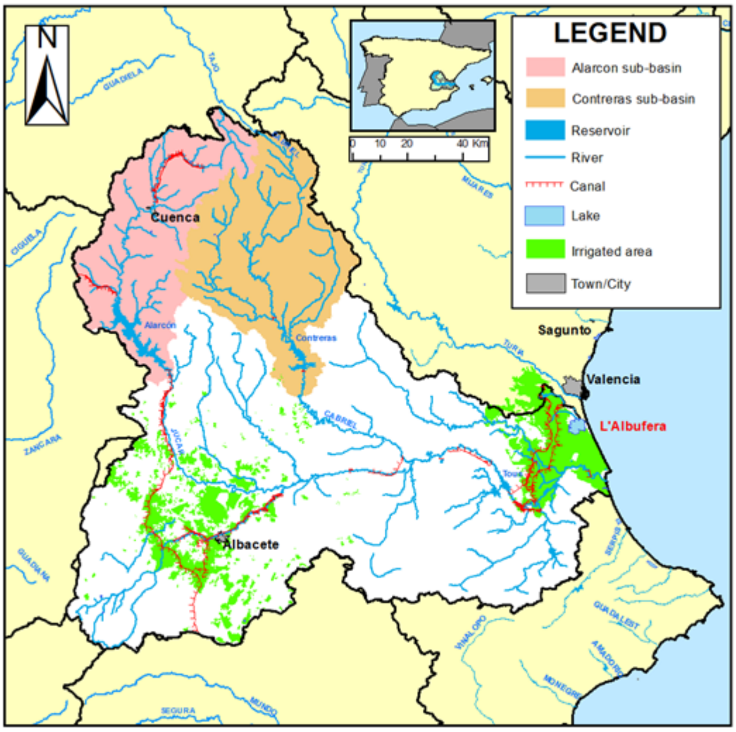

Figure II.1: Jucar River Basin location.

In lithological terms, Alarcon and Contreras sub-basins are characterized by existing of important limestone formations, dolomites, conglomerates, sandstones and Tertiary detritus (IGME, 2020a). Hydrogeology speaking, Alarcon sub-basin presents impermeable or very low permeability formations, together with extensive, discontinuous and local aquifers of moderate permeability and production. In contrast, Contreras sub-basin is characterized by very permeable aquifers, generally extensive and productive with other ones impermeable or very low permeability zones (IGME, 2020b). Moreover, both sub-basins show a piezometric gradient towards the coastal area, from West to East (CHJ, 2006,2020) (Figure II.2).

The annual consumptive demand of the Jucar river system is 1,557 Mm^3 for the 2015-2021 period (CHJ, 2015). The major consumptive use is agriculture (90%), followed by urban (8%) and industrial (2%) uses. The most important urban districts correspond to Valencia, Albacete and Sagunto. Surface irrigation demands concentrate on the lower basin (Riberas del Jucar and Canal Jucar-Turia), while the main groundwater-irrigated area is the Mancha Oriental, in the middle basin. The aquifer overdraft from this demand has caused an inversion of the stream-aquifer interaction found between the Mancha Oriental aquifer and the Jucar river, moving from gaining to losing river. Furthermore, minimum flows are set on 18 streams by environmental reasons (CHJ, 2015).

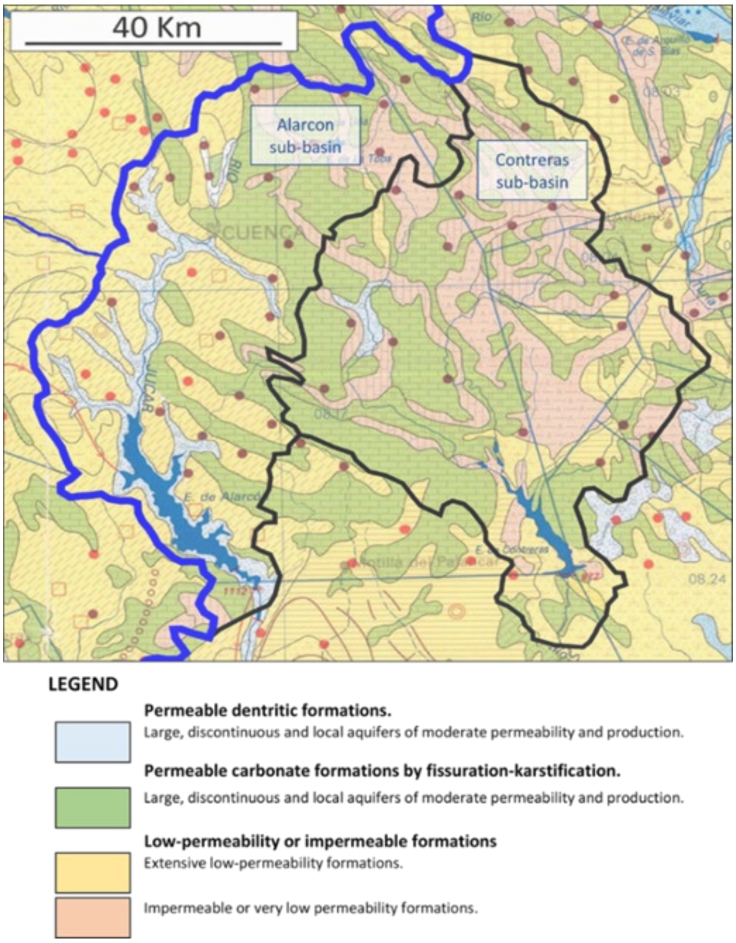

Figure II.2: Hydrogeological maps of Alarcon and Contreras sub-basin IGME. Source (2020b).

The planning and operation of the Jucar River Basin is the main responsibility of the Jucar River Basin Authority (in Spanish Confederacion Hidrográfica del Júcar, CHJ). Once environmental requirements are met, the current operating rules give priority to urban uses over agricultural areas. Among the latter, the users with elder rights from the lower basin, gathered together in the users' union USUJ (*Unidad Sindical de Usuarios del Júcar*), are given the highest surface priority. The remaining demands, with access to both surface and ground waters, can only use surface water if the Alarcon storage is higher than the limits established by the Alarcon Agreement (CHJ, 2015).

II.3.2 Available and processed data

The BCM analysis of spatio-temporal inflow dependence has been applied to the Alarcon and Contreras sub-basins, which correspond to the upper part of the Jucar River Basin and are the main contributors to the water discharge that can be regulated through the Alarcon and Contreras reservoirs (see Figure II.1). The available data consists of monthly inflow time series to the reservoirs for the 1940-2012 period (72 hydrological years; please note: in Spanish hydrological years the first month is October and the last is

September of following year), obtained from the Spanish Ministry of Agriculture, Fishery, Food and Environment (http://ceh-flumen64.cedex.es/anuarioaforos/default.asp). They have been naturalized by removing the effect of evaporation and seepage losses in Alarcon and Contreras, given that anthropic modifications in the upper basins of the Jucar and the Cabriel rivers are negligible. Figure II.3 and Table II.1 display the monthly time series considered and their main statistic parameters respectively, as well as the probability distribution functions of both time series and their correlograms are presented in Figure II.4.

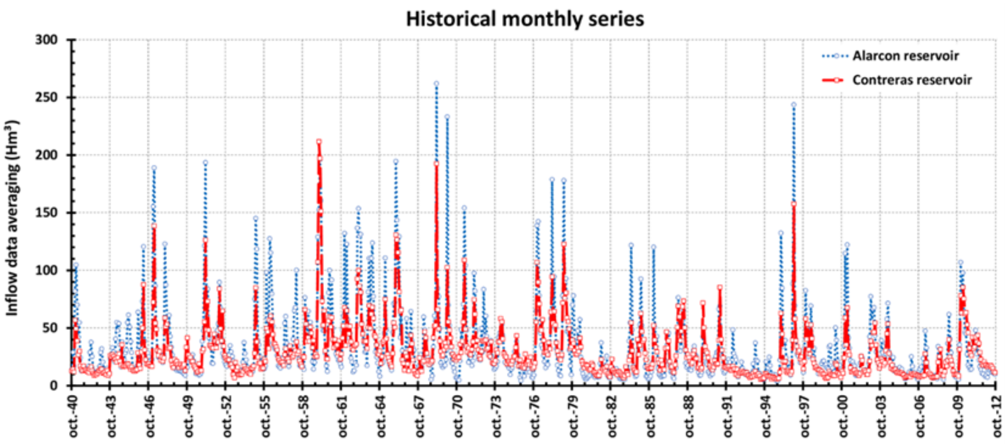

Figure II.3: Alarcon and Contreras historical monthly series after removing effect of evaporation and seepage losses, according to Spanish hydrological years (first month October and the last one is September of following year).

Table II.1: Alarcon and Contreras monthly time series. Main statistic parameters.

Statistic parameters	Sub-basins	
	Alarcon	**Contreras**
Monthly mean (Hm³):	33.01	28.51
Annual mean (Hm³):	396.09	342.12
Minimum (Hm³):	3.86	5.52
Maximum (Hm³):	262.14	211.70
Range (Hm³):	258.28	206.18
Variance:	1099.39	532.31
Standard deviation (Hm³):	33.16	23.07
Variation coefficient (%):	100.5	80.9
Skewness coefficient:	2.78 Positive skewness	2.98 Positive skewness
Kurtosis:	10.12	14.30

The similarity exposed by their probability distributions is the result of its spatial proximity and their resemblance in physical, meteorological and hydrological properties. Their correlograms show a strong spatial and spatio-temporal dependence. The temporal dependence of Contreras runoff is higher than in Alarcon. On the contrary, the spatio-temporal correlograms show a higher influence of Alarcon on Contreras inflow values than in the opposite. The main reason behind these differences seems to be the role of groundwater discharge (CHJ, 2006, 2020). These relationships will be explored more deeply with the BCM analysis.

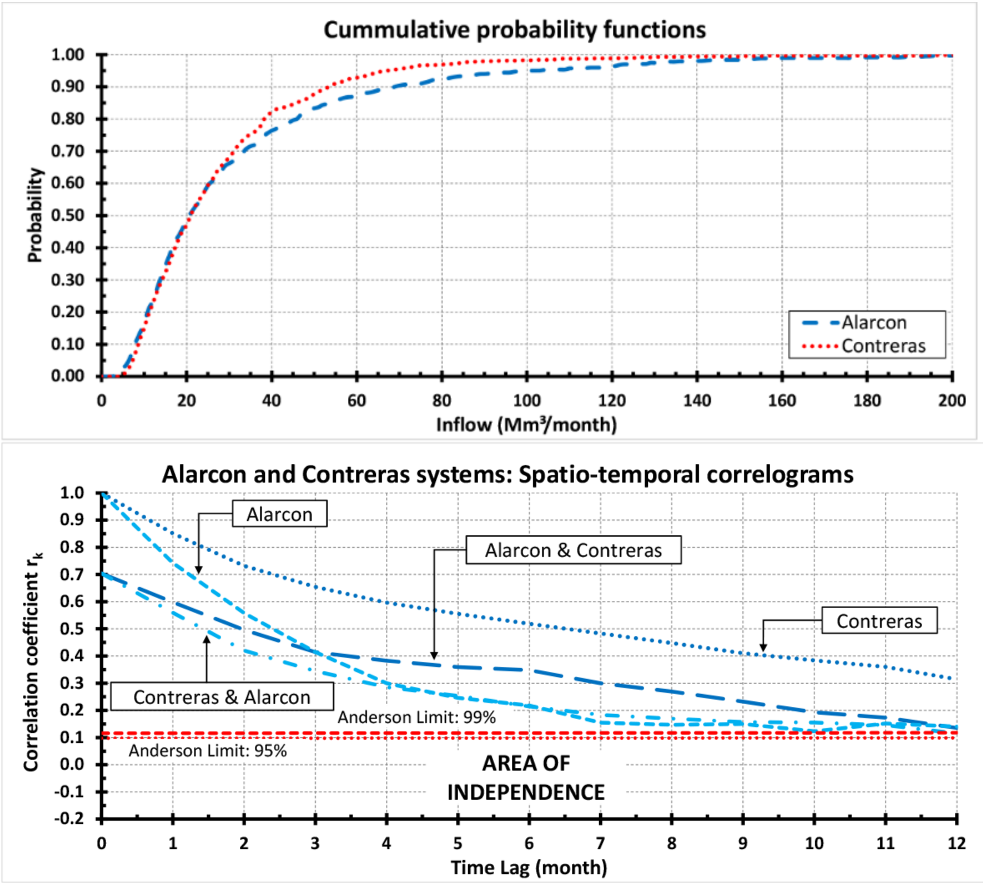

Figure II.4: Preliminary assessment of the spatial and temporal dependencies of the Alarcon and Contreras sub-basins. Upper: Probability distribution functions. Bottom: Temporal and Spatio-temporal correlograms with Anderson probability limits for an independent series (95 and 99 percent probability level). Please note that the Anderson limits define independence area of a correlogram.

II.4 Methodology

This research was articulated in three consecutive and interrelated sequential steps (Figure II.5). Step-1 comprises the treatment and analysis of the raw inflow data, in order to adapt it to the subsequent steps and to the goals pursued by the study. After that, Step-2 corresponds to the building of the BN_PGM models applied to perform the spatio-temporal BCM analysis; and they models are populated and trained by the treated data previously. Finally, Step-3 is fully entirely devoted to calculating and analyzing the causal relationships through “concept-proof” BCM. This last step is crucial because of it will allow discovering, extracting and quantifying of the logical and non-trivial time-dependency structure that inherently underlies into hydrological series and that define of the behavior of the adjacent sub-basins.

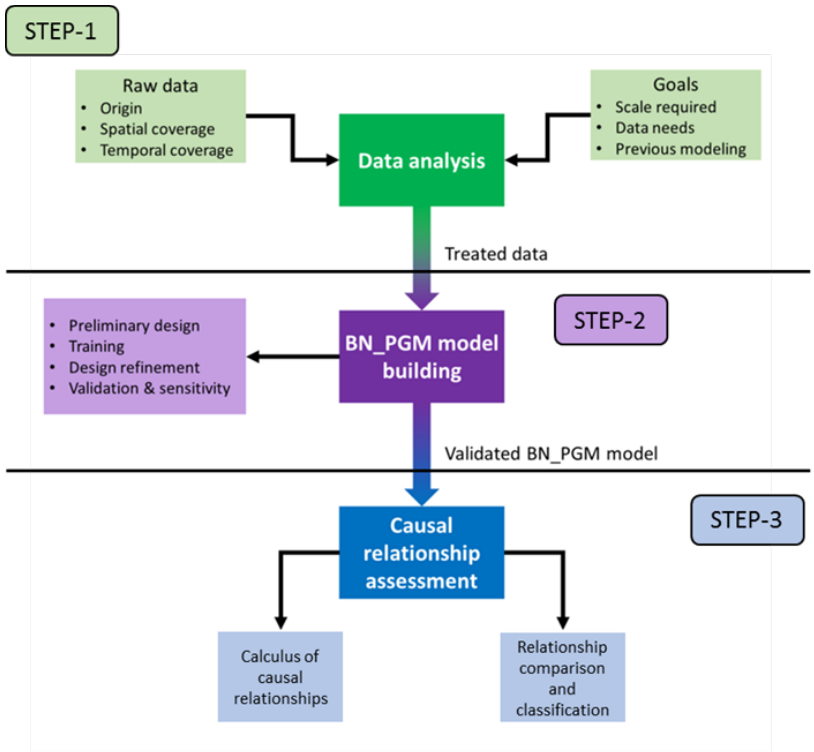

Figure II.5: General methodology.

II.4.1 Step-1. Data analysis

The key factors of this step are the origin of the data (historical records, outputs from hydrological modeling, results obtained by stochastic models and so on), its spatial coverage (e.g. the entire hydrological basin as a lumped unit, the entire basin divided into sub-basins, certain sub-basins, …) and its temporal coverage (period of analysis, time scale of the data, etc.). They should be shaped according to the objective of the analysis. For example, the evaluation of climate change impacts would require the obtaining of future inflow scenarios through hydrological modeling, while analyses based on the current hydrology may be done employing historical records. One aspect that should also be considered is the data needs of a BN, which may require to extend the available records using modelling techniques (e.g. Molina et al., 2016).

In the case of the Jucar river basin, the analysis has been developed at the seasonal scale, dividing the monthly inflows into two different periods per year. This division has been made in accordance with the operational practices of the Jucar River Basin Authority (CHJ). The Irrigation Period (IP; to May from September) corresponds to the irrigation season, in which agricultural demands concentrate and rainfall is reduced, so reservoirs are lowered to satisfy them. The Non-Irrigation Period (NIP; to October from April of next year) is characterized by low agricultural demands and higher rainfalls than the summer one. The Jucar river system operation by the CHJ Operation Office is supported by projections on inflows during the irrigation period based on the hydrological discharge on the past months (Macian-Sorribes and Pulido-Velazquez, 2017). Based on them, deliveries from the reservoirs to the farmers are scheduled for the upcoming irrigation season. Consequently, this division aligns the analysis with the practices of the system operators.

II.4.2 Step-2. Causal model building

This step involves developing BN-PGM model by means of other four sub-steps:1) Preliminary design; 2) training; 3) design refining; and 4) validation and sensitivity analysis. At the beginning of the process, a first design of the PGM is proposed. A training process on this draft is performed to refine the design of the BN-PGM model and make sure it captures the spatio-temporal relationships shown by the data. Once the model is set, it is necessary to validate and to perform a sensitivity analysis, based on the perspective of the Theory of Information.

Given the novelty of application of this BCM methodology, there were not previous references on how to proceed regarding the application of the PGMs for the triple dimension of analysis pursued by this research, so it was built in an iterative way. After a period of analysis within the preliminary design phase, an initial draft was developed. Once the network design was set, supported by a powerful training through Learning Wizard (HUGIN ® version 7.3), a fully connected PGM was built for wholly capturing and modelling the double dimension (spatio-temporal) of both sub-basins. This is consistent with the strong relationships found in the previous data analysis (please see Fig 4 bottom, correlograms). Finally, model validation was developed through the calculation of some important parameters belonging to Information Theory discipline. In particular, it has been used Total Entropy, Conditional Entropy and Mutual information. In the Jucar river basin two different BN-PGM models have been built: one describing the average and lumped behavior of the upper sub-basins and another specific one used to obtain the spatio-temporal relationships during a dry period.

II.4.3 Step-3. Bayesian Causal Modelling

This is a key step in this research and consists in calculating and analyzing the causal relationships using the BCM developed in the last step, following the process explained in section II.2.2. The estimation of the relationships embedded in each BN-PGM consisted in alternatively modifying (maximizing) one node of the model and evaluate how the remaining nodes change in response (Molina et al., 2016). A remarkable change in one particular node associated with a change in another would imply a strong causal relationship between them, whereas a little one would mean the absence of a bond. The analysis of these relationships consists in comparing and sorting the changes previously calculated, considering the type of relationship that each pair of nodes has (e.g. spatial, temporal, spatio-temporal).

This step was also tackled from a triple dimension that comprises spatial, temporal and spatio-temporal analysis. Drawn results from these dimensions show important differences among them. Furthermore, due to the flexibility of design and the back propagation of the probability, the BN-PGM was able to evaluate the influence of both sub-basins each other in both ways. This is a relevant characteristic, which is essential for developing an accurate and rigorous water rivers basins management. This is highlighted through two different analyses. First one dedicated to a lumped analysis of dependence, and the second one by means of a specific analysis over dry periods focused on time-horizon of the Jucar basin typical drought (3 years; (CHJ, 2007)). Both analyses comprise the development of two fully connected Bayesian Networks (BNs), designed at a season-scale and grouped in two different periods, Temporal Irrigation and Non-Irrigation ones, according to Jucar River Basin Authority operational practices. Furthermore, it was considered a year as dry year if either Alarcon or Contreras runoff during the winter season falls below the percentile 33 of the whole historical period.

A novel variation ratio (*VR*) has been proposed that allows a dependence analysis between the 2 subbasins at the three dimensions (spatial, temporal and spatio-temporal) at seasonal scale. This index is obtained as the division between the expected value of the probability function after maximization of the probability intervals from designed BN-PGM models and the one from before. In order to facilitate its compression, the outcomes were normalized, in this way that variation ratio had the same physical sense as a classical correlation coefficient. That is, the higher the value departs from zero (0), the stronger the dependence is. In contrast, values lower than 0 indicate an inverse dependence, and 0 value displays non-dependence.

II.4.4 BCM Concept-proof. Applied conceptual frameworks

Due to the absence of previous references on this type of application, it is essential to describe the applied conceptual frameworks (Figure II.6). Each node of the BN represents the runoff of an upper Jucar sub-basin for a given season. Alarcon NIP is the runoff of the Alarcon sub-basin for the non-irrigation period; Contreras NIP is the runoff of Contreras for the non-irrigation period; Alarcon IP corresponds to the runoff from the Alarcon sub-basin during the irrigation season; and Contreras IP represents the runoff from Contreras for the irrigation period.

On the other side, the data used to populate and train this BN corresponds to the available monthly historical records presented in Section II.3.2., obtained from the Jucar River Basin Authority (CHJ), upscaled to seasonal periods (months from October to April added to form the non-irrigation runoff and months from May to September to form the irrigation runoff).

Consequently, in order to propagate the Bayes' Theorem in both space and time the Figure II.6 summarizes the applied conceptual frameworks both for lumped analysis and specific ones focused on dry cycle analysis.

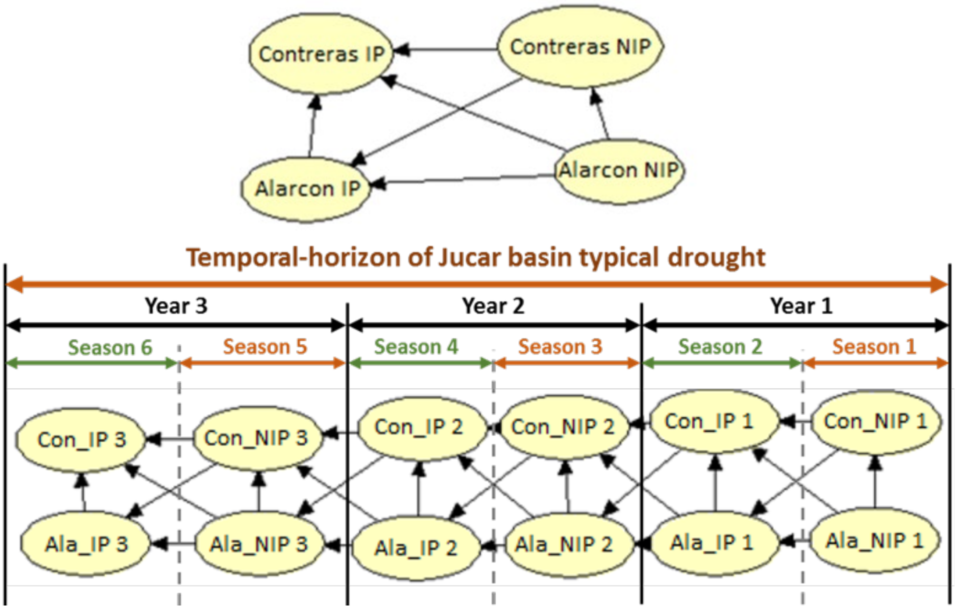

Figure II.6: BCM conceptual frameworks to upper Jucar river sub-basins. Direct Acyclic Graph considered between one season and the subsequent one. Upper lumped analysis. Bottom specific analysis over dry cycle. Abbreviations used: Non-irrigation period (NIP). Irrigation period (IP). Contreras reservoir (Con). Alarcon reservoir (Ala). Please note that the numbers indicate the year of the dry cycle analyzed.

The BCM was built using the Learning Wizard of HUGIN Expert ® (V 7.3), which generated probabilistic distributions of the variables associated with each node, as well as a logic structure according to the internal dependences and relationships detected. The Learning Wizard result was a fully connected network (each node interacts with the remaining three), which is in accordance to the strong dependences shown by the statistical analysis performed before (please see Figure II.4 bottom, correlograms). Therefore, each node of the network shows a causal relationship with the remaining three. Another reason for this fully connected design is that it is the best way for assuring the complete capture of the runoff dependence for the double dimension: space and time.

Finally, although this conceptual framework, by itself could be understood as results of the research, it has been considered appropriate to show them as part of the methodological section, given the novelty of these approaches, in this way the reader is facilitated to understand of the developed process.

II.4.5 Concept-proof. Sensitivity Analysis and Validation of results

Sensitivity analysis and validation of results is addressed through the development of an Entropy approach, based on the perspective of the Theory of Information. In this sense, Conditional Entropy, Mutual information is calculated for the Bayesian causal models.

Sensitivity analysis can be performed using two types of measures: entropy and Shannon's measure of mutual information (Pearl, 1988). The entropy measure assumes that the uncertainty or randomness of a variable *X*, characterized by probability distribution *P(x)*, can be represented by the entropy function *H(X)* (Molina et al., 2016):

$$H(X) = -\sum_{x \notin X} P(x) log P(x)$$

Entropy of a probability distribution can be defined as a measure of the associated uncertainty to that random process that this distribution describes. Consequently, a score of uncertainty/certainty level of events can be made attending to this entropy, *H(X)*.

Reducing *H(X)* by collecting information in addition to the current knowledge about variable *X* is interpreted as reducing the uncertainty about the true state of *X* (Molina et al., 2016; Zazo, 2017). The entropy measure therefore enables an assessment of the additional information required to specify a particular alternative. Shannon's measure of mutual information is used to assess the effect of collecting information about one variable (*Y*) in reducing the total uncertainty about variable *X* using:

$$I(Y.X) = H(Y) - H(Y \mid \mathrm{X})$$

where *I(Y.X)* is the mutual information between variables. This measure reports the expected degree to which the joint probability of X and Y diverges from what it would be if X were independent of Y. If *I(Y.X)* = 0, X and Y are mutually independent. *H(Y|X)* is conditional entropy which means the uncertainty that remains about Y when X is known to be x.

According to the entropy approach presented, mutual information values higher than 0 would imply some dependence between the variables analyzed, while the opposite would mean that they are independent from each other (Pearl, 1988). Therefore, this analysis represents an alternative way to characterize the dependences between variables. In this research, this validation is useful because its results can be compared with the temporal dependence analysis carried out.

Assessments of the entropy associated to each variable, the conditional entropy and mutual information for each variable and connection were performed supported by HUGIN Expert ® software.

II.5 Results

II.5.1 Average spatio-temporal dependences

The average spatio-temporal dependence analysis has been done by maximizing the probability distribution of one variable of the BN each time and measuring how this perturbation affects the probability distributions of the rest of the network. This dependence has been evaluated using a novel and normalized developed variation ratio, for each remaining node of the network, as the division between the expected value of the probability function after the perturbation and the one from before (Figure II.7). Moreover, the dependences obtained have been divided into spatial (same season, different sub-basin), temporal (different season, same sub-basin) and spatio-temporal (different season, different sub-basin). The considered seasons are non-irrigation (*NIP*) and irrigation (*IP*); while the sub-basins correspond to Alarcon (*A*) and Contreras (*C*).

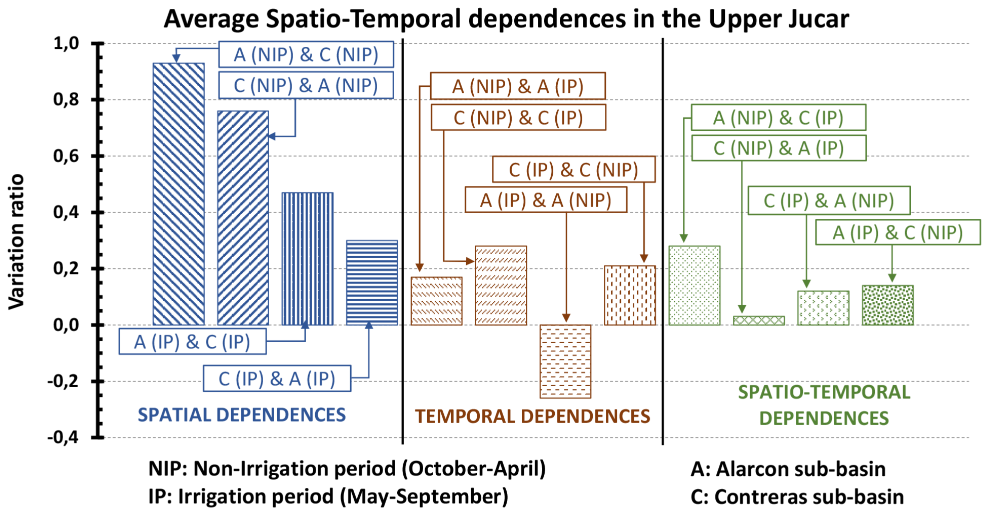

Figure II.7: Average spatio-temporal dependences for the upper Jucar river basin.

It can be observed that spatial dependences (blue bars) are the strongest ones, with values distinctly higher than 0 and higher than the temporal and the spatio-temporal dependences. This bond is in accordance with the geographical proximity of both sub-basins. Furthermore, dependences are higher for the non-irrigation season than during irrigation. This may be caused by the higher rainfalls in the non-irrigation season, since its geographic proximity drives similar rainfall events, strengthening the bond between them. Another interesting aspect (also noticed in the correlograms, see Figure II.4 bottom) is the fact that the influence of Alarcon subbasin on Contreras' inflows is higher than in the opposite way, for both seasons. This asymmetry in their dependences may be caused by groundwater flows (please see Figure II.2), which show an underground discharge from Alarcon sub-basin to Contreras sub-basin, according to piezometric levels as it is shown CHJ (2006,2020).

Considering the temporal dependences, Contreras shows a higher bond than Alarcon, given the higher variation ratio noticed in Contreras. This agrees with the correlograms, in which this influence is clearly shown by the significant statistical evidence (see Figure II.4 bottom; Alarcon & Contreras correlogram displays higher correlation coefficients, r_k, than Contreras & Alarcon correlogram in all analyzed monthly time lags). The reason behind this may be the geological differences found between both sub-basins, which can be explored using the information provided by the Geological Survey of Spain (Instituto Geológico y Minero de España, IGME, http://www.igme.es/default.asp). In this sense, the groundwater bodies under the Alarcon sub-basin present a significant portion of detrital sedimentary rocks, while the aquifers related with the Contreras sub-basin are mainly chemical sedimentary rocks. Given that detrital rocks are associated with quicker hydrological responses than chemical ones, the geological differences noticed may cause a slower hydrological response (and thus with longer time spans) in Contreras.

Regarding the spatio-temporal dependences, the prevalence pattern observed for the spatial ones (more influence on Alarcon in Contreras than the opposite) is maintained from the non-irrigation to the irrigation season. In fact, Contreras runoff on non-irrigation does not seem to play any influence on the Alarcon runoff during irrigation, as the variation ratio is approximately 0. The reason behind this behavior may be the maintenance across time of the bond observed in the spatial analysis. The lack of influence of Contreras on Alarcon seems to be caused by the limited groundwater flow from the Contreras sub-basin to the Alarcon one. It is also interesting notice that the spatio-temporal dependence from Alarcon to Contreras (A (NIP) & C (IP)) is similar to the temporal dependence of Contreras (C (NIP) & C (IP)).

Overall, results show a relevant asymmetry on the spatial and spatio-temporal influence of both basins each other. This may be due to the fact that Alarcon sub-basin plays more influence on Contreras than the opposite, probably by the existence of groundwater flows following mainly the Alarcon-Contreras direction (piezometric gradient towards the coastal area, from West to East (CHJ, 2006,2020)).

II.5.2 Spatio-temporal dependence on dry years

Given that dry spells in the Jucar river basin last more than one year, a new BCM has been developed extending its temporal-horizon up to 3 years (6 seasons, see Figure II.6 Bottom). According to dry year definition a set of 27 years were considered. In the most of them, both Alarcon and Contreras inflow during winter fall below the threshold, as well as during the summer season.

Figure II.8 shows the results of the causal relationship analysis done for dry periods, starting at a dry year and spanning to 2 years after a dry one. Most of the years after a dry year were dry too, but a 3-year dry spell was only found for the case of an extreme drought.

The main difference between the average dependences and the ones in a dry year is the absence of significant spatial relationships during the non-irrigation season, as the variation ratios are similar to 0 (please see Figure II.8 upper; A (NIP) & C (NIP) and C (NIP & A (NIP)). This may be caused by the absence of rainfall and the lowering of groundwater tables. The decrease in heads is steeper in the Alarcon sub-basin due to having more detrital rock areas than Contreras, causing the interruption of the groundwater flow from Alarcon to Contreras. During irrigation, on the other hand, spatial dependences are similar to the average ones. This seems to be caused by the fact that rainfall during the irrigation season is low even during wet years, so the differences among years are less relevant than the ones found for the non-irrigation season. Another change between normal and dry years is that Contreras plays more influence on Alarcon than Alarcon on Contreras during dry years (C (IP) & A (IP) is greater than A (IP) & C (IP)). This inversion is also shown in the spatio-temporal relationships (C (NIP) & A (IP) is greater than A (NIP) & C (IP)). The temporal relationships do not suffer significant modifications, although Contreras does not show higher temporal dependences than Alarcon.

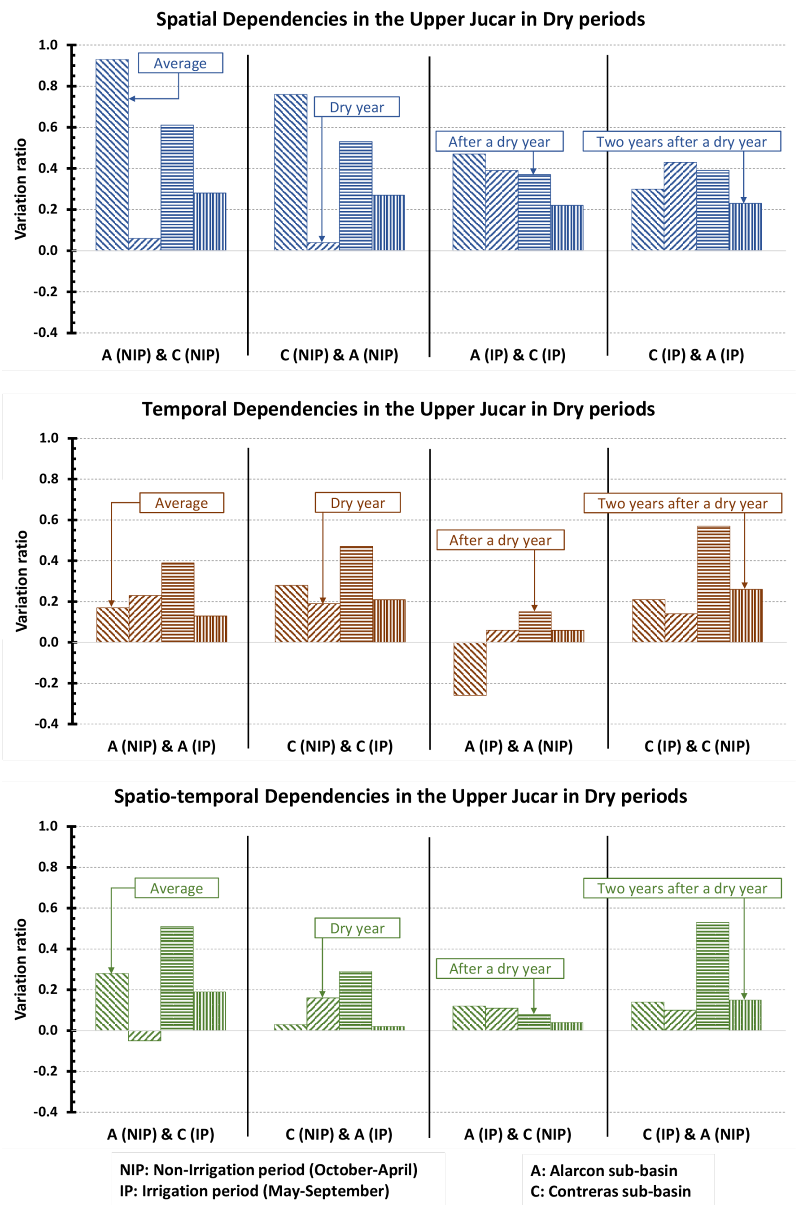

Figure II.8: Spatio-temporal dependence on the upper Jucar river basin during dry periods.

The causal relationships observed after a dry year (which in most cases corresponds to a dry year) present a remarkable increase in temporal and spatio-temporal relationships with respect to the average dependences. This increase in the relationships with temporal component may be caused by groundwater discharge, since its importance grows during long periods without rainfall. Spatial relationships show higher levels than the ones found for the first dry year, but do not reach the levels shown on average. This seems to point that groundwater exchanges between sub-basins increase after a dry year, may be because the geological differences between both sub-basins cause an unbalance between piezometric heads again (due to different hydrological response times).

Two years after the start of the dry spell (which except for the most severe droughts found, is not dry) the temporal and spatio-temporal dependences are, on a broader view, similar to the average. This is consistent with the ending of a dry period. However, spatial dependences are lower than the average while showing similar levels regardless of the sub-basin and season. This may be caused by a rise in precipitations, since its influence in the bond between sub-basins is the same regardless of the direction of the relationship (from Alarcon to Contreras or from Contreras to Alarcon).

II.5.3 Sensitivity and Validation Analysis

Calibration of causal reasoning process is done through a comparative analysis with traditional techniques such as correlation. In this sense, the results obtained from the causal reasoning analysis for the average BN-PGM model resemble the ones provided by correlation (please see Figure II.4 Bottom), as explained previously.

On the other side, assessments of the entropy associated to each variable, the conditional entropy and mutual information for each variable and connection were done for the average BN-PGM model (please see Figure II.6 Upper, BCM conceptual framework for lumped analysis). In this sense, Figure II.9 summarizes the main achieved results. These outcomes of the entropy analysis agree with the causal relationship analysis (see Figure II.7). In particular, the same prevalence pattern is observed: spatial dependences show the highest values of mutual information, then temporal and finally spatio-temporal dependences, whose values are the lowest.

Regarding the mutual information values of the spatial dependences are higher in the non-irrigation period, as the causal relationships. Similarly, mutual information values on the temporal dependences of Contreras are higher than the ones in Alarcon. Regarding the spatio-temporal dependences, the one between A (NIP) and C (IP) has the highest mutual information value, in accordance with the strongest causal relationship found between both nodes in comparison to the rest of spatio-temporal dependences. In spite of the similarity between them, there exist some differences. The most important is that the results of the mutual information between two nodes are the same regardless of the direction considered (e.g. A (NIP) & C (NIP) has the same value than C (NIP) & A (NIP)), while the causal relationship analysis is sensitive to it. Moreover, the remarkable differences found between the spatial and the remaining causal relationships do not appear in the entropy analysis, in which only slight modifications are found.

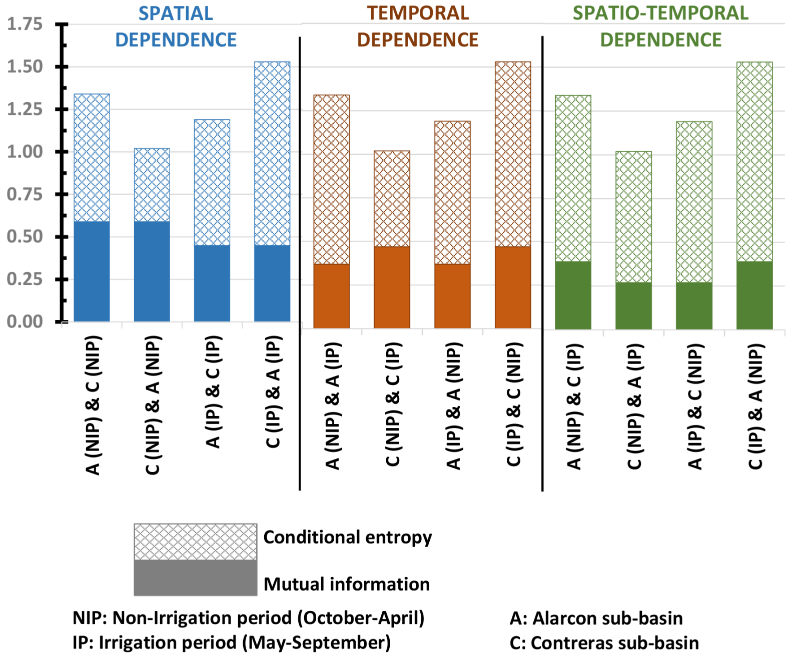

Figure II.9: Sensitivity analysis results for the average behavior of Alarcon (Ala) and Contreras (Con) sub-basins.

On the other hand, Figure II.10 shows an entropy analysis of the BN-PGM model for a dry period, which is also supported through HUGIN Expert ® software. The entropy results clearly reflect the temporal mitigation of dependences, since the mutual information values decrease when moving forward or backward in time. The mutual information values distinctly decrease when moving more than one year apart from the hypothesis node. This is in line with the correlograms (see Figure II.4), which show dependence for 12 months. The fact that Contreras has more temporal dependence than Alarcon is also shown in the entropy analysis, since mutual information values associated with temporal dependences are higher in Contreras than in Alarcon (although with slight increases).

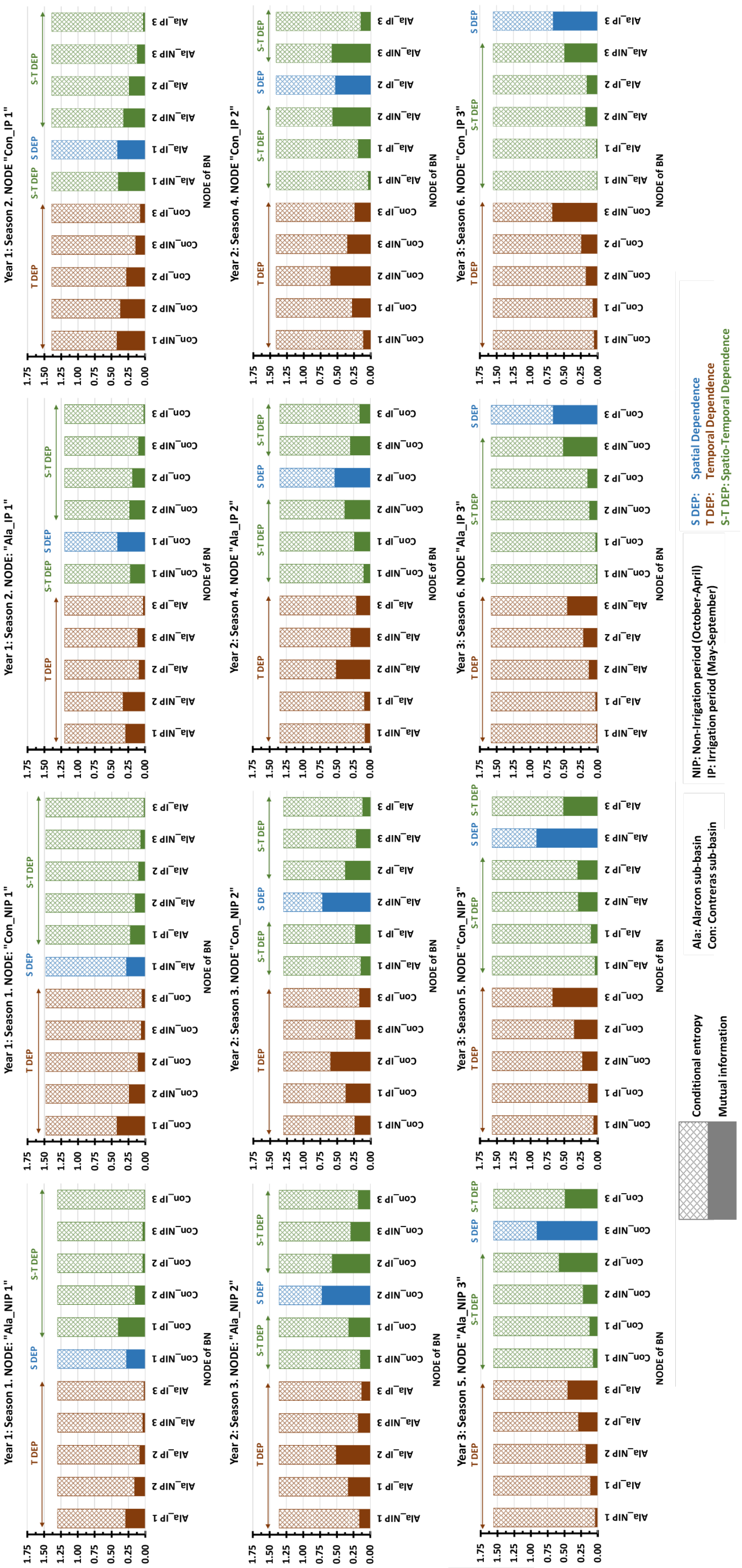

Figure II.10: Entropy analysis over dry cycle analysis performed over time-horizon of 3 year (6 seasons).

On a broader view, the results of the entropy analysis agree with the causal relationship analysis. The mutual information values for the first year of a dry cycle are lower than on average, in accordance with the causal relationship analysis, as well as the increase noticed in the mutual information values after the first year. Similarly, temporal mutual information values after a dry year increase, as causal relationships do. However, there are also points in which both analyses depart. For example, the mutual information values for the third year are in general similar to the second, while the causal relationships showed a decrease between those years.

With respect to the spatio-temporal relationships, the mutual information values for the non-irrigation season are higher in Alarcon than in Contreras, while during the irrigation season they are similar except for the second year, in which Contreras shows higher values. This is consistent with the causal relationship analysis (see Figure II.8) except for the first dry year, in which they disagree (entropy points at a higher influence from Alarcon on Contreras while the causal relationship shows the opposite). In spite of the differences found, most of the pattern changes noticed between the average behavior and a dry year found by the causal relationship analysis can be drawn from the entropy analysis. Given this, the BN-PGM for dry years can be considered valid.

II.5.4 Comparison between BCM and traditional statistical analysis

Although their distinct differences in terms of setup and interpretation, BCM results (Figure II.7) agree in general terms with the ones obtained from a traditional statistical correlation analysis (Figure II.4). In particular, both procedures find out that Contreras shows higher temporal dependence than Alarcon (the correlogram of Contreras takes higher values than Alarcon, as well as the temporal variation ratios), that the dependence from Alarcon to Contreras is higher than from Contreras to Alarcon (the correlogram between Alarcon and Contreras takes higher values than the one from Contreras to Alarcon, as the spatial and spatiotemporal variations ratios); and that these dependences hold for the whole hydrological year (correlograms rise above the Anderson limits while variation ratios depart from zero). An advantage of statistical analysis is their well-developed theory, which is able to clearly identify when a relationship is significant (using the Anderson limits), in contrast to the use of variation ratios by BCM, since they are unbounded and no precise threshold can be set to infer its significance. Although both methodologies are sensitive to the amount of available data, BCM is more data-demanding than statistical analyses in general.

However, BCM outperforms statistical analysis in other aspects. First of all, it is able to offer context-dependent information in a straightforward way (e.g. how the relationships vary between normal and dry years, or between the irrigation season and the rest of the year), being also possible to determine when this general behavior changes better than statistical analysis. Moreover, BCM does not require prior data transformations or standardizations before and after running the analysis, being also not bound to a particular distribution function or set of distribution functions. Although not explored in this research, BCM can also generate probability functions conditioned to previous observations of related variables in an efficient way compared to statistical procedures.

II.6 Discussion and conclusions

Bayesian Causal Modelling, evaluated from Bayesian Networks perspective, has demonstrated in this "concept-proof" to be able to identify which relationships between variables are important, as well as how they change between an average behavior and a dry year. Compared with classic statistical analysis, neither prior knowledge nor assumptions on the probability distribution of the variables involved is required. On the contrary, Bayesian Networks learn it by themselves, being also able to recursively add more information as soon as it is available (Molina et al., 2016).

The spatio-temporal dependences in the upper Jucar river sub-basins analyzed through causal reasoning have been compared with an entropy analysis. Although some differences were found, both of them agreed in most of the main patterns found in the data, as well as the modifications suffered by these for a dry year. However, CR considers the direction of each relationship. This advantage is a distinct feature of causal reasoning, making it able to determine which variables are playing the highest influence on the spatio-temporal relationships found in the system. If the influence of each variable can be assessed and ranked with respect to the others, one can determine where investments in reducing uncertainty (e.g. increasing the monitoring or the quality of the measurements) would be efficient.

BN models developed in this research have been populated, trained and validated using historical data. This could be done due to the existence of enough records (72 years for the whole historical period and 27 dry years). However, they would exist situations in which historical records would not reach the minimum size to ensure a safe training. In this case, suitable alternatives to extend the available time series would consist in using stochastic processes like Monte Carlo simulation or stochastic models, as done by Molina et al. (2016). However, these techniques assume a specific spatio-temporal dependence structure, so they would influence the analysis of the causal relationship performed, given that the generated data would follow a pattern that may not be in line with the one intrinsic to the historical records.

Another alternative to extend the available runoff data would be the use of hydrological models, whose assumptions are less tight in terms of spatio-temporal dependences. However, these models would require enough historical records of meteorological variables (e.g. temperature and rainfall) and information about the hydrological properties of the sub-basins to be analyzed. Furthermore, hydrological models usually need more time to be set up than stochastic models.

The changes found out by BCM at the beginning of the dry period open the possibility of predicting droughts from examining the evolution of these dependences. In fact, BNs' assessment of dependence is able to determine how each variable depends on previous measurements, enabling its use as a predictor (Molina and Zazo 2017). For the Jucar River basin in particular, the absence of spatial dependence between Alarcon and Contreras sub-basins can be used to foresee water scarcity periods and start activating drought management measures in advance.

Using the BCM defined in combination with water resource management models, one can automatically trigger these measures according to the evolution of the causal relationship. These possibilities of predictive potential will be explored in upcoming research.

From the methodology developed in this research and its application to the case study, the following conclusions can be drawn:

- Causal reasoning has been successfully applied to the upper Jucar river basin. The BN_PGM model developed has been able to identify the dependences existing between runoff variables in both time (in-year seasons) and space (sub-basins). These dependences are similar to the ones provided by an entropy analysis and agree with the ones found by a previous statistical analysis.
- Causal reasoning identified how dependences change between average and dry years for the upper Jucar River basin. They were also able to characterize how these dependences evolve during a dry period. This ability to determine the entrance and exit of a drought enables the use of BNs as drought forecasting tool or as drought scenarios generation technique.

Additionally, this research demonstrates the suitability of BCM methodology for spatial-temporal analysis of water resource behavior of one or several basins, in a dynamic and stochastic way, because of BCM is able to reveal a logical, hidden and non-trivial structure of interdependence underlying in the hydrological historical records.

On the other hand, the spatial approach proposed in this “concept-proof” based on BCM, and focused on dry periods (droughts), may be a suitable starting point for its application to other types of extreme events such as floods, within a context of flood damage prediction.

Finally, this “concept-proof” reinforces that past information will provide prior knowledge of the future, particularly useful in water resources planning and management of highly dependent basins.

CAPÍTULO III
Optimización de la modelización causal bayesiana

Este Capítulo III reproduce la versión de autor, adaptada al formato tesis, del artículo científico, del artículo científico "Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework", publicado en la revista científica *Journal of Hydrology* (ISSN: 0022-1694) el día 8 de abril 2022.

Las innovaciones en la aplicación de los Modelos Probabilísticos Gráficos en la modelización hidrológica, y en particular las RBs al amparo del paradigma de la Inteligencia Artificial, suponen avanzar en el establecimiento de marcos metodológicos robustos para analizar en detalle las dependencias temporales en series hidrológicas.

La investigación que integra este capítulo ha supuesto la definición de un nuevo marco metodológico para el análisis de la estabilidad temporal de las series hidrológicas que optimiza los dos principales factores implicados en la modelización causal bayesiana, que son el número de series sintéticas (cantidad de datos) y el número de intervalos de las distribuciones de probabilidad para los procesos de entrenamiento y aprendizaje. Para esto se han definido dos nuevos indicadores, llamados "Índice de similitud" e "Índice de estabilidad", que permiten evaluar el rendimiento global del proceso de optimización. La combinación óptima de ambos factores se lleva a cabo mediante un enfoque recursivo bi-objetivo basado en los dos índices definidos.

Los resultados obtenidos ponen de manifiesto una elevada relación entre el nivel de rendimiento de la modelización, evaluado en términos de estabilidad, y el comportamiento temporal de la aportación, determinado en términos de dependencia temporal. Esta investigación contribuye a una modelización hidrológica causal más rigurosas y robustas, lo que permitiría mejorar la gestión de los recursos hídricos debido a una mejor comprensión de su funcionamiento.

[19] Zazo, S., Martín, A. M., Molina, J. L., Macian-Sorribes, H., Pulido-Velázquez, M. 2022. Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework. Journal of Hydrology, 610, 127832. https://doi.org/10.1016/j.jhydrol.2022.127832.
Se omiten los apartados: "CRediT authorship contribution statement", "Declaration of Competing Interest" y "Acknowledgements". La sección "References" se integra en la Bibliografía de esta Tesis.
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III.0 Abstract

A strong innovative tendency is nowadays emerging that largely comprises new hydrological modelling approaches, based on Causal Reasoning through Probabilistic Graphical Modelling (PGM), because its ability to support probabilistic reasoning from data with uncertainty. These novel modelling frameworks are quite diverse and disperse not only in terms of techniques but also regarding its aims. It seems necessary to find a general and robust methodology for assessing its performance. This research aims to provide a novel general methodology for assessing the performance of PGM based on Bayesian Causality for modelling and analysing the rivers´ runoff behaviour. For it, a structured four-step approach is developed and showed throughout the paper. The proposed methodology begins with the identification of the two main factors that condition the Bayesian Causal (BC) Modelling: the number of synthetic series (data amount) and the number of intervals for probability distributions for training and learning processes. The developed analysis comprises the definition of three levels for the first factor and seven levels for the second one, as well as the design of an innovative stability framework that assesses the level of BC Modelling performance. Furthermore, it has been necessary to create-define two novel indexes, named "Similarity and Stability Indexes" from 21 scenarios arising from the combination of the levels of the both factors. The optimal combination of factors is identified through a bi-objectives recursive approach based on previous indexes. Main results drawn successfully show a high relationship between the level of modelling performance, measured in terms of stability, and the river runoff temporal behaviour, measured in terms of temporal dependence. This research may help water managers and engineers to develop more rigorous and robust hydrological causal modelling implementations.

III.1 Introduction

Probabilistic Graphical Models (PGMs) since their emergence in the 1980s, within the statistical and artificial intelligence reasoning communities (Javidian et al., 2020), have been increasingly getting more notoriety in scientific community. This is mainly because they are an intuitive formalism to capture the probabilistic (in)dependence information of a domain (Pearl, 1988; Vogel et al., 2018) through the combination of probability-graph theories (Vogel et al., 2014), as well as a powerful framework for reasoning under uncertainty in knowledge-based systems (Cabañas de Paz, 2017; Javidian et al., 2020).

According to Koller and Friedman (2009), a PGM "*use a graph-based representation as the basis for compactly encoding a complex distribution over a high-dimensional space*". Formally, it is defined by a joint probability distribution $P(X)$ on the set of variables of the problem X, and a graph G that represents the (in)dependence relationship amongst variables (Cabañas de Paz, 2017). At its core, they are characterized by a "*qualitative*" part which encodes a set of (conditional) (in)dependence relationships amongst variables, and a second "*quantitative*" one that measures the (in)dependence strength (Cabañas de Paz, 2017).

PGMs have been widely applied to a variety of reasoning tasks related to prediction, diagnosis, classification and risk assessment under original approaches and applied to different scientific disciplines. Engelke and Hitz (2020) introduces a general theory of conditional independence applied to graphical models for extremes. For its part, Javidian et al., (2020) propose a new algorithm (named LCD-AMP) applied to chain graphs, that overcomes the problems of data order dependence. Ramos Fernandez (2018) designs a Naïve Bayes PGM as a medical tool for predicting the severe course of acute bronchitis in infants. Lehikoinen et al., (2019), by Bayesian network (BN) classifiers, assesses the effects of multiple natural and anthropogenic factors on marine ecosystems simultaneously. For the first time, Macian-Sorribes et al., (2020) addresses the spatio-temporal dependence dimensions of inflows in hydrology through BNs. In Vogel et al., (2018) is identified the driving factors of flood loss at residential buildings applying novel PGMs approaches, based on BNs and Markov Blankets. On the other side, the relation among probability distribution and the graph defines the PGM type, existing three classes basically (Diez et al., 2018): (a) undirected graphs (e.g. Markov Networks), (b) directed acyclic graphs (e.g. BNs) and (c) chain graphs which are a unification of the first two (Javidian et al., 2020). Of these, the most widely used is the one based on BNs (Cabañas de Paz, 2017; Javidian et al., 2020), due to its ability to describe the overall behaviour of a system through the propagation of (in)dependence among the variables throughout the whole graphical structure (Vogel et al., 2018). In addition, the fact that BNs are based on the notion of conditional (in)dependence (Steck, 2001) makes them particularly useful for dealing with forecasting and analysing of the general behaviour in complex natural processes (Molina et al., 2019).

Referring specifically to hydrology and water resources, BNs have been satisfactorily applied to issues such as water planning of catchments (Mamitimin et al., 2015; Xue et al., 2017), integrated groundwater management (Carmona et al., 2011; Molina et al., 2013), reservoir management (Malekmohammadi et al., 2009), assessment of environmental risk on large dams (Ahmadi et al., 2015), flood damage (Schroeter et al., 2014) and drought forecasting and management (Shin et al., 2019), among others.

Recently, new hydrological challenges have begun to be addressed through the potential that BNs offer to discover causal structures in observed data (Spirtes, 2010), because the intrinsic (in)dependence relationships within of temporal series are not known in depth (Molina and Zazo, 2018; Molina et al., 2019). This is performed under a novel framework named Bayesian Causal (BC) Modelling, based on Causality, and which is addressed in form of Causal Reasoning (CR), supported by Bayesian modelling (Macian-Sorribes et al., 2020; Zazo, 2017). BC Modelling is a suitable technique for modelling the temporal behaviour of water resources of a basin when: (1) the approach is done from top to down, (2) the analysis is focused on the cause and (3) the objective comprises the prediction of the consequence (Macian-Sorribes et al., 2020: Pearl, 2009), as in the case of Bayesian Causality.

By means of BC Modelling it is highlighted the hidden logical temporal (in)dependence structure, that inherently underlies into hydrological historical records (Macian-Sorribes et al., 2020; Zazo et al., 2020). Under this approach, some noteworthy contributions have emerged in the field of stochastic hydrology. In Molina et al. (2016), a preliminary dynamic analysis of temporal dependence propagation was presented. For its part, Molina and Zazo (2018) discovered and quantified, for the first time, two opposite temporal-fractions within annual runoff time series, one conditioned by time and other no. Molina et al. (2019) developed a dynamic predictive runoff model based on the temporal behaviour trends of previously discovered runoff temporal fractions. Zazo et al. (2019) showed a qualitative approach for assessing temporal dependence through a novel dependence graph. Recently, Macian-Sorribes et al., (2020) analysed and assessed, simultaneous and completely, of spatio-temporal dimension of inflows across two adjacent and parallel river basins. In this sense, BC Modelling framework deliver much more accurate and powerful hydrological simulations and predictions, in line with new trends in stochastic hydrological research based on hybrid approaches between "traditional-novel techniques" (Mohammadi et al., 2006; Nourani et al.,2011; Valipour et al., 2012).

At this point, it is worth highlighting that PGMs are characterised by learning directly from the data when the structure of the network is unknown (Javidian et al., 2020; Malone and Yuan, 2012), and that such learning comprises not only the quantitative dimension of the data but also its intrinsic structure (Koller and Friedman, 2009; Steck, 2001). Therefore, issues such as the number of data or the modelling structure itself are crucial for suitable and reliable model performances (Koller and Friedman, 2009; Vogel et al., 2018). In this sense, there are significant algorithm-based developments for learning model structure from sampled data, which are well known-stablished in the scientific community. For instance, inductive causation (IC) algorithm (Verma and Pearl, 1991,1992), a similar approach independently developed by Peter Spirtes and Clark Glymour, known as PC algorithm (Spirtes et al., 2000; Madsen et al., 2003), based on conditional independence decisions (Le et al., 2016), and the improvement of the latter, named NPC learning algorithm, that introduces the notion of a Necessary Path Condition (Madsen et al., 2003; Steck, 2001). Nevertheless, in respect of the data there are two key driving factors for building a reliable dataset for learning and/or training which have not yet been addressed in depth. These are: (1) “number of synthetic series” and (2) “number of intervals” for discrete probability distributions.

The aim of this research is to provide a methodological framework for achieving an optimal combination between the different considered levels of two main driving factors that condition Learning-Training Processes of BC Modelling. This approach was applied to increase knowledge of the temporal behaviour of water resources in a river basin and have not yet been addressed by any hydrological research based on Bayesian Causality. The first, external one, is “number of synthetic series” that populates the Bayesian causal models (Factor 1; three considered levels in annual synthetic data). The second, internal one, is “number of intervals” for discrete probability distributions of synthetic data (Factor 2; with seven considered levels). This was developed to improve the performance of causal models with respect to their analytical and predictive capacity in the context of temporal behaviour of water resources of a basin. The influence between the levels of both factors was measured through two innovative indices, named "Similarity Index" and "Stability Index". These allowed the identification of the optimal combination between the levels of both factors through a bi-objectives recursive approach, in terms of overall stability of the BC Modelling process. These findings may be extrapolated to other approaches based on this type of PGMs for improving their analytical and forecast capabilities.

III.2 Methodological approach

The framework for assessing the BC Modelling performance, in terms of overall stability process comprises a four-step approach (Figure III.1). Step-1 implies the generation of synthetic data from historical records through a parametric Autoregressive Moving Average Model (ARMA) model or any alternative model approach able to generate synthetic time series. Use of observational data would only be possible if enough data to populate the BNs is available. Step-2 designs the BC Modelling by 4 sequential phases (Learning, Preprocessing, Constraints and Structure-Learning Process). In Step-3, probability propagation is addressed by Dependence Mitigation Graphs (DMGs), obtaining also its uncertainty bands through a Bootstrap approach. Finally, Step-4 assesses the BC Modelling performance innovatively. Firstly, a novel Similarity index is defined through an in-depth analysis of the overlap between uncertainty bands of wrap-around averages of DMGs. Secondly, a Stability index is created for assessing global BC Modelling performance of all possible combinations between the levels of both factors. Then, a bi-objectives recursive approach identifies the optimal combination of factors.

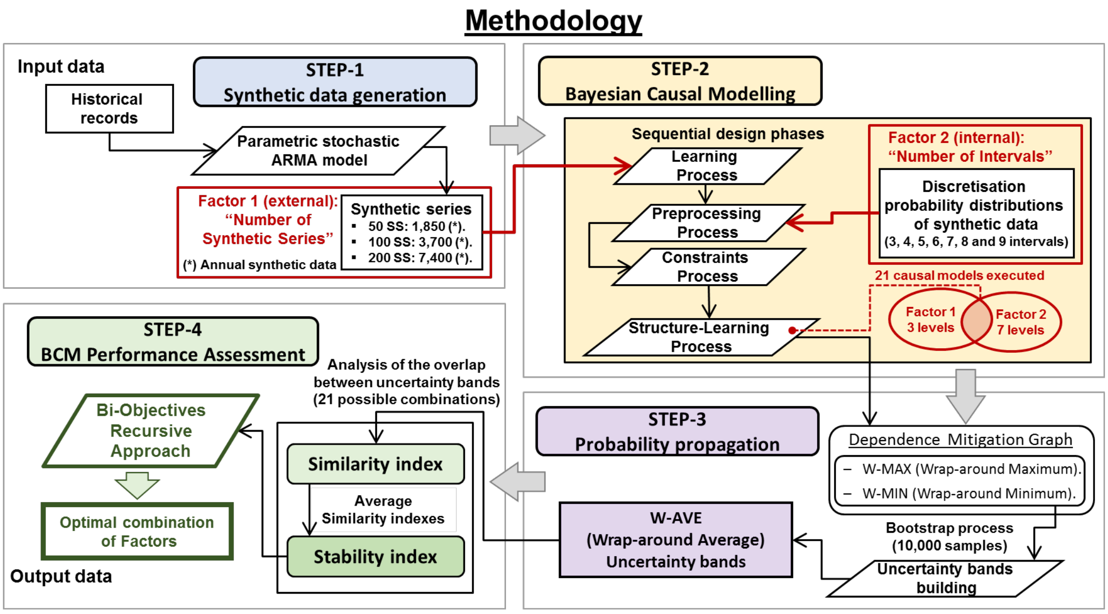


Figure III.1: General methodology.

As DMG supposes an innovative way for assessing probability propagation, for understanding of the reader Uncertainty Band generation and their overlap analysis are facilitated by exemplary figures.

On the other side, the application of ARMA models to hydrological analysis/simulation and prediction reveals a wide heterogeneity of data samples. For example, in Srinivas and Srinivasan (2006) is assessed a hybrid model for stochastic simulation of multi season stream flows through 100 synthetic data seasonal-threshold model. Borgomeo et al., (2015) presented a method to generate synthetic monthly streamflow through random sampling from a parametric or a nonparametric distribution, assessed by 100 flow sequences. In Molina et al., (2019) a dynamic predictive model which was populated with 200 synthetic annual runoff series from an ARMA model is developed.

Based on the review of the scientific literature and in the expertise acquired in the development of causal models applied to the analysis and prediction of spatio-temporal behaviour of water resources in a river basin(s) three different numbers of annual synthetic series (Factor 1; 50, 100 y 200) were generated in each case study, all of them with the same length of the historical datasets. In contrast, Factor 2 (number of intervals for probability discretization) and whose influence has not yet been addressed within the framework of hydrological research, was given seven levels (3, 4, 5, 6, 7, 8 and 9 intervals). This led to the design, execution and analysis of the results of 21 causal models for each case study, which ensures the robustness of the findings and the designed methodological framework.

Data description - Case studies

The framework in which this research is conducted involves that the case studies form part of the methodological section. In order to define a robust methodological approach that would allow extrapolating the research findings to the field of prediction based on Bayesian causal models, two headwater case studies were chosen according to the following key aspects: (1) their completely opposite temporal behaviour, temporal (in)dependence, (2) same time period of analysis and (3) lack of spatial correlation between them.

Both headwaters (Porma in the north, and Adaja in the south) belong to Duero River Basin (the largest international river basin between Spain and Portugal). Furthermore, they are defined by gauging stations, located upstream the first regulating reservoir (flows under natural regime). They are: Camposolillo (code 2078) in the first case, and Adaja (code 2046) in the second one (Figure III.2a). The time period covered 37 hydrological years (from October to September) 1974/75 and 2010/11. The historical records (without missing data) were supported by the network of gauging stations of Duero river basin Authority (MITECO, 2021). Table III.1 summarizes the main statistical parameters.

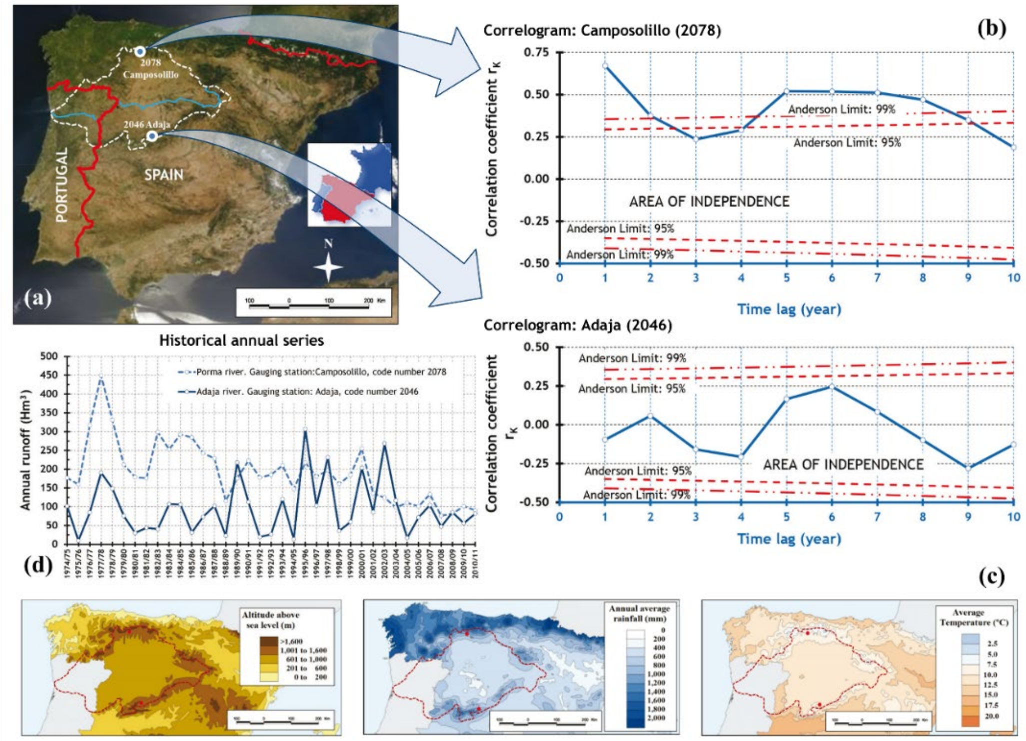


Figure III.2: (a) Case studies location. (b) Correlograms and Anderson probability limits for an independent series (95 and 99 percent probability level). (c) Main geomorphology (left) and climatic factors (center and right) of both case studies. (d) Historical annual series of runoff (time period: 1974/75 to 2010/11). Note: Hydrological year in Spain begins in October and ends in September of the following year.

Table III.1: Historical records. Main statistical parameter.

Main statistic parameters	Sub-basins: Porma "Camposolillo" (2078)	Adaja "Adaja" (2046)
Annual mean (Hm^3):	191.29	95.90
Standard deviation (Hm^3):	80.92	73.44
Skewness coefficient:	0.98	1.25

Porma case study displays a temporal behaviour completely dependent, with its correlation coefficients outside the Anderson limits of the correlogram or very close it. In contrast, Adaja case study, exhibits an opposite behaviour, clearly independent, with all correlation coefficients within the independence area of the correlogram. Figure III.2b displays both correlograms.

Both case studies are characterized by a cold Mediterranean climate, highly continental. Porma case study shows an annual average rainfall of 1430 mm. Geologically, there are important formations of limestones, sandstone and alluvial deposits in the fluvial courses. Hydrogeological speaking, it is characterized by low permeability or impermeable materials and low productivity and small extension aquifers (Molina and Zazo, 2018). Adaja case study presents an average annual about 400 mm.

Geologically, it shows important areas of arkoses, granitic blocks and alluvial deposits at the bottom of the valley. Regarding hydrogeology, impermeable or very low permeability formations are present (Molina and Zazo, 2018). Figure III.2c displays the main climatic factors and Figure.2d shows the graphic of both historical annual series.

III.2.1 Step-1. Synthetic data generation

This step is addressed through a parsimonious ARMA (1,1) model for each sub-basin, developed according to Molina et al., (2016). ARMA model plays a crucial role in this research because it provides reliable data to populate the BC Modelling process. In this sense, the purpose of this initial phase is to generate, in form of synthetic series all of them equiprobable to the historical series considered, the amount of information necessary to populate the subsequent Bayesian causal models. This stochastic, parsimonious and unconditioned model confers the highest degree of freedom to Bayesian modelling. An ARMA (p,q) is expressed as (Salas et al., 1980):

$$Y_t = \mu + \sum_{j=1}^{p} \emptyset_j \left(Y_{t-j} - \mu\right) + \epsilon_t - \sum_{j=1}^{q} \theta_j \, \epsilon_{t-j}$$

where Y_t is the value of the temporal series at a certain time-step t, μ is the mean of the time series; (p,q) are the number of autoregressive (AR) and moving average (MA) average parameters, $\emptyset_j$, θ_j are the coefficient of AR and MA average model respectively and ϵ_t represents the historical residuals.

Before the postulation of the model, a normalization process was applied using three different methods: square root, natural logarithm plus one and natural double logarithm plus one (Salas et al., 1980). These functions are commonly applied to operational hydrology (Ochoa-Rivera et al., 2007). The natural logarithm plus one method was chosen in both cases, as it yielded the lowest skewness coefficient. Afterwards, the synthetic data (equiprobable to historical records) were generated.

The validation of synthetic time series was carried out comparing their relevant statistics to those of historical records (Ochoa-Rivera et al., 2007). In this case, due to use annual time series, this process was focused on mean values (Molina et al., 2021). Given that the levels considered for Factor 1 (50, 100 and 200 synthetic series) and the length of the historical data (37 years) a total of 1850, 3700 and 7400 annual synthetic data were respectively generated in each case study.

III.2.2 Step-2. Bayesian causal model design

Conceptually BC Modelling, as PGM based on BNs, is defined as a direct acyclic graph (DAG) in which conditional probability among variables is computed (Molina et al., 2021) and propagated omnidirectionally supported by Bayes' Theorem (Zazo et al., 2020). Mathematically, BC Modelling is expressed as (Madsen et al., 2003):

$$P(V) = \prod_{X \in V} P\big(X|pa(X)\big) \ ,$$

where *P(V)* is the joint probability distribution over set of nodes V (random variables, *X*) present in the graph and which are defined through DAG and P(*X*|*pa(X)*) is the conditional probability distribution for each variable $X \in V$ that belongs to a set of probability distributions.

BC Modelling application to hydrological time series makes possible to determine/quantify the strength of (in)dependence relationships between variables in a dynamic and step-by-step manner (Macian-Sorribes et al., 2020). This is performed through modifying and analyzing the evolution of the probability distribution over time (Macian-Sorribes et al., 2020), by maximizing the statistical evidence of highest discrete probability distributions interval in each BN´s variable (Molina et al., 2016). After this maximization over a particular variable (node), the change (its influence) in the expected value of the other ones is assessed and quantified (Molina et al., 2016).

BC Modelling design was developed in 4 phases: (1) learning from synthetic data from ARMA (*1*,*1*) models (Factor 1); (2) preprocessing that implies the discretization of the synthetic data into discrete probability distributions (Factor 2), all of them with the same amplitude; (3) considering constraints initially that the main relationship among variables is natural (consecutive variables linking, time-lag=1); and (4) structure learning, which highlights the real structure of interdependence of runoff series by a constraint-based approach (Steck, 2001; Vogel et al., 2018), which finds a DAG structure from synthetic data through conditional independence statistical tests.

This final stage is the core of BC Modelling because it reveals the hidden, non-trivial and logical interdependence structure (time lag > 1) that underlies into hydrological series. It was done through NPC learning algorithm (Madsen et al., 2003) which allows efficient simplifications to find net-structures (Steck, 2001) under the condition of not including links between conditionally independent nodes (HUGIN, 2021).

BC Modelling design was supported by software HUGIN® Expert (version 7.3) with a significance level of 0.05 for Structure Learning Process. All BC Modelling parameters were fixed except the two factors analyzed.

III.2.3 Step-3. Probability propagation

This step comprises probability propagation analysis over the time throughout the network. through an innovative Dependence Mitigation Graphs (DMG, Zazo et al., 2019). DMG encompasses two variables: (1) "time" (X-axe; in form of time-lag) and (2) "% relative of change" (Y-axe; propagation of temporal dependence strength over the time). Conceptually, DMG is obtained through the relative percentage of change produced in the child variable, connected with the parent (Molina et al., 2016; Zazo et al., 2019).

Figure III.3 shows two DMGs for both sub-basins. Temporally dependent basins tend to present a dominant positive part (Figure III.3a Porma). In contrast, temporally non-dependent basins show a tendency towards symmetric wrap-around results; positive or Wrap-around Maximum (W-MAX), and negative or Wrap-around Minimum (W-MIN), as found in Figure III.3b Adaja (Molina et al., 2016).

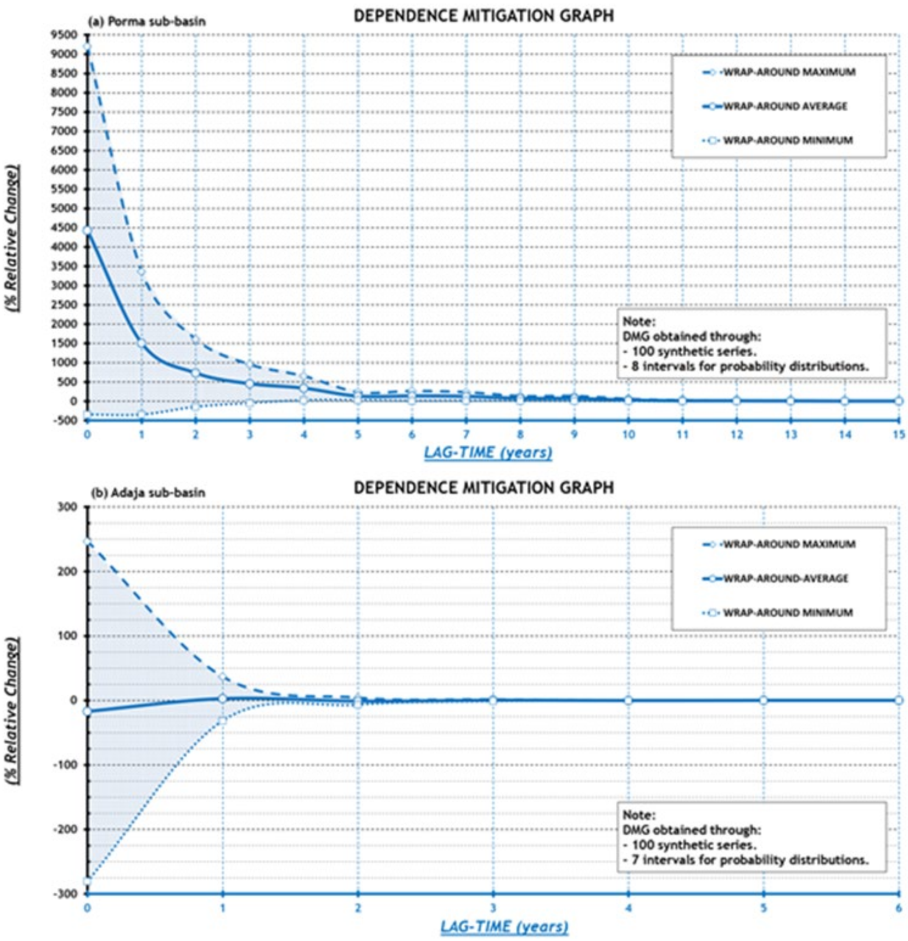


Figure III.3: Dependence Mitigation Graphs for Porma (a) and Adaja (b) case studies.

III.2.3.1 Uncertainty bands generation

In order to study the uncertainty of the wrap-around results before changes in the levels of the two parameters/factors studied, 95 % uncertainty bands for W-MAX and W-MIN series were generated by Bootstrap estimation (Efron and Tibshirani, 1993).

For the band around W-MAX, let $\boldsymbol{x_1, x_2, \dots, x_n}$ be the values used for getting $\mathbf{\max_i}\, \boldsymbol{x_i}$ for a particular lag. From these values, 10,000 bootstrap samples $\boldsymbol{x_1^*, x_2^*, \dots, x_n^*}$ were generated and the maximum value $\mathbf{\max_i}\, \boldsymbol{x_i^*}$ was calculated for each one. Then, 2.5th and 97.5th percentiles of those maximum values were obtained. Those percentiles were named $(\mathbf{max}\, \boldsymbol{x}^*)_{\mathbf{0.025}}$ and $(\mathbf{max}\, \boldsymbol{x}^*)_{\mathbf{0.975}}$ respectively. Finally, the 95% confidence interval for this particular time-lag is developed as:

$$\left(\mathbf{2}\, \mathbf{\max_i}\, \boldsymbol{x_i} - (\mathbf{max}\, \boldsymbol{x}^*)_{\mathbf{0.975}};\ \mathbf{2}\, \mathbf{\max_i}\, \boldsymbol{x_i} - (\mathbf{max}\, \boldsymbol{x}^*)_{\mathbf{0.025}}\right)$$

Then 95% uncertainty band for W-MAX series is calculated by joining the upper and lower limits from the confidence intervals. Similarly, it is determined W-MIN 95% confidence intervals. From both bands the 95% uncertainty band for the Wrap-around Average (W-AVE) can be constructed.

The usefulness of W-AVE is based on the application of the three-fold criterion “statistical-comparability-representativeness”: (1) Statistically, of the three wrap-arounds, W-AVE exhibits the lowest dispersion; (2) in river basins with temporally dependent behavior, W-MAX is clearly predominant with a minimal influence of W-MIN. By contrast, in independent ones, W-MAX and W-MIN tend to compensate each other (Molina et al., 2016; Zazo et al., 2019). Consequently, W-AVE can compare both types of river basins through a unique "wrap-around"; and (3) W-AVE is also able to capture/represent the temporal behavior of water basins. When W-AVE is generally positioned above the DMG X-axis the basin exhibits a dependent behavior; whereas if W-AVE is positioned in both sides of the X-axis the behavior is independent.

Finally, uncertainty band for W-AVE is built by averaging the 95% uncertainty bands for W-MAX and W-MIN series. In other words, the upper (lower) limit of the uncertainty band for the W-AVE series become the average of the upper (lower) limits of the uncertainty bands for the W-MAX and MIN series. In this manner, a single wrap-around (with its uncertainty band) is available. For a better understanding of this process Figure III.4 schematizes the W-AVE generation process and its uncertainty band.

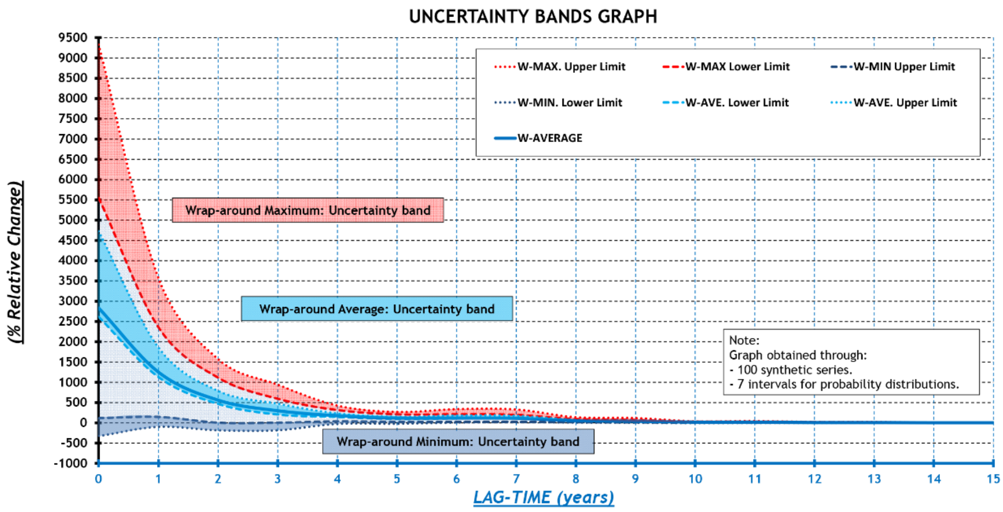


Figure III.4: Graph of uncertainty bands. Wrap-around Maximum (W-MAX), Minimum (W-MIN) and Average (W-AVE). Note: Uncertainty bands at 95% confidence level. Example Porma case study.

III.2.4 Step-4. BC Modelling performance assessment

This step determines how the W-AVE built depends on Factors 1 and 2 of BC Modelling. For this purpose, for each of the 21 scenarios (3x7) considered, W-AVE and 95% uncertainty band are constructed and then the overlapping between all of them is analysed. In this regard, two novel indexes have been defined: (1) Similarity index and (2) Stability index. The first one analyses in depth the overlap between uncertainty bands for the W-AVE, and the second one assesses the overall performance of the process.

Moreover, in the scientific literature there are a variety of indices based on Bayesian approaches, such as the Bayesian Information Criterion (Schwarz, 1978) one of the most widely applied to model selection, those arising from the combination of different indices and causes (Bradley et al., 2015; Kim et al., 2018), or from the combination of different causes to assess a particular problem (Giné-Garriga et al., 2018), among others.

III.2.4.1 Similarity index

For each pairwise comparison of scenarios a Similarity Index is calculated through a complete Uncertainty Bands Overlapping Analysis (UBOA) as follows:

1. If the two uncertainty bands overlap for a certain time-lag, the value 1 is assigned to that time-lag. Otherwise, a 0 value is assigned. This is mathematically expressed by a Boolean Factor of Overlap (F_o).
2. A weighted sum of the overlaps of all time-lag is obtained through following weights (w_i): 0.5 for lag_0 and lag_1 ($w_0=w_1=0.5$), 0.1 for lag_2 to $lag4$ ($w_2=w_3=w_4=0.1$) and 0.01 for the rest $lags$ (w_i=0.01 for $i > 4$). This weight

structure is based on the acquired knowledge on DMG (Zazo et al., 2019). DMG allows us to identify two regions of higher and lower mitigation of time dependence. Of these, lag_0 and lag_1 are those that present a higher mitigation gradient, for that $w_0=w_1=0.5$. The limit between these regions has been observed in lag_4 or lag_5, mainly in lag_4, which justifies the assignment of weight 0.1 to lag_{2-4}. From lag_5 the mitigation gradient is gradual, up to a relative percentage of change equal to 0.

3. The weighted sum is corrected through a multiplicative factor (0, 1, 2, 3, 4, 5) that considers the consecutiveness of the overlap of uncertainty bands for the first 5 time-lags, denoted as $F_{(c)}$. If the bands are overlapped within the first 5 lags, multiplier $F_{(c)}$ is 5; 4 if the overlap is within the first 4 lags, and successively. $F_{(c)}=0$ if no overlap in the first 5 lags. This threshold (first 5 time-lags, up to lag_4) is defined according to the limit between the two regions of dependence mitigation indicated above.

4. The Similarity Index of each pairwise comparison is obtained by the normalization of the previous rate to be enclosed within 0 (no overlap) and 1 (total overlap). This normalization is done by dividing the previous rate by the summation of all time-lag weights and multiplying the result by 5 (maximum F_o value). Figure III.5 schematizes UBOA process for a Similarity index value of 0.71. Similarity Index is formally expressed as:

$$Similarity\ Index = \frac{F_{(c)} \cdot \sum(w_i \cdot F_o)}{5 \cdot \sum w_i}$$

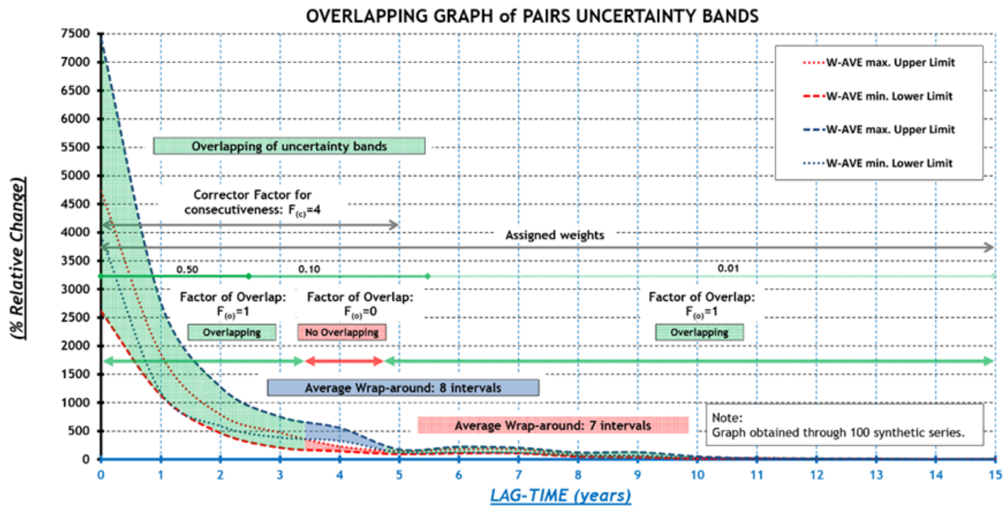


Figure III.5: Uncertainty Bands Overlapping Analysis. Example Porma case study of overlapping between uncertainty bands. Note: This analysis process is repeated for each of the 21 possible combinations resulting from Factor levels 1 and 2.

Then, Similarity index values were arranged in matrix form and grouped on two categories and five classes (Table III.2). For each case study 10 different matrices were defined: seven 3x3 matrixes for grouping the results of Factor 1 vs Factor 2, and three 7x7 matrixes in the case of Factor 2 vs Factor 1 results.

Table III.2: Similarity Index. Categories and classes.

Similarity categories	Classes	Color code	Description
Similarity Index ≥ 0.50 High evidence of similarity	[1.00 , 0.90]		Fully
	(0.90 , 0.80]		Highly
	(0.80 , 0.65]		Similar
	(0.65 , 0.50]		Slightly
Similarity Index < 0.50 Null or Low evidence of similarity	(0.50 , 0.00]		

III.2.4.2 Stability index

The Stability Index is computed by averaging the Similarity indexes of each scenario with the others (including the scenario in hand) in the form of a transposed matrix. Consequently, the previous ten matrixes for each case study are summarized in only two: one of dimensions 3x7 in the case of Factor 1, and second one of 7x3 for grouping the results of Factor 2. Both matrixes are expressed as:

$$\boldsymbol{S}_{F-1\,(3x7)} = \begin{pmatrix} \left(\frac{\sum_{m=1}^{3}\left(SI_{L1,F2}\right)_{m,1}}{3}\right)_{L1,F1} & \cdots & \left(\frac{\sum_{m=1}^{3}\left(SI_{L7,F2}\right)_{m,1}}{3}\right)_{L1,F1} \\ \left(\frac{\sum_{m=1}^{3}\left(SI_{L1,F2}\right)_{m,1}}{3}\right)_{L2,F1} & \cdots & \left(\frac{\sum_{m=1}^{3}\left(SI_{L7,F2}\right)_{m,1}}{3}\right)_{L2,F1} \\ \left(\frac{\sum_{m=1}^{3}\left(SI_{L1,F2}\right)_{m,7}}{3}\right)_{L3,F1} & \cdots & \left(\frac{\sum_{m=1}^{3}\left(SI_{L7,F2}\right)_{m,7}}{3}\right)_{L3,F1} \end{pmatrix}$$

$$\boldsymbol{S}_{F-2\,(7x3)} = \begin{pmatrix} \frac{\sum_{m=1}^{7}\left(SI_{L1,F1}\right)_{m,1}}{7} & \frac{\sum_{m=1}^{7}\left(SI_{L2,F1}\right)_{m,1}}{7} & \frac{\sum_{m=1}^{7}\left(SI_{L3,F1}\right)_{m,1}}{7} \\ \vdots & \vdots & \vdots \\ \frac{\sum_{m=1}^{7}\left(SI_{L1,F1}\right)_{m,7}}{7} & \frac{\sum_{m=1}^{7}\left(SI_{L2,F1}\right)_{m,7}}{7} & \frac{\sum_{m=1}^{7}\left(SI_{L3,F1}\right)_{m,7}}{7} \end{pmatrix}$$

where $SI_{Li,F-1}$ and $SI_{Li,F-2}$ are the mean values of Similarity Index (*SI*) of each levels of Factors 1 and 2 respectively.

Then, overall performance of Stability indexes was recursively analysed through trend graphs, according to their classification in two categories and five classes (Table III.3).

Table III.3: Stability Index. Categories and classes.

Stability categories	Classes	Description
Stability Index ≥ 0.50 High evidence of stability	[1.00 , 0.90]	Fully
	(0.90 , 0.80]	Highly
	(0.80 , 0.65]	Stable
	(0.65 , 0.50]	Slight stable
Stability Index < 0.50 Null or Low evidence of stability	(0.50 , 0.00]	

III.2.4.3 Stability framework

The influence of the factors over the BC Modelling Performance is analyzed through a recursive process that provides the highest possible stability:

1. The process starts with the evaluation of Factor 1, through plotting the performance of the Stability Index (Y-axis) versus Factor 2 (X-axis). In this graph, the Factor 1 level with the highest Stability Indexes is selected.
2. The level value of Factor 2 is determined through plotting the trend of the Stability Index (Y-axis) versus Factor 1 (X-axis). The number of intervals (Factor 2 levels) is chosen so that the Stability Index for the previously determined value of Factor 1 displays the highest value. This is done recursively if there are several values that satisfy the indicated condition.

III.3 Results

III.3.1 Generation of synthetic time series

Average values of mean, standard deviation and skewness coefficient were determined from each historical records and synthetic data time series of each case study (Table III.4). It is worth to highlight the maintenance of the mean value, according to the average behaviour that annual data offer. Figure III.6 shows the spectrum (wrap-arounds of each set of synthetic data of Factor 1), which will populate the BC Modelling.

Table III.4: Main statistical parameters: Historical records vs. Synthetic data generation.

Gauging station / Parameters				
Camposolillo	**Historical time series**	**50 SS**	**100 SS**	**200 SS**
Annual mean (Hm^3):	191.29	195.88	192.57	189.64
Standard deviation (Hm^3):	80.92	75.32	74.72	72.55
Skewness coefficient:	0.96	0.90	0.88	0.85
Adaja	**Historical time series**	**50 SS**	**100 SS**	**200 SS**
Annual mean (Hm^3):	95.90	102.16	100.93	101.11
Standard deviation (Hm^3):	73.44	100.68	97.26	97.77
Skewness coefficient:	1.25	2.19	2.14	2.15

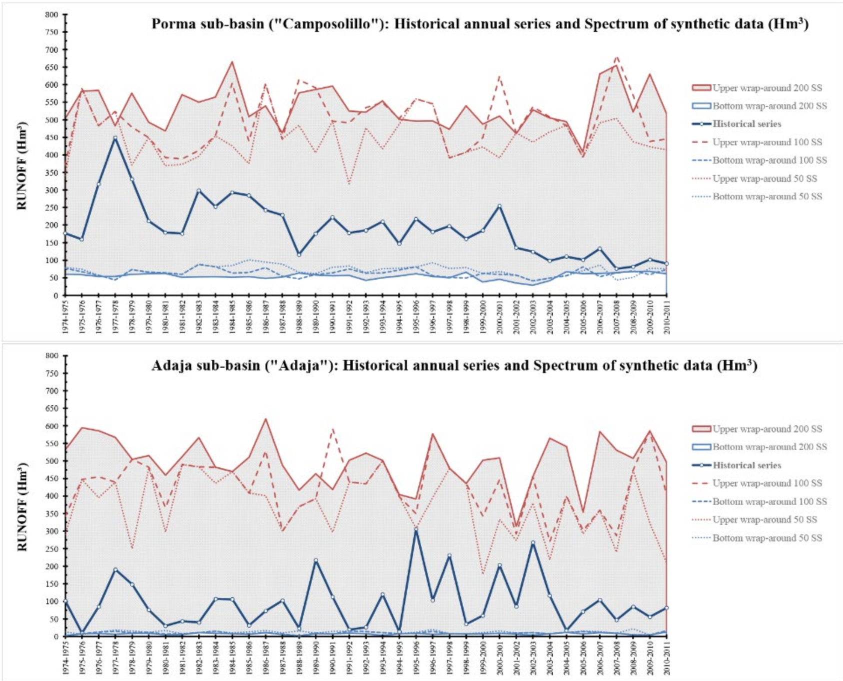


Figure III.6: Historical records and Spectrum of synthetic data (3 level) to populate Bayesian Causal Modelling. (Upper) Porma sub-basin. (Bottom) Adaja sub-basin.

III.3.2 Similarity indexes

Figure III.7 shows Similarity Indexes obtained in matrix form. In general, it is noticeable that the values are relevant for 6 intervals and beyond (Figure III.7 left). For this reason, the analysis of the resulting 7x7 dimension matrixes (Factor 1 vs. Factor 2) focuses on intervals 6 to 9. In contrast, 3x3 matrixes of the Factor 2 vs. Factor 1 are analysed for all of them.

In Porma case study, the highest values are obtained with 50 and 200 SS (Factor 1), with the combination of 200 SS and intervals 6 to 9 (Factor 2) showing the highest indexes [(6-7=0.94), (6-8=0.94), (6-9=0.97), (7-8=0.97), (7-9=0.99) and (8-9=0.74)]. In contrast, in the case of 50 SS the highest values are only obtained with the combination of 7 to 9 intervals [(7-8=0.96), (7-9=0.94) and (8-9=1.00)]. In both cases (50-200 SS), the values are homogeneous, with minimal variability, high evidence of similarity and belonging principally to the “Fully similar” class.

On the other hand, the matrixes (Factor 1 vs. Factor 2) for Adaja case study are less homogeneous, although the highest values are also associated with 50 and 200 SS. Moreover, the 200 SS level shows that for 6 to 9 intervals there is an alternation between values with null or low evidence of similarity [(6-8=0.34), (7-8=0.32), (8-9=0.34)] and values belonging to class slight similarity [(6-7=0.75), (6-9=0.75), (7-9=0.75)]. In the 50 SS level the disparity of values is meaningful, where values of practically null evidence of similarity [(7-8=0.12, 8-9=0.39)] are alternating with values of total similarity [(7-9=0.99)].

In both case studies, the 100 SS level Factor 1 shows the highest variability of indexes, even with the lowest values (the lowest evidence of similarity), Porma: [(6-9=0.07, (7-9=0.08), (8-9=0.19)], Adaja: [(6-8=0.10), (7-8=0.39), (8-9=0.10)]. On the other hand, the analysis of the 3x3 matrixes (Factor 2 vs. Factor 1) highlights clearly that the highest indexes were found for 7 intervals except for the combination of 5 intervals with 100 and 200 SS in the Adaja case study (value of 0.75). In the rest of combinations, the values show null or low evidence of similarity.

Finally, it is evident that the highest similarity is achieved with 200 SS, being its combinations with 7 to 9 intervals the ones that "a priori" offer the greatest similarity. The assessment of the overall performance of both factors through the Stability Indexes, and by means bi-objectives recursive process, will allow defining the optimal combination of both factors.

Factor 1 (Synthetic series) vs. Factor 2 (Intervals)

Porma sub-basin — 50 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.30	0.07	0.08	0.00	0.00	0.00
4	0.30	1.00	0.94	0.33	0.00	0.00	0.00
5	0.07	0.94	1.00	0.97	0.08	0.09	0.08
6	0.08	0.33	0.97	1.00	0.35	0.10	0.33
7	0.00	0.00	0.08	0.35	1.00	0.96	0.99
8	0.00	0.00	0.09	0.10	0.96	1.00	1.00
9	0.00	0.00	0.08	0.33	0.99	1.00	1.00
μ	0.21	0.37	0.46	0.45	0.48	0.45	0.49

Adaja sub-basin — 50 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.09	0.08	0.09	0.09	0.08	0.69
4	0.09	1.00	0.18	0.37	0.54	0.11	0.97
5	0.08	0.18	1.00	0.04	0.21	0.09	0.48
6	0.09	0.37	0.04	1.00	0.55	0.99	0.39
7	0.09	0.54	0.21	0.55	1.00	0.12	0.99
8	0.08	0.11	0.09	0.99	0.12	1.00	0.39
9	0.69	0.97	0.48	0.39	0.99	0.39	1.00
μ	0.30	0.47	0.30	0.49	0.50	0.40	0.70

Porma sub-basin — 100 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.17	0.00	0.00	0.00	0.00	0.00
4	0.17	1.00	0.08	0.00	0.01	0.00	0.00
5	0.00	0.08	1.00	0.34	0.92	0.31	0.27
6	0.00	0.00	0.34	1.00	0.72	0.92	0.07
7	0.00	0.01	0.92	0.72	1.00	0.71	0.08
8	0.00	0.00	0.31	0.92	0.71	1.00	0.19
9	0.00	0.00	0.27	0.07	0.08	0.19	1.00
μ	0.17	0.18	0.42	0.44	0.49	0.45	0.23

Adaja sub-basin — 100 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.46	0.08	0.08	0.08	0.08	0.07
4	0.46	1.00	0.09	0.09	0.09	0.09	0.09
5	0.08	0.09	1.00	0.34	0.75	0.12	0.51
6	0.08	0.09	0.34	1.00	0.75	0.10	0.51
7	0.08	0.09	0.75	0.75	1.00	0.39	0.51
8	0.08	0.09	0.12	0.10	0.39	1.00	0.10
9	0.07	0.09	0.51	0.51	0.51	0.10	1.00
μ	0.26	0.27	0.41	0.41	0.51	0.27	0.40

Porma sub-basin — 200 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.27	0.00	0.00	0.00	0.07	0.00
4	0.27	1.00	0.30	0.07	0.08	0.07	0.07
5	0.00	0.30	1.00	0.30	0.32	0.89	0.31
6	0.00	0.07	0.30	1.00	0.94	0.96	0.94
7	0.00	0.08	0.32	0.94	1.00	0.97	0.99
8	0.07	0.07	0.89	0.96	0.97	1.00	0.74
9	0.00	0.07	0.31	0.94	0.99	0.74	1.00
μ	0.19	0.27	0.45	0.60	0.61	0.67	0.58

Adaja sub-basin — 200 Synthetic series

	3	4	5	6	7	8	9
3	1.00	0.37	0.11	0.37	0.49	0.30	0.71
4	0.37	1.00	0.53	0.49	0.49	0.30	0.70
5	0.11	0.53	1.00	1.00	0.52	0.34	0.75
6	0.37	0.49	1.00	1.00	0.75	0.34	0.75
7	0.49	0.49	0.52	0.75	1.00	0.32	0.75
8	0.30	0.30	0.34	0.34	0.32	1.00	0.34
9	0.71	0.70	0.75	0.75	0.75	0.34	1.00
μ	0.48	0.55	0.61	0.67	0.62	0.42	0.71

Factor 2 (Intervals) vs. Factor 1 (Synthetic series)

Porma sub-basin	50 SS	100 SS	200 SS	Adaja sub-basin	50 SS	100 SS	200 SS
3 intervals							
50 SS	1.00	0.08	0.00	50 SS	1.00	0.21	0.00
100 SS	0.08	1.00	0.10	100 SS	0.21	1.00	0.02
200 SS	0.00	0.10	1.00	200 SS	0.00	0.02	1.00
μ	0.36	0.39	0.37	μ	0.40	0.41	0.34
4 intervals							
50 SS	1.00	0.00	0.00	50 SS	1.00	0.09	0.29
100 SS	0.00	1.00	0.10	100 SS	0.09	1.00	0.00
200 SS	0.00	0.10	1.00	200 SS	0.29	0.00	1.00
μ	0.33	0.37	0.37	μ	0.46	0.36	0.43
5 intervals							
50 SS	1.00	0.08	0.00	50 SS	1.00	0.19	0.19
100 SS	0.08	1.00	0.30	100 SS	0.19	1.00	0.75
200 SS	0.00	0.30	1.00	200 SS	0.19	0.75	1.00
μ	0.36	0.46	0.43	μ	0.46	0.65	0.65
6 intervals							
50 SS	1.00	0.00	0.00	50 SS	1.00	0.23	0.23
100 SS	0.00	1.00	0.50	100 SS	0.23	1.00	0.37
200 SS	0.00	0.50	1.00	200 SS	0.23	0.37	1.00
μ	0.33	0.50	0.50	μ	0.49	0.53	0.53
7 intervals							
50 SS	1.00	0.95	0.04	50 SS	1.00	0.12	0.55
100 SS	0.95	1.00	0.49	100 SS	0.12	1.00	0.75
200 SS	0.04	0.49	1.00	200 SS	0.55	0.75	1.00
μ	0.66	0.81	0.51	μ	0.56	0.62	0.77
8 intervals							
50 SS	1.00	0.03	0.21	50 SS	1.00	0.97	0.10
100 SS	0.03	1.00	0.33	100 SS	0.97	1.00	0.00
200 SS	0.21	0.33	1.00	200 SS	0.10	0.00	1.00
μ	0.41	0.45	0.51	μ	0.69	0.66	0.37
9 intervals							
50 SS	1.00	0.29	0.03	50 SS	1.00	0.99	0.99
100 SS	0.29	1.00	0.31	100 SS	0.99	1.00	0.51
200 SS	0.03	0.31	1.00	200 SS	0.99	0.51	1.00
μ	0.44	0.53	0.45	μ	0.99	0.83	0.83

Figure III.7: Similarity Indexes. (Left) Matrixes (7x7): Factor 1 vs. Factor 2. (Right) Matrixes (3x3): Factor 2 vs. Factor 1. Please note it additionally includes the mean value of each scenario denoted by μ, which justifies the posterior Stability Index.

III.3.3 BC Modelling performance assessment

III.3.3.1 Stability indexes

Table III.5 summarizes the Stability indexes of Factor 1 vs. Factor 2. In contrast, Table 6 shows the Stability indexes resulting according to the levels of Factor 2 for fixed levels of Factor 1. It is observed that the highest values of the Stability Index are mainly associated with the combination of 200 SS (Factor 1) with 7 to 9 intervals (Factor 2). In particular, for Porma case study: [200 SS vs. (7 intervals: 0.61), (8 intervals: 0.67)], and for Adaja case study: [200 SS vs. (6 intervals: 0.67), (7 intervals: 0.62), (9 intervals: 0.71)] (see Table III.5).

On the other side, it is worth noting that in Porma case study no stability index is above 0.5 (lower limit of the stability threshold) for the levels 50 and 100 SS of Factor 1, and almost the same result is observed in Adaja save two combinations: [(50 SS, 9 intervals): 0.70] and [(100 SS, 7 intervals): 0.51]. Furthermore, in Adaja stability indices for all combinations of Factor 1 with 8 intervals are lower than the preceding and following ones (0.40, 0.27, 0.42).

Table III.5: Stability Indexes of levels of Factor 2 fixing the levels of Factor 1. Note: The highest values are indicated in bold type. Please see Figure III.7 where the Stability Index values are justified.

	Gauging stations					
	Porma (2078)			Adaja (2046)		
	Synthetic series			Synthetic series		
Intervals	50	100	200	50	100	200
3	0.21	0.17	0.19	0.30	0.26	0.48
4	0.37	0.19	0.27	0.47	0.27	0.55
5	0.46	0.42	0.45	0.30	0.41	0.61
6	0.45	0.44	0.60	0.49	0.41	**0.67**
7	0.48	0.49	**0.61**	0.50	0.51	**0.62**
8	0.45	0.45	**0.67**	0.40	0.27	0.42
9	0.49	0.23	0.58	**0.70**	0.40	**0.71**

Additionally, in both case studies the Stability Indexes for 200 SS and 7 intervals exhibit a high and almost equal evidence of stability (0.61 and 0.62 respectively), being the combination that offers the greatest stability of results with the minimum spread of values.

Regarding the Stability Indexes of Factor 1 levels after setting the levels of Factor 2 (Table III.6), the highest stability indexes are achieved, in general, from 7 intervals in all levels of Factor 1. In this sense, the highest values are observed in Adaja case study for 9 intervals (0.99, 0.83 and 0.83) and in Porma case study for 100 SS and 7 intervals

(0.81). However, a detailed analysis reveals that the level of the 7 intervals of Factor 2 is the only one for which the resulting values are all higher than 0.50 in both cases. In particular, Adaja case study shows increasing values, from 0.56 to 0.77.

Table III.6: Stability Indexes of levels of Factor 1 fixing the levels of Factor 2. Note: The highest values are indicated in bold type.

		Number of intervals						
		3	**4**	**5**	**6**	**7**	**8**	**9**
Porma	50 SS	0.36	0.33	0.36	0.33	**0.66**	0.41	0.44
	100 SS	0.39	0.37	0.46	0.50	**0.81**	0.45	0.53
	200 SS	0.37	0.37	0.43	0.50	0.51	0.51	0.45
		Number of intervals						
		3	**4**	**5**	**6**	**7**	**8**	**9**
Adaja	50 SS	0.40	0.46	0.46	0.49	0.56	**0.69**	**0.99**
	100 SS	0.41	0.36	**0.65**	0.53	**0.62**	**0.66**	**0.83**
	200 SS	0.34	0.43	**0.65**	0.53	**0.77**	0.37	**0.83**

III.3.3.2 Bi-objective recursive process. Optimal combination of levels

The influence of both factors over the general BC Modelling Performance is analysed through a bi-objective recursive approach inspired by a One-Way ANOVA.

As indicated previously, the highest stability index for Factor 1 level is determined firstly, and then the stability trend for the levels of Factor 2 is observed for the set level. In this manner, both factors are controlled simultaneously and recursively. Figure III.8 displays the overall stability framework of the process.

The choice of the level of Factor 1 (upper Figure III.8) is clear. In both case studies the highest overall Stability indexes and trends are only achieved for the level 200 SS of Factor 1. In the case of Porma sub-basin, the values display an increasing trend from 0.19 (minimum value; 3 intervals) to 0.60 (6 intervals). From this point a stability is observed, with a maximum of 0.67 (8 intervals) and a gradual decrease to 0.58 (9 intervals). In the case of the other two levels of Factor 1 (50 and 100 SS), the described behavioural pattern is generally maintained, but always inside the category of null or low evidence of stability. On the other hand, in the Adaja sub-basin case, the highest overall stability trend is found for the levels of 6 and 7 intervals of Factor 2 (0.67 maximum and 0.62 respectively). The other two levels for Factor 1 exhibit an irregular stability behaviour.

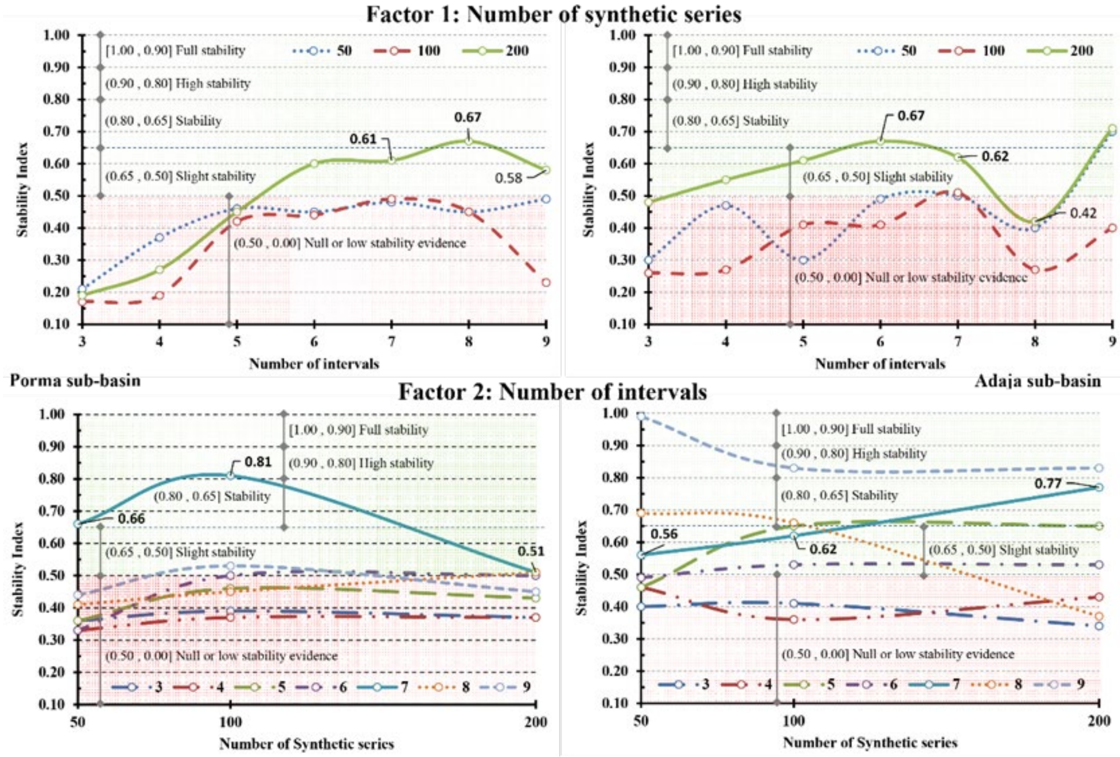


Figure III.8: Overall stability framework. (Upper) Factor 1 (3 levels) vs. Factor 2. (Bottom) Factor 2 (7 levels) vs. Factor 1. Please note that the category of null or low evidence of stability, (0.50 , 0.00], is coloured in light red. In contrast, the category of high evidence of stability, [1.00 , 0.50], is coloured in light green. For Stability index thresholds please see Table III.3.

Once set the level of Factor 1 (200 SS), the best level of Factor 2 is determined the graphs at the bottom of Figure III.8. In Porma case study, all levels of Factor 2 display a pattern of lack of relevant stability in the results, excluding the level of 7 intervals. The overall stability indexes of this level are higher than 0.50 in all cases. In contrast, in Adaja case study is not so evident with two meaningful levels. Whilst the 9-interval level shows the highest stability values, with a clearly stable trend at the value 0.83 for 100 and 200 SS (see Table III.6), the 7-interval level shows a clearly increasing trend of stability up to 0.77 (200 SS). Considering the minimal difference between both values of the stability index (0.83 vs. 0.77, roughly 7%), both values confirm a high evidence of stability and, for consistency and homogeneity of results with the previous case, the best level of intervals is achieved for 7 ones.

Consequently, the optimal combination of levels of both factors is obtained with 200 SS and 7 intervals.

III.4 Discussion and Conclusions

This research proposes an innovative methodological framework for assessing and improving the performance of BC Modelling, applied to the analysis and the prediction of runoff temporal behaviour of a river basin, based on Causality. For that, a robust stability framework to assess performance Learning-Training Processes of BC Modelling is set up employing an innovative bi-objective recursive approach. This is conditioned by two main factors: the number of synthetic series that populate the causal models (Factor 1), and the number of intervals defined for discrete probability distributions of synthetic data (Factor 2). These factors have not yet been addressed by any hydrological research based on Bayesian Causality.

This innovative stability framework has led to the development of two novel indicators. The first one, named “Similarity Index”, enables an in-depth analysis of the overlap between wrap-around of DMGs (in this case focused on W-AVE uncertainty bands). The second one, called “Stability Index”, assesses the overall BC Modelling performance process. In addition, the number of causal models executed/analyzed together with the strong mathematical foundations applied highlights the robustness and reliability of the findings.

Moreover, this research has revealed, for the first time, the influence of the number of intervals of probability distributions of synthetic data (Factor 2) on the BC Modelling process, and by extension to Bayesian PGMs, by means of Similarity and Stability indexes. This factor had not yet been analysed in a hydrological causal reasoning context.

This research, focused on two exemplary temporal case studies through bi-objective recursive developed approach, highlights that the most stable combination of factors is achieved through the combination of the 200 SS level of Factor 1 and 7-interval level of Factor 2.

As the improvement of BC Modelling performance has been conducted on the decision variables of the process itself, in this case annual normalizable runoff time series, the optimal combination of levels achieved may also be effective for other temporal scales such as seasonal and/or monthly, normalizable ones as well. Furthermore, the fact that the case studies show opposite, and exemplary temporal behaviors indicates that the conclusions of this research can be extrapolated to other river basins.

On the other hand, the optimal combination of factor levels will allow a better understanding of statistical evidence propagation between the model variables. This will undoubtedly make possible to predict future events and analyze the temporal and spatio-temporal behaviour of water resources in a river basin in a more reliably way.

Furthermore, the optimization of the BC Modelling will enable progressing in future work on the DMG by incorporating uncertainty bands and developing new indicators of temporal and even spatio-temporal behaviour, these latter addressed by means of multivariate analysis.

Additionally, the framework developed might be applied to both flow classification and prediction. It provides an in-depth knowledge of the historical flow patterns, as an alternative to standard statistical analyses, and maybe automatized (subject to data requirements) to classify river reaches according to how the conditioned and the unconditioned fraction behave and interact. In addition, BC Modelling might be used to predict streamflows in an alternative way compared to traditional hydrometeorological forecasting methods (e.g. Ensemble Streamflow Prediction, use of stochastic models, use of meteorological forecasts to force a hydrological model). In fact, it is one of the most promising applications of the methodology proposed.

Finally, the methodological framework may serve as a basis for further advances in the field of classification applied to Bayesian PGMs.

CAPÍTULO IV
Modelización causal bayesiana aplicada a la predicción de aportaciones

Este Capítulo IV reproduce la versión de autor, adaptada al formato tesis, del artículo científico "Assessment of the predictability of inflow to reservoirs through Bayesian Causality", publicado en la revista científica *Hydrological Sciences Journal* (ISSN: 0262-6667) el día 14 de julio 2023.

La investigación que se presenta en este capítulo evalúa, por primera vez, la capacidad predictiva de la causalidad bayesiana bajo las hipótesis simultáneas y restrictivas de cuencas hidrográficas caracterizadas por un comportamiento temporal independiente de sus recursos hídricos superficiales, y con un limitado número de registros históricos.

Este reto se aborda mediante una "prueba de concepto" basada en una metodología estocástica híbrida, que combina un modelo paramétrico autorregresivo con un modelo causal bayesiano. La capacidad analítica de este enfoque ha permitido poner de manifiesto la estructura lógica temporal de dependencia que define el comportamiento general de cualquier aportación. A partir de ésta, se han cuantificado las dos fracciones temporales que componen cualquier aportación (una debida al tiempo y otra no), y que son la base para la generación de sendos modelos predictivos.

Los resultados obtenidos en cuencas con un fuerte comportamiento temporal independiente abren nuevas posibilidades para el desarrollo de modelos hidrológicos predictivos basados en la causalidad bayesiana. Por otro lado, esta investigación propone un nuevo enfoque para evaluar la dependencia temporal de las series desde un punto de vista cuantitativo, a través de la definición del "Índice de simetría". Dicho índice expresa la relación entre las áreas de los envolventes, positiva y negativa ajustadas a funciones matemáticas, que sintetizan las curvas de propagación de la dependencia temporal a lo largo de la red bayesiana definida para modelar la serie temporal.

[20] Zazo, S., Molina, J.L., Macian-Sorribes, H., Pulido-Velazquez, M. 2023. Assessment of the predictability of inflow to reservoirs through Bayesian Causality. Hydrological Sciences Journal, 68:10, 1323-1337. https://doi.org/10.1080/02626667.2023.2200143.
Se omiten los apartados: "Acknowledgements", "Disclosure statement", "Funding" y "ORCID". La sección "References" se integra en la Bibliografía de esta Tesis.
Nota: La utilización del artículo científico en esta tesis cumple con el "Publishing Agreement" firmado entre los autores y la editorial Taylor & Francis Online.

IV.0 Abstract

This research assesses the predictive capacity of Bayesian Causality through Causal Reasoning (CR), which has been successfully applied to the study of reservoir inflows. It was done by combining an autoregressive development with a causal modelling approach through a "proof of concept" which assesses the predictive capacity of approach. The analytical CR power revealed the logical temporal-structure that defines general behaviour of inflows, which was latent in the historical records. This allowed identifying-quantifying through a dependence matrix, two temporally runoff fractions, one due to time and the other not. Finally, a predictive model for each temporal fraction was implemented, evaluating its forecasting skills through Mean Absolute Error and Root Mean Square Error. This was applied to the reservoirs that supply water to the city of Ávila (Spain), whose watersheds present a strong independent temporal behaviour. These results open new possibilities for developing hydrological predictive models within CR modelling framework.

IV.1 Introduction

There is growing evidence that the availability of water resources is experiencing major alterations with respect to its traditional cyclical patterns, due mainly to the phenomenon of global change (O'Gorman 2015; Pfahl et al., 2017). This fact implies that the stationarity hypothesis in hydrological time series is not strictly kept anymore (Donat et al., 2016; Guinard et al., 2015). In this sense non-stationarity becomes a common characteristic to be addressed that increases the uncertainty of hydrological processes (Molina and Zazo 2018). This situation leads towards to an intensification of extreme hydrological phenomena, such as heavy rainfall, floods and prolonged droughts, among others (Jyrkama and Sykes 2007; Marcos-Garcia 2017; Vogel et al., 2018) which are becoming more frequent and unpredictable (Zazo, 2017). These issues challenge the spatiotemporal analyses and forecasts and requires powerful analytical strategies to provide reliable predictive models (Hao and Singh 2016; Recio et al., 2018) to anticipate water management strategies (Rubio-Martin et al., 2020).

On the other side, temporal dependence analysis in Hydrology has been thoroughly studied through concepts such as Persistence, strongly related to time series long term memory through Hurst coefficient (Hurst, 1951), storage and drought statistics or time series modeling by means of AutoRegressive Moving Average (ARMA) models (Salas et al., 1980). However, over the last decades the methodologies based on Artificial

Intelligence have gained force in Hydrology (Giuliani et al., 2019; Kousari et al., 2017). Within these ones, Probabilistic Graphical Models (PGMs) are strongly emerging, and in particular Bayesian Networks (BNs). This is due to BNs are a graphical and compact representation of a joint probability distribution over a finite set of random variables, where the nodes of the network are the variables of a reasoning problem, and the links denote the (conditional) (in)dependencies between the variables (Pearl, 1985, Pearl and Russell 1998). Thus, in a BN the joint probability distribution of all variables is modelled by the propagation of the strength of (in)dependencies between the variables throughout the whole network, which may be seen as a general description of the behavior of a system (Macian-Sorribes et al., 2020). By means of the combination of probability-graph theories (Vogel et al., 2014), BNs have become not only increasingly popular but the most used PGMs (Cabañas de Paz, 2017). Besides, their capability to support probabilistic reasoning from data with uncertainty (Javidian et al., 2020) makes them especially interesting for the forecast of complex natural processes such as hydrological ones (Molina et al., 2019).

Specifically on water resources management, BNs have been successfully implemented to deal with problems such as water resources planning (Xue et al., 2017), integrated groundwater management (Hosseini and Kerachian 2019), reservoir management (Mediero et al., 2007), assessment of environmental risk on large dams (Ahmadi et al., 2015) and flood damage (Schroeter et al., 2014).

On the other hand, Causality, as methodological approach for searching patterns of reasoning in data, has not been deeply applied to hydrological records (Macian-Sorribes et al., 2020). In fact, Causality has a high potential of application for discovering causal structures in an observed dataset by means of techniques such as Causal Reasoning (CR), Evidential Reasoning (ER) and Intercausal Reasoning (IR). In this sense, CR is a top-down approach which is applied when the objective is the prediction of the effect and the analysis puts the focus on the cause. However, ER is a bottom-up approach since the analysis is focused on the effect and the cause is inferred; whereas IR comprises the interaction of several causes for the same effect. Nevertheless, CR, addressed under a Bayesian framework, highlights over the others (Pearl, 2014). Currently, this is under development through the Bayesian Causality (Molina et al., 2016; Spirtes 2010), which has led to the emergence of new approaches for modelling and forecasting the temporal behaviour of water resources in river basins. The rationales of these methods are mainly based on discovering the logical-latent temporal dependence structure into hydrological historical records that defines the overall behaviour of the observed dataset (Macian-

Sorribes et al., 2020; Zazo et al., 2022). In this sense, Molina et al., (2016) and Molina and Zazo (2017) assessed the ability of the CR supported by BNs to model temporal behaviour. Molina and Zazo (2018) highlighted for the first time two-opposite temporal-fractions within an annual runoff time series, named Temporally Conditioned Runoff (TCR, fraction due to time) and Non-conditioned Runoff (TNCR, uninfluenced by time). In parallel, Molina et al., (2019) implemented a dynamic predictive runoff model, based on the observed temporal behaviour trends of TCR and TNCR. Furthermore, this research highlighted their importance through the analysis of probability distribution functions on which the development of predictive models was based. Macian-Sorribes et al., (2020) developed a comprehensive spatiotemporal dependence analysis of inflow across two adjacent and parallel river basins, broadening the potential application of this causal approach. Recently, Molina et al., (2022) have proposed a bivariate causal methodology, named HydroPredicT_Extreme, to improve the predictive capacity of extreme rainfall-runoff events.

The novelty of this research lies in assessing, for the first time, the predictive capacity of Bayesian Causality applied to reservoir inflows in river basins with a highly independent temporal behaviour. For this reason, this challenge was addressed in form of "proof of concept" through a stochastic hybrid methodology, which combines an autoregressive development with a causal model based on CR supported by Bayesian modelling. By doing so, it was possible to obtain the hidden logical and non-trivial temporal dependence structure that inherently underlies into hydrological series. From this logical structure, the strength of the temporal dependencies was characterized through a dependence matrix, and then the two temporal fractions that compose an annual runoff (TCR and TNCR) were identified and computed. Based on this temporal conditionality two predictive models, one for each runoff fractions, were developed. Their forecasting skills were evaluated through the Mean Absolute Error (MAE) and Root Mean Square Error (RMSE). To conclude, this research proposes a new approach to assess the temporal dependence of the series from a quantitative perspective, based on symmetry index, which is obtained from Dependence Mitigation Graph (DMG).

IV.2 Case study

The international Duero river basin is located in the north-western part of the Iberian Peninsula with a surface area of 98,103 km² (80.4 % in Spain and 19.6 % in Portugal), which makes it the largest peninsular basin, and where the Spanish management of the basin is divided into 5 zones (A-E) with a total of 13 subsystems (Figure IV.1a,b; CHD 2015). The southern subsystems in the Duero river basin are undergoing significant changes in their behaviour, as evidenced by its River Basin Management Plan (CHD 2015). In particular, the Eresma and Adaja subsystems are experiencing a severe decrease in the availability of water resources (CHD 2015), which has significantly affected the city of Ávila, with an estimated population of 60,000 inhabitants. The urban supply to Ávila relies on two hydraulic infrastructures, Becerril and Serones reservoirs (Figure IV.1c). The Becerril reservoir, in the Adaja subsystem, has a small upstream area (20.7 Km²) with a storage capacity of 1.79 Hm³. The Serones reservoir, in the Eresma subsystem, has an upstream area of 109 Km² and a capacity of 6.30 Hm³ (IDEDuero 2022; SEPREM 2022). Both reservoirs are the upstream regulation facilities in both subsystems.

The Becerril reservoir has traditionally supplied water to the city of Ávila from the beginning of the 20th century, and it was not until the 1990s, when Serones reservoir also began to be used for the same matter (SEPREM 2022), to the point that it has become the main water supply for Ávila city, leaving the Becerril reservoir water supply almost insignificant, according to the managers of the reservoir system.

The study area is traditionally characterized by a cold Mediterranean climate, highly continental, with moderately warm summers and severe winters due to the altitude conditions (CHD 2015). The relatively high elevation of the area (average altitude of 1,200 meters) has an influence over the temperature, with an annual mean of 11 ºC (MITECO 2022). The precipitations present a high interannual and annual irregularity, with an annual average of approximately 450 mm (with annual minimum and maximum values between 173 and 718 mm respectively), corresponding to a semi-arid area, mainly concentrated between October to December and March to June. In the winter months part of the precipitation usually falls as snow (MITECO 2022).

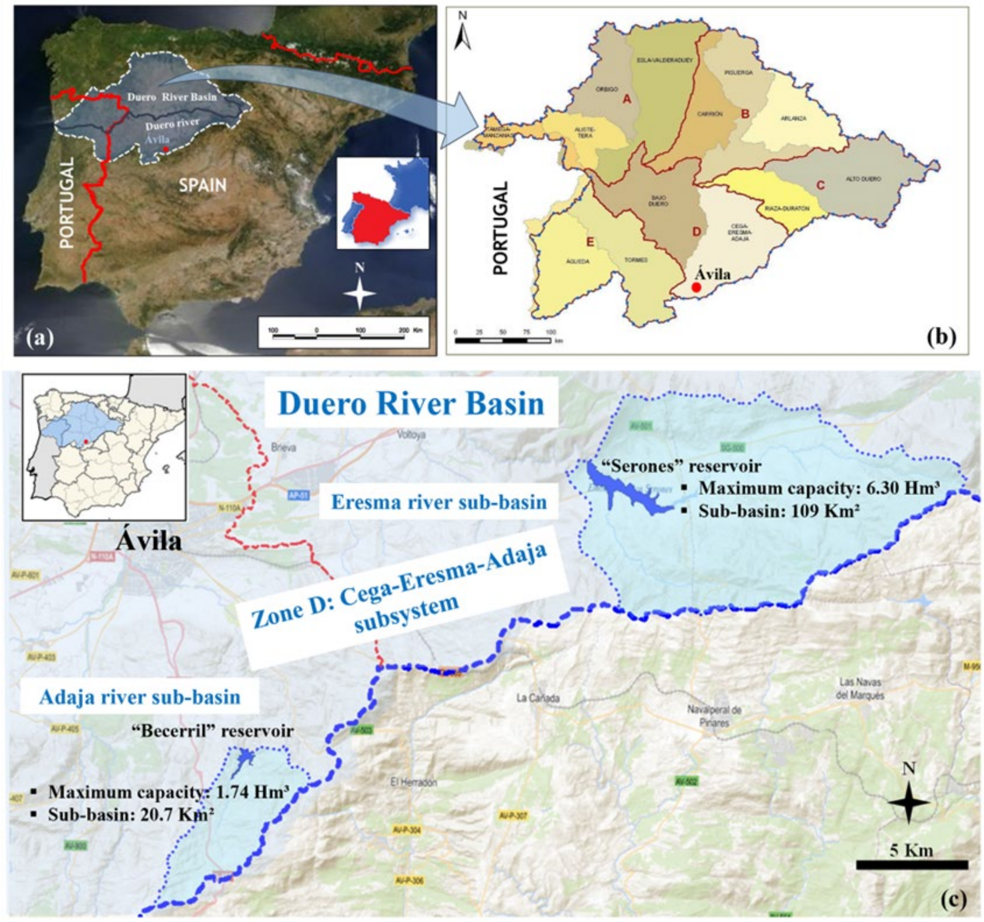


Figure IV.1: (a) Situation of case studies; (b) zones (A to E) and subsystems of the Spanish management of the Duero basin; (c) scheme of current system of reservoirs that supply water to the city of Ávila. Map source: CHD (2015) and IGN (2022). Open sources data. No additional permissions are required (INSPIRE European Directive).

In lithological terms, the Becerril reservoir basin consists of extensive granite and granodiorite formations in form of blocks. In contrast, the Serones reservoir basin displays a major heterogeneity of formations with blocks of granites and granodiorites mainly, as well as micaschists, phyllites, slates, quartzites, greywackes and gneisses in the northern area. In this case, the bottom of the valley is dominated by detrital formations of high and medium permeability. In hydrogeological terms (Figure IV.2), both basins are characterized by generally impermeable or very low permeability formations, with the possibility of containing superficial aquifers due to alteration or fissuring, mostly not very extensive and with low productivity (IGME, 2022a,b), with scare river-aquifer interactions, largely producing temporally independent behaviour of the river (Molina and Zazo 2018).

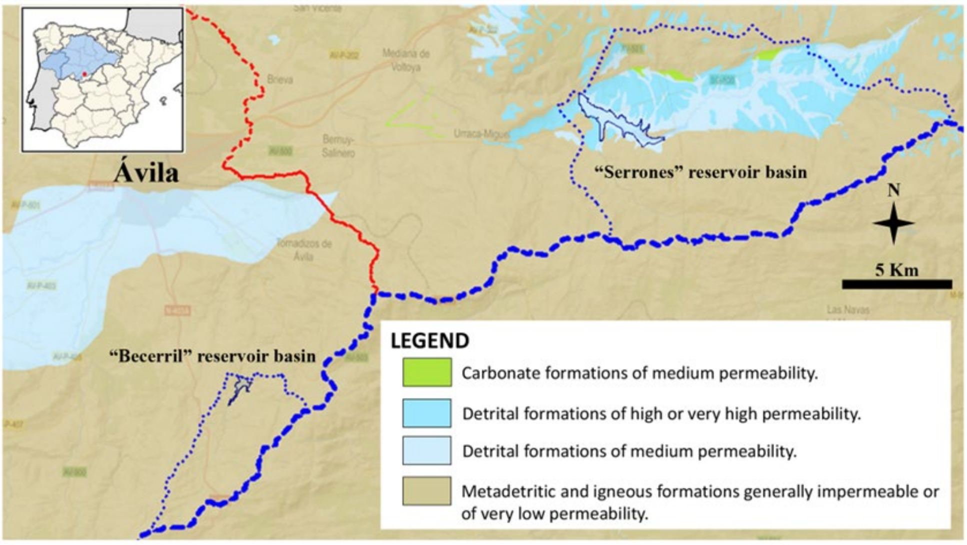


Figure IV.2: Hydrogeological maps of Becerril and Serones sub-basin. Source: IGME (IGME, 2022a). Open sources data. No additional permissions are required (INSPIRE European Directive).

Annual runoff historical records (without missing data) were provided by Ávila City Council (Figure IV.3a). The time period covers from 2003 to 2018, 16 years (see Table IV.A1). Regarding the annual hydrological response of the watershed to rainfall, the upstream area of both reservoirs show independent behaviour, as highlighted by the temporal correlograms in Figure IV.3b,c. This is especially conspicuous in the case of Serones reservoir, where all its lags are within the area of independence defined by the Anderson limits. This availability data reinforces the "proof of concept" framework in which the research is developed.

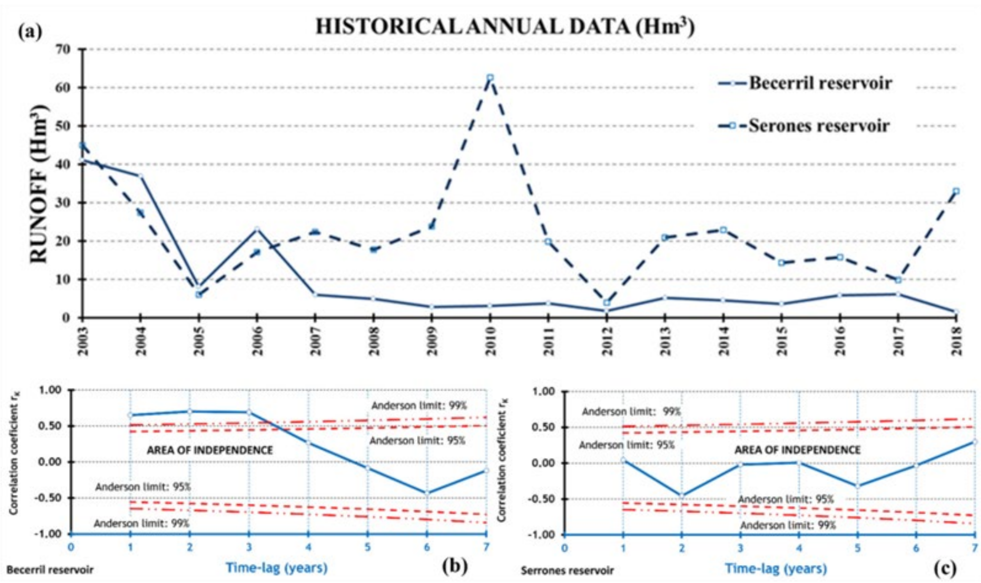


Figure IV.3: (a) Historical annual runoff data (time period: 2003 to 2018); source: Ávila City Council; (b) temporal correlogram of annual runoff "Becerril" reservoir; (c) temporal correlogram of annual runoff "Serones" reservoir.

IV.3 Methodology

The enforced methodology comprises the subsequent five consecutive stages that contain several sub-stages (Figure IV.4):

- Stage 1 implies an initial analysis of the main statistical parameters of the time series considered as well as the generation of consistent equiprobable synthetic runoff series that will populate the subsequent CR process.
- Stage 2, an exhaustive Causality process is conducted through CR approach. This was based on Bayesian modelling which confers a strong dynamism and stochasticity to the methodology. Here, the analytical power of CR is key, due to its ability to identify the logical and non-trivial structure of temporal interdependence that defines general behaviour of the series. Next, the propagation of the temporal dependence is performed and evaluated by DMG approach.
- Stage 3 focuses on the identification and quantification of temporally runoff fractions, named Temporal Conditioned Runoff (TCR) or fraction due to time, and Temporal Non-Conditioned Runoff (TNCR) fraction or uninfluenced by time.
- Stage 4 two predictive models, one for each temporally runoff fractions, were developed based on the approach proposed by Molina et al. (2019).
- Stage 5, forecasting skills validation. First, in an overall way through Mean Absolute Error (MAE) and Root Mean Square Error (RMSE), and secondly, in a much more detailed approach provided by the metrological perspective.

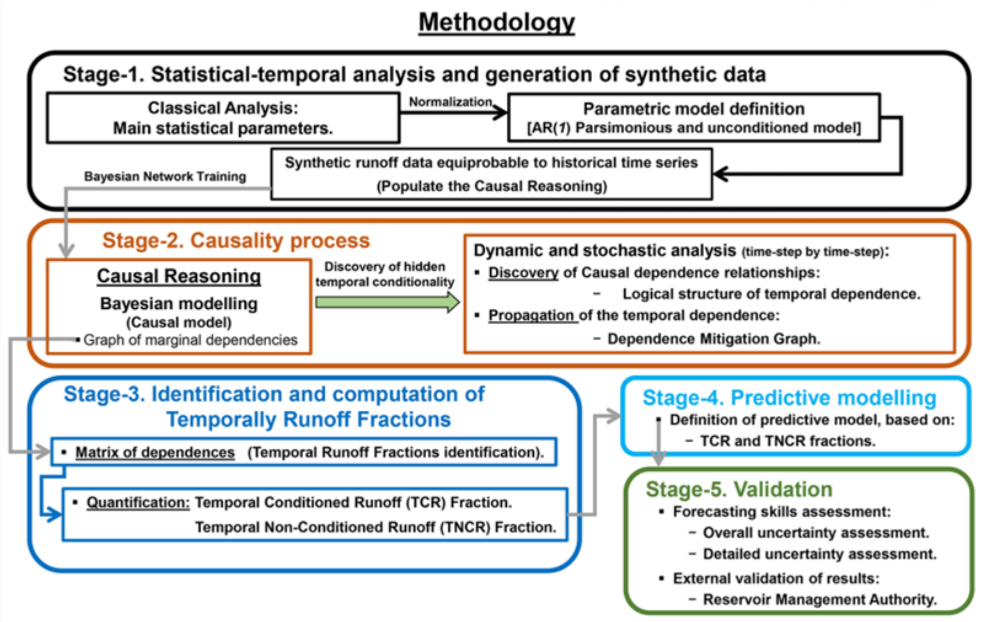


Figure IV.4: General methodology.

IV.3.1 Stage 1. Statistical-temporal analysis and generation of synthetic data

Firstly, a statistical analysis of the annual time series was performed and the assumption of stationarity of time series was tested. This hypothesis was verified, based on Hipel and McLeod, (1994), through an ARMA model selection process, supported by TRASERO ® software (version 2.3.0). In this process the coefficients of the models are obtained by means of the Least Squares Method, minimizing the Error Function using the Gauss-Newton algorithm and model selection is performed by Akaike Information Criterion (AIC, Akaike 1974), where is the one with the lowest AIC value (TRASERO 2015).

Secondly, based on Molina et al., (2016), a set of 200 synthetic runoff data were generated through an AR (1) model according to the framework by Salas et al., (1980). All synthetic series have the same length as the historical records for each sub-basin. The purpose of the of AR (p) model is exclusively providing reliable data to populate the subsequent Causality process (Zazo et al., 2022). It should be noted that without this observational data it would not be possible to generate Bayesian causal models, due to this information is necessary to define the probability distribution functions, “a priori” and “a posteriori”, of Bayes´ Theorem. However, and seemingly difficult, if enough data to populate the Causality process is available the generation of equiprobable time series through a generic ARMA (p,q) model or any alternative approach able to generate synthetic time series would be omitted (Zazo et al., 2022).

This stochastic, parsimonious and unconditioned parametric AR (*1*) model confers a higher degree of freedom to Causality process (Molina et al., 2019; 2016) and implies that the variable of interest regresses according to its previous values (Boulariah et al., 2021), which is mathematically expressed as (Salas et al., 1980):

$$Y_t = \mu + \sum_{j=1}^{p} \emptyset_j \left(Y_{t-j} - \mu\right) + \epsilon_t$$

where Y_t is the value of the temporal series at a certain time-step t, μ is the mean of the time series; (p) is the number of autoregressive (AR) parameters, $\emptyset_j$ is the coefficient of AR model and ϵ_t represents the historical residuals.

Afterwards the model definition, a normalization process is applied by means of three different mathematical functions: square root, natural logarithm plus one and natural double logarithm plus one, which are usually applied to operational hydrology (Ochoa-Rivera et al., 2007). The selection criterion for the functions is based on the coefficient of skewness closest to zero (0). Next, the synthetic data is generated. In order to the generation process of synthetic series to be "non-conditioned" and to avoid "boundary effects" a warm-up period of 20 years was defined (Molina et al., 2016). Validation of synthetic data was performed comparing its relevant statistics to those of historical records (Ochoa-Rivera et al., 2007).

IV.3.2 Stage 2. Causality process

From the methodological perspective this stage is key. Causality, addressed through CR and supported by Bayesian modelling in form of BN, allows to highlight the logical and non-trivial structure of interdependence, latent in the historical data (Molina et al., 2019; Molina and Zazo 2018). In addition, this internal structure describes the general behaviour of the temporal records (Macian-Sorribes et al., 2020).

This methodological strategy is a suitable technique not only for modelling but also for forecasting the general behaviour in complex natural processes (Molina et al., 2019), due to CR addressed through Bayesian modelling is mainly characterized by: (1) searching reasoning patterns in a hierarchical way from top to bottom, (2) focusing the analysis on the cause and (3) the objective comprises the prediction of the consequence (Pearl 2009, Macian-Sorribes et al., 2020). In addition, the ability of BNs to describe the overall behaviour of a system through the propagation of (in)dependence among the variables throughout the whole structure (Vogel et al., 2018) as well as the fact that these are based on the notion of conditional (in)dependence (Steck 2001) makes this approach particularly useful in the general framework of this research.

Conceptually, Bayesian Causality process is based on the definition of a BN in which conditional probability among decision variables is computed and propagated omnidirectionally supported by Bayes' Theorem (Zazo et al., 2022). According to Madsen et al., (2003) is expressed as:

$$P(V) = \prod_{X \in V} P\big(X|pa(X)\big)$$

where P(V) is the joint probability distribution over set of nodes V (random variables, X) present in the graph and which are defined through direct acyclic graph, and $P(X|pa(X))$ is the conditional probability distribution for each decision variable $X \in V$ that belongs to a set of probability distributions.

In this research, the nodes are each of the annual historical records of the time series, which are consecutively interconnected by means of "links" (natural connection, time-lag = 1). In order to propagate Bayes´ Theorem the variables were partitioned into 5 discrete probability intervals, all with the same range (Molina et al., 2016). The real, hidden and non-trivial structure of interdependence (time-lag > 1) was highlighted by a constraint-based approach (Steck 2001; Vogel et al., 2018), which finds a direct acyclic graph structure from synthetic data through conditional independence statistical tests (Zazo et al., 2022). This was supported through NPC (Necessary Path Condition) algorithm (Madsen et al., 2003), which is based on the condition of not including links between conditionally independent nodes (HUGIN 2021). Causality process was developed through software HUGIN® Expert (version 7.3) with a significance level of 0.05.

The application of Bayesian Causality to hydrological time series is performed through analysing the evolution (change) of the probability distribution, "a priori" and "a posteriori", over time and throughout the BN (Macian-Sorribes et al., 2020). This is done by maximizing the whole probability distribution of highest discrete probability distributions interval in each BN´s decision variable (Molina et al., 2016; Macian-Sorribes et al., 2020; Zazo et al., 2022). In this way, after the maximization over a particular variable (node), the induced change in the other ones may be suitably assessed and quantified through the relative percentage of change produced in the "child" variable, connected with the "parent" (Molina et al., 2016; Zazo et al., 2022). This approach provides a curve of propagation of temporal dependence for each decision variable over the time and throughout the whole network (Zazo et al., 2019). In this sense, relevant modifications (changes) in a node associated with a change in another, would imply a strong causal evidence (relationship) between both. In contrast, a little one would mean the absence of a bond (Macian-Sorribes et al., 2020).

On the other side, the overall analysis of strength of dependence between variables were conducted through DMG (Zazo et al., 2019,2022). This graph, where X axis represent “time” (time-lag) and Y axis is “relative percentage of chance”, summarizes all the curves of propagation of temporal dependence by means of two wraparounds, one positive and other negative, denoted W-MAX and W-MIN respectively, which are fitting to mathematical functions. The analysis of symmetry of both wraparounds provides initially a qualitative method to assess temporal dependence (Zazo et al., 2019), where DMG asymmetry shows a dependent behaviour and the symmetry reveals an independent one (Molina et al., 2016; 2019, Molina and Zazo 2017,2018, Zazo et al., 2022). Furthermore, a more detailed analysis of the DMG allows defining two regions dependence, based on the gradient of propagation of the temporal dependence. A first one, of major mitigation where the gradient is higher, and a second one of lower gradient (Zazo et al., 2019,2022). Additionally, the convergence of W-MAX and W-MIN to 0 on X axis (time-lags) defines the temporal horizon of the dependence influence (Zazo et al., 2019). This qualitative approach is completed from a quantitative point of view through the Symmetry Index of the enclosed areas between both wraparounds (W-MAX and W-MIN) with respect to the X-axis. This index is defined by the integration of both ones from time-lag0 (point with the highest strength of dependence over time.) to the maximum time-lag (temporal-horizon, point where the relative percentage change is 0). Symmetry Index is mathematically expressed as:

$$Symmetry\ Index = \frac{\left|\int_0^{TH_{W-MAX}} W - MAX\right|}{\left|\int_0^{TH_{W-MIN}} W - MIN\right|}$$

where $TH_{W\text{-}MAX}$ and $TH_{W\text{-}MIN}$ are respectively the temporal horizon of both wraparounds. In this index, a value of one (1) would imply total symmetry between W-MAX and W-MIN and therefore a fully independent behaviour. In contrast, as this value is significantly different from 1 the asymmetry increases, revealing an increasingly dependent behaviour and therefore one of the two wraparounds predominates over the other.

IV.3.3 Stage 3. Identification and computation of Temporally Runoff Fractions

A first sub-stage was performed with the aim of obtaining the matrix of temporal dependence. This one, initially proposed by Molina and Zazo (2017), is a compact representation of the dynamic temporal behaviour of a hydrological basin, which summarizes the interactions between one target variable (year in this cases) and the previous ones (Zazo 2017). This matrix is generated from all the (in)dependence relationships highlighted in the causal model through the graph of marginal dependencies and for a 100% independence level threshold (Molina et al., 2019). The reason for this is that: (1) Causality process is based on statistical tests of conditional independence (Steck 2001) and (2) in the graph of marginal dependencies each detected connection (link) represents a temporal (in)dependence relationship (Molina and Zazo 2017). Thus, the strength of dependence in each causal relationship is evaluated by Dependence Rate (DR; from 0 to 1). According to Molina and Zazo (2017) DR is expressed as:

$$DR = 1 - (P_{value})$$

where *P_value* represents the strength of evidence against the independence relationship and a DR value equal to one (1) implies a total dependence or total probability of being dependence (Molina and Zazo 2017). Based on Molina et al., (2019) DR values were also classified in two classes and grouped in 5 intervals (Table IV.1).

Table IV.1: Dependence Rate (DR). Classes and intervals.

Similarity categories	Classes	Color code	Description
DR ≥ 0.50. High evidence dependencies	[1.00 , 0.95]		Totally dependent
	(0.95 , 0.90]		Highly dependent
	(0.90 , 0.75]		Dependent
	(0.75 , 0.50]		Slightly dependent
DR < 0.50. Low evidence dependencies	(0.50 , 0.00]		

The second sub-stage comprises the identification and computation of temporally runoff fractions. This is because in any runoff two opposite temporal behaviour fractions may be considered (Molina and Zazo, 2018, Molina et al., 2019). The first one, denoted by TCR fraction and due to time, and the second one, TNCR fraction, or uninfluenced by time. According to Molina et al., (2019) both ones are expressed an annual scale as:

$$TCR_i = \frac{\sum_{j=0}^{i-1} w_j \cdot Y_j}{\sum_{j=0}^{i-1} w_j}, \qquad i = 1, \dots, TD$$

$$TNCR_i = (R_i - TCR_i), \qquad i = 1, \dots, TD$$

where TCR_i is the weighted average conditioned runoff of the Target Year (i); w_j expresses in weight form the dependence of year j on Target Year (i); Y_j is the conditioned runoff for the year j; TD is the temporal interval in years; R_i is the runoff of the time series in the target year; and $TNCR_i$ is the uninfluenced by time fraction for the target year.

Once temporally runoff fractions were quantified, different scenarios were generated according to a past temporal horizon of four years, which also made it possible to assess internally the predictive capabilities of the Causality process. In each defined scenario, the values of both fractions and its respective percentages over the runoff were obtained. Consequently, the modelling and forecasting ability of the Causality process was jointly assessed.

IV.3.4 Stage 4. Predictive modelling

This stage encompasses the implementation of two predictive models, one for each temporally runoff fractions (TCR and TNCR). Both ones were based on the hidden temporal conditionality of the historical runoff series, highlighted through Causality process (Molina et al., 2019).

The predictive models were developed based on a stochastic hydrological parametric AR (1) model, one for each temporal fraction. Both were developed from a TCR and TNCR temporal series obtained in Stage 3 for each past temporal horizon of four years. This is because several studies have displayed the validity of stationary assumptions and stochastic parametric models applied to the generation of hydrological predictive models (Papacharalampous et al., 2019, Tyralis and Koutsoyiannis 2014). Given the extremely high annual variability that characterizes the availability of Spanish water resources (CEDEX 2017, Garrote et al., 2007) the predictive models were generated by forecast horizon of one (1) year (Dep-1). Then, Monte Carlo simulations from AR (1) models with 5000 data were done. The probabilistic approach was based on Gringorten probability, expressed as (Jiménez Álvarez 2016):

$$F_{(y_i)} = \frac{i - 0.44}{n + 0.12}$$

where $F_{(yi)}$ is the value of the data distribution function y_i, i the occupied position by the data in the series ordered from lowest to highest, and n the total number of data in the series.

IV.3.5 Stage 4. Validation

Finally, forecasting skills were assessed through the observed and predicted values obtained previously by means of two ways. The first one, general through the Mean Absolute Error (MAE) and Root Mean Square Error (RMSE), based on a comprehensive analysis of the probability distribution functions of observed data in each one temporal horizon of the four years considered. The second one, based on a metrological approach because of the TNCR fraction does not depend on time and therefore it may be considered as a source of uncertainty to the forecast. In this sense, MAE is a widely accepted approach to assess the accuracy of forecasting (Feroz et al., 2020, Kumar et al., 2022, Foran Quinn et al., 2021). It represents the absolute average error between observed and forecasted values and it is the most important parameter used to check the precision of the prediction skill of a model (Feroz et al., 2020). For its part, RMSE measures the absolute deviation of the predicted values from the observed values (Feroz et al., 2020):

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |Obs_i - f_i|$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Obs_i - f_i)^2}{n}}$$

where Obs_i and f_i are observed and forecasted values respectively and n is the total number of observations.

This final stage was completed with an external validation based on the expert knowledge of the reservoir system managers.

IV.4 Results

IV.4.1 Statistical analysis of historical and synthetic data

Table IV.2 summarizes the main statistical parameters of historical time series versus synthetic ones. The comparison clearly shows how the AR (1) model maintains the main statistical parameters of the historical records, validating the process of generating synthetic data. Furthermore, the differences in absolute value present nonrelevant values. Particularly noteworthy is the minimal difference existing in the mean value of both inflows, with errors of 1.3% in the case of the Serones reservoir and 3.8% in the Becerril one.

Table IV.2: Validation of synthetic data generation process based on AR(1) models. CI: Confidence intervals.

Reservoir case study	Parameters	Historical records	Synthetic data	
			Average value	CI (95%)
Serones	Annual mean (Hm^3):	22.69	22.39	[15.53 , 29.85]
	Standard deviation (Hm^3):	14.62	16.28	[10.80 , 22.63]
	Variation coefficient (%):	64.44	72.71	
	Skewness coefficient:	1.51	1.28	
Becerril	Annual mean (Hm^3):	9.91	9.53	[3.82 , 16.00]
	Standard deviation (Hm^3):	12.43	9.80	[9.18 , 19.23]
	Variation coefficient (%):	125.42	102.83	
	Skewness coefficient:	1.97	1.71	

Table IV.3 shows the results of the model selection process. All coefficients, with an absolute value less than the unit, satisfy the stationarity condition for ARMA (*p*,*q*) models. It is worth noting the minimal difference in the case of model selection between an AR(*1*) and ARMA (*1*,*1*) models as well as the value of the coefficient of the MA part in both cases. In consequence, and based on the principle of parsimony, historical records are adequately modelled by means of AR (*1*) models.

Table IV.3: Stationarity condition of annual historical records. AIC: Akaike Information Criterion.

ARMA (*p*,*q*) model		AIC	$\emptyset_1$ / $\emptyset_2$	θ_1 / θ_2
Serones reservoir	(1 , 0)	-5.359105	0.9975	
	(1 , 1)	-5.358764	0.9975	0.0012
	(1 , 2)	-5.358423	0.9975	0.0012 / 0.0012
	(2 , 0)	-5.358765	0.9988 / -0.0013	
	(2 , 1)	-5.358423	0.9988 / -0.0013	-0.0001
	(2 , 2)	-5.358082	0.9988 / -0.0013	-0.0001 / 0.0012
Becerril reservoir	(1 , 0)	-6.391680	0.9986	
	(1 , 1)	-6.391338	0.9986	0.0001
	(1 , 2)	-6.390996	0.9986	0.0001 /0.0001
	(2 , 0)	-6.391338	0.9993 / -0.0007	
	(2 , 1)	-6.390996	0.9993 / -0.0007	-0.0006
	(2 , 2)	-6.390655	0.9993 / -0.0007	-0.0006 / 0.0001

IV.4.2 Propagation of the temporal dependence

Temporal dependence propagation was performed by a qualitative and quantitative analysis of symmetry of DMGs. From a qualitative perspective, both graphs reveal a high degree of symmetry (Figure IV.5) and therefore display an independent temporal behaviour. Noteworthy is the case of the DMG of the Becerril reservoir, which is practically symmetrical at time-lags 0 and 1 (405.13 versus -384.36 and 195.93 versus -

252.52 respectively). From this time-lag the mitigation of the dependence decreases gradually until time-lag = 4, where the relative percentage of change is zero (0).

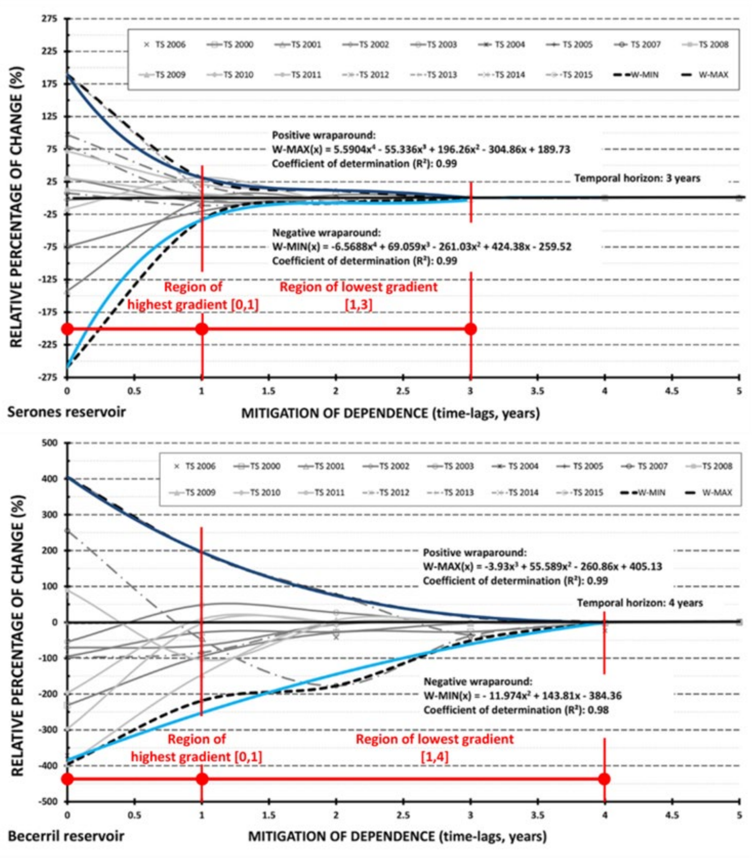


Figure IV5: Dependence mitigation graphs. Upper: Serones reservoir; lower: Becerril reservoir.

Serones DMG, with a slight asymmetry at time-lag = 0 (189.73 versus -259.52) displays a rapid decrease in temporal dependence up to time-lag = 1, with a positive value of 31.38 and negative one -33.67. From this point and until time-lag = 3, where the value is 0, the symmetry is practically total, showing purely independent behaviour, and with no significant dependence mitigation. Furthermore, in both DMGs the region the highest dependence mitigation gradient is in the interval [0,1]; in contrast, the lowest dependence is defined by the interval [1,3] (Serones) and [1,4] (Becerril). It is worth noting the high values of the coefficients of determination of the W-MAX and W-MIN polynomial fitting (0.99 and 0.98).

Quantitatively, Serones Symmetry Index presents a value of 0.82 (|114.799| / |-138.919|), which reinforces the clearly independent behaviour shown in the qualitative analysis. In contrast, Becerril Symmetry Index, with a value of 0.73 (|468.019| / |-642.405|), although very close to unity (1), shows a slightly less independent behaviour than in the case of Serones. This implies a major influence of one of the wraparound, in this case W-MIN. Nevertheless, it should be noted that the Bayesian Causality has been able to capture this singularity in the temporal behaviour, highlighted in the temporal correlogram (please see Figure IV.3b,c), where the correlation coefficients r_1, r_2 and r_3 are outside the zone of independence of the correlogram, but very close to the Anderson limits that define it.

IV.4.3 Identification and quantification of Temporally Runoff Fractions

Figure 6 shows the analytical ability of Bayesian Causality. It shows the set of all causal relationships that are established between the decision variables of the model. It is remarkable the high number of non-trivial relationships (time-lag >1) detected versus the natural ones (time-lag = 1). In this sense, each “link” represents a temporal (in)dependence relationship whose strength is evaluated through its p-value (please note that Causality process, supported by NPC algorithm, is developed through statistical tests of conditional independence).

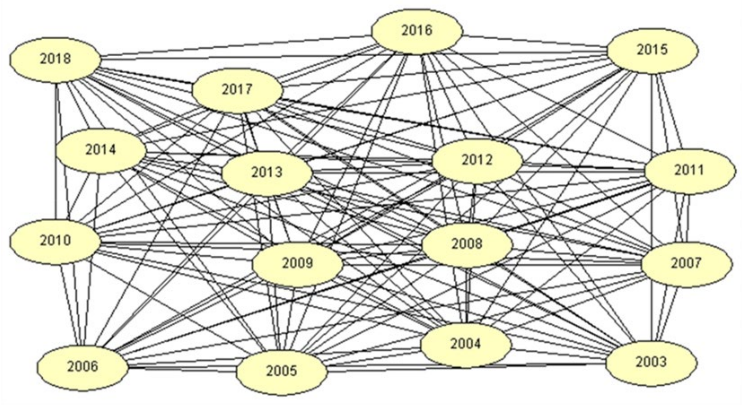


Figure IV.6: Serones causal model. Graph of marginal dependencies for a 100% independence level threshold. The Becerril causal model displays a similar dependence scheme.

For its part, Figure IV.7 presents (in)dependences matrixes which are obtained through the graph of marginal dependencies of Causality process. By the dependence matrix and focusing on a target year (an element of the main diagonal of matrix), the influence of the previous one is revealed. Furthermore, an analysis of these matrixes clearly shows that in the case of the Becerril reservoir the dependences are higher than in the case of Serones, especially in the short term (time-lag =1). This highlights a higher “dependence signal” which is evidenced by means of a major influence of TCR fraction. In contrast, a lower dependence reveals a higher influence of TNCR fraction on the total runoff. In this sense, the fact that a higher influence of the TCR fraction is associated with a significant "dependence signal" was already highlighted in the research work Molina et al., (2019).

Serones reservoir

Matrix of independences

	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
2003	0.0000															
2004	0.6848	0.0000														
2005	0.3559	0.2642	0.0000													
2006	0.2574	0.1537	0.6942	0.0000												
2007	0.9992	0.2692	0.8428	0.6727	0.0000											
2008	0.9095	0.4502	0.7113	0.8248	0.8864	0.0000										
2009	0.3507	0.9024	0.9894	0.7658	0.5690	0.6222	0.0000									
2010	0.4846	0.9765	0.6848	0.7941	0.9300	0.3467	0.3168	0.0000								
2011	0.9305	0.0211	0.8363	0.9188	0.6810	0.3421	0.7460	0.1407	0.0000							
2012	0.9507	0.6790	0.1254	0.9982	0.9820	0.9654	0.5914	0.9859	0.9643	0.0000						
2013	0.9565	0.6501	0.5790	0.4809	0.9248	0.8269	0.6752	0.2616	0.0350	0.7619	0.0000					
2014	0.2693	0.4266	0.0489	0.2551	0.8297	0.5811	0.8196	0.2356	0.2660	0.2466	0.9799	0.0000				
2015	0.0299	0.2960	0.7523	0.9270	0.9911	0.9490	0.9601	0.1021	0.7267	0.9467	0.6961	0.8145	0.0000			
2016	0.9846	0.2101	0.4561	0.4264	0.4615	0.0910	0.4533	0.7488	0.5137	0.5862	0.5719	0.6018	0.4719	0.0000		
2017	0.8842	0.0708	0.3598	0.3577	0.9436	0.9323	0.9695	0.5226	0.3878	0.9855	0.3931	0.5976	0.9929	0.6557	0.0000	
2018	0.3094	0.6233	0.2947	0.4302	0.9417	0.6720	0.3519	0.1998	0.6365	0.4425	0.8903	0.2003	0.7057	0.7775	0.7494	0.0000

Matrix of dependences

	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
2003	1.0000															
2004	0.3152	1.0000														
2005	0.6441	0.7358	1.0000													
2006	0.7426	0.8463	0.3058	1.0000												
2007	0.0008	0.7308	0.1572	0.3273	1.0000											
2008	0.0905	0.5498	0.2887	0.1752	0.1136	1.0000										
2009	0.6493	0.0976	0.0106	0.2342	0.4310	0.3778	1.0000									
2010	0.5154	0.0235	0.3152	0.2059	0.0700	0.6533	0.6832	1.0000								
2011	0.0695	0.9789	0.1637	0.0812	0.3190	0.6579	0.2540	0.8593	1.0000							
2012	0.0493	0.3210	0.8746	0.0018	0.0180	0.0346	0.4086	0.0141	0.0357	1.0000						
2013	0.0435	0.3499	0.4210	0.5191	0.0752	0.1731	0.3248	0.7384	0.9650	0.2381	1.0000					
2014	0.7307	0.5734	0.9511	0.7449	0.1703	0.4189	0.1804	0.7644	0.7340	0.7534	0.0201	1.0000				
2015	0.9701	0.7040	0.2477	0.0730	0.0089	0.0510	0.0399	0.8979	0.2733	0.0533	0.3039	0.1855	1.0000			
2016	0.0154	0.7899	0.5439	0.5736	0.5385	0.9090	0.5467	0.2512	0.4863	0.4138	0.4281	0.3982	0.5281	1.0000		
2017	0.1158	0.9292	0.6402	0.6423	0.0564	0.0677	0.0305	0.4774	0.6122	0.0145	0.6069	0.4024	0.0071	0.3443	1.0000	
2018	0.6906	0.3767	0.7053	0.5698	0.0583	0.3280	0.6481	0.8002	0.3635	0.5575	0.1097	0.7997	0.2943	0.2225	0.2506	1.0000

Becerril reservoir

Matrix of independences

	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
2003	0.0000															
2004	0.0049	0.0000														
2005	1.0000	0.7308	0.0000													
2006	0.1475	0.7752	0.5179	0.0000												
2007	0.4423	0.5511	0.6040	0.0727	0.0000											
2008	0.9998	0.9818	1.0000	0.7728	0.5296	0.0000										
2009	0.9965	0.9510	0.9998	0.7584	0.5522	0.0001	0.0000									
2010	0.7892	0.9512	0.9686	0.9707	0.3951	0.1100	0.0044	0.0000								
2011	0.9817	0.0967	0.9321	0.9006	0.8793	0.7241	0.9639	0.3873	0.0000							
2012	0.9368	0.5558	0.9683	0.9390	0.9962	0.5160	0.8186	0.3476	0.0431	0.0000						
2013	0.9415	0.9358	0.7789	0.9918	0.9856	0.9975	0.9646	0.7891	0.3201	0.0050	0.0000					
2014	0.7247	0.9913	1.0000	0.9999	0.9336	1.0000	1.0000	0.4146	0.9440	0.3177	0.0065	0.0000				
2015	0.9990	0.9808	0.9999	0.9799	0.9859	0.9990	0.9926	0.5208	0.7689	0.4321	0.2358	0.0117	0.0000			
2016	1.0000	0.9994	1.0000	0.9991	0.8060	0.6464	0.5486	0.9686	0.9999	0.9998	0.9999	1.0000	0.9999	0.0000		
2017	0.9670	0.6935	0.8422	0.9445	0.9388	0.8873	0.9698	0.5877	0.8673	0.9252	0.9810	0.8175	0.2506	0.4790	0.0000	
2018	0.8884	0.8145	0.9996	0.1622	0.9244	0.7795	0.8382	0.3392	0.5714	0.7312	0.9856	0.8185	0.2965	0.7896	0.0092	0.0000

Matrix of dependences

Influential year

Target year

	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
2003	1.0000															
2004	0.9951	1.0000														
2005	0.0000	0.2692	1.0000													
2006	0.8525	0.2248	0.4821	1.0000												
2007	0.5577	0.4489	0.3960	0.9273	1.0000											
2008	0.0002	0.0182	0.0000	0.2272	0.4704	1.0000										
2009	0.0035	0.0490	0.0002	0.2416	0.4478	0.9999	1.0000									
2010	0.2108	0.0488	0.0314	0.0293	0.6049	0.8900	0.9956	1.0000								
2011	0.0183	0.9033	0.0679	0.0994	0.1207	0.2759	0.0361	0.6127	1.0000							
2012	0.0632	0.4442	0.0317	0.0610	0.0038	0.4840	0.1814	0.6524	0.9569	1.0000						
2013	0.0585	0.0642	0.2211	0.0082	0.0144	0.0025	0.0354	0.2109	0.6799	0.9950	1.0000					
2014	0.2753	0.0087	0.0000	0.0001	0.0664	0.0000	0.0000	0.5854	0.0560	0.6823	0.9935	1.0000				
2015	0.0010	0.0192	0.0001	0.0201	0.0141	0.0010	0.0074	0.4792	0.2311	0.5679	[illegible]	0.9883	1.0000			
2016	0.0000	0.0006	0.0000	0.0009	0.1940	0.3536	0.4514	0.0314	0.0001	0.0002	0.0001	0.0000	0.0001	1.0000		
2017	0.0330	0.3065	0.1578	0.0555	0.0612	0.1127	0.0302	0.4123	0.1327	0.0748	0.0190	0.1825	0.7494	0.5210	1.0000	
2018	0.1116	0.1855	0.0004	0.8378	0.0756	0.2205	0.1618	0.6608	0.4286	0.2688	0.0144	0.1815	0.7035	0.2104	0.9908	1.0000

Figure IV.7: Matrixes of independences (cell value is *p* value) and matrixes of dependences (cell value is *DR*). Note that row values indicate year interactions with respect to target year (main diagonal cell). Colour code according to Table IV.1.

Table IV.4 summarises the quantitative assessment of both temporary runoff fractions according to past temporal horizon of four years. It should be emphasized the stability of the results of the fractions in both cases. The maintenance of the “dependence signal” over time would suggest a persistence in the temporal behaviour of water resources that could condition their availability in the short and medium term. Therefore, the higher or a lower influence of the internal temporal dependence structure would imply a higher or a lower influence of one of the two temporally conditional fractions as Table IV.4 has highlighted. This would explain the differentiated and opposite behaviour of the TNCR fraction in both case studies. In this sense, it is worth noting that the fraction with the most influence conditions the general behavior of the runoff.

Table IV.4: Quantitative assessment of temporary runoff fractions (TCR and TNCR).

	Up to	TCR (%)	TNCR (%)
Serones reservoir	2015	32.6	67.4
	2016	34.3	65.7
	2017	33.3	66.7
	2018	32.6	67.4
Becerril reservoir	2015	70.2	29.8
	2016	63.9	36.1
	2017	62.9	37.1
	2018	63.6	36.4

IV.4.4 Predictive models and forecasting reliability

Due the importance of Serones reservoir for the supply of the city of Ávila the predictive models were developed on this case study. Figure IV.8 shows the ability that Bayesian Causality offers from of the minimum “dependence signal” highlighted by the dependence matrix of Serones reservoir. It is evident that the temporal fraction with the highest influence in the annual runoff is TNCR, which presents the lowest slope in all cumulative distribution functions. This fact was also observed in Molina et al., (2019). This effect has important implications for water resources management, because TNCR is uninfluenced by time, and it may be considered as a source of uncertainty in forecasting.

Figure IV.9 summarizes the fitting process of the observed data to cumulative distribution functions (CDFs), as well as Table IV.5 shows forecasting skills based on MAE and RMSE in each predictive model.

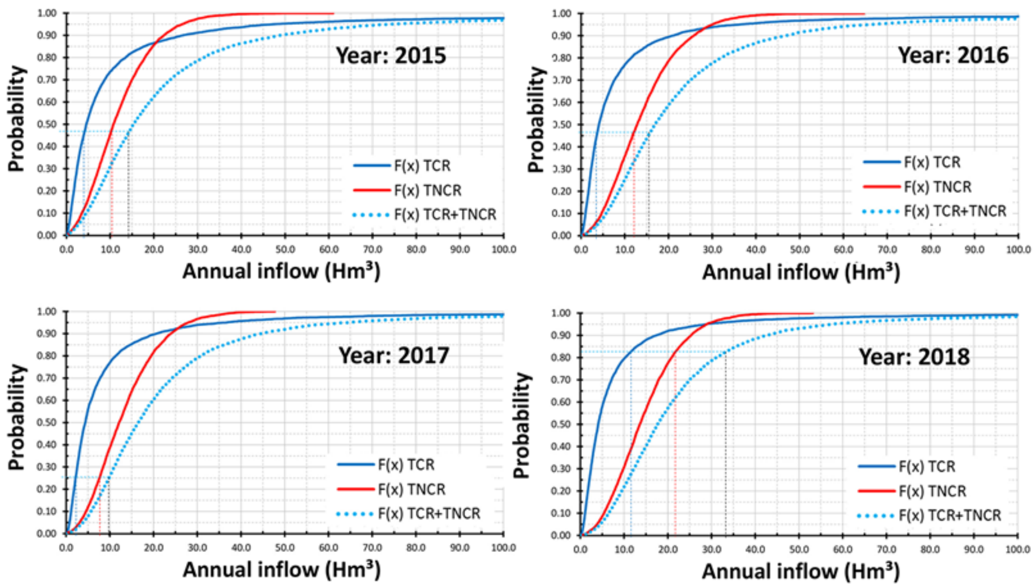


Figure IV.8: Serones reservoir predictive models for a forecast horizon of one year (Dep-1). F(x): Cumulative probability functions for each runoff fractions.

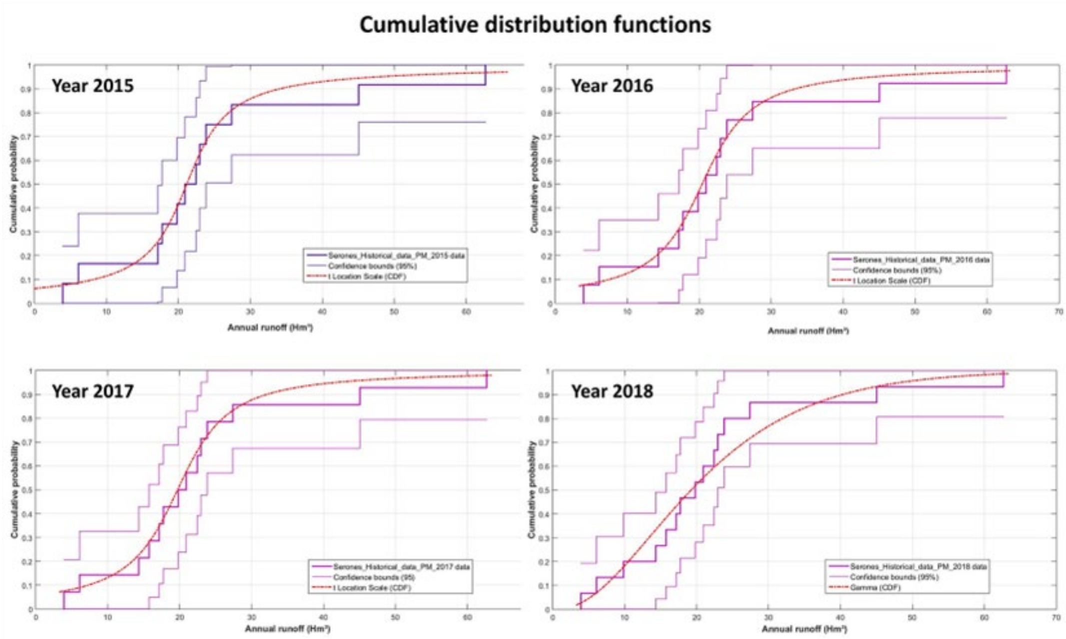


Figure IV.9: Cumulative distribution functions of Serones reservoir runoff data.

Table IV.5: Forecasting skills based on mean absolute error (MAE) and root mean square error (RMSE).

	Probability	Cumulative Distribution Function: Historical data	Cumulative Distribution Function: Predictive model	|$Obs_{(i)}$ - $Pre_{(i)}$|
Predictive model. Year 2015	0.85	29.4	37.9	8.5
	0.80	27.0	31.6	4.6
	0.75	25.4	27.1	1.7
	0.70	24.2	23.8	0.4
	0.60	22.6	19.1	3.5
	0.50	21.1	15.3	5.8
	0.40	19.8	12.4	7.4
	0.30	18.1	9.8	8.3
	0.25	16.9	8.6	8.3
	0.20	15.3	7.4	7.9
	0.15	12.9	6.1	6.8
				MAE: 5.7
				RMSE: 6.3
Predictive model. Year 2016	0.85	29.2	37.8	8.6
	0.80	26.8	32.2	5.4
	0.75	25.1	28.2	3.1
	0.70	23.9	25.1	1.2
	0.60	22.0	20.6	1.4
	0.50	20.4	17.0	3.4
	0.40	18.8	14.0	4.8
	0.30	16.9	11.3	5.6
	0.25	15.7	10.0	5.7
	0.20	14.0	8.7	5.3
	0.15	11.7	7.3	4.4
				MAE: 4.4
				RMSE: 4.9
Predictive model. Year 2017	0.85	28.3	36.5	8.2
	0.80	26.0	31.0	5.0
	0.75	24.4	27.3	2.9
	0.70	23.2	24.3	1.1
	0.60	21.3	19.9	1.4
	0.50	19.7	16.6	3.1
	0.40	18.1	13.6	4.5
	0.30	16.2	11.0	5.2
	0.25	15.0	9.9	5.1
	0.20	13.4	8.6	4.8
	0.15	11.2	7.2	4.0
				MAE: 4.1
				RMSE: 4.5
Predictive model. Year 2018	0.85	35.5	35.9	0.4
	0.80	31.9	31.3	0.6
	0.75	29.1	27.9	1.2
	0.70	26.6	25.1	1.5
	0.60	22.6	21.0	1.6
	0.50	19.2	17.7	1.5
	0.40	16.2	15.0	1.2
	0.30	13.4	12.3	1.1
	0.25	12.0	10.9	1.1
	0.20	10.5	9.5	1.0
	0.15	9.0	8.1	0.9
				MAE: 1.1
				RMSE: 1.2

The usefulness of the metrological approach on temporally conditioned fractions and their influence for the management of water resources in a basin is highlighted in Table IV.6.

Table IV.6: Reliability of the predictive model from a metrological perspective.

Predictive model (year)	Recorded inflow	Probability	TCR	TNCR	Runoff forecast
2015	14.32 Hm^3	46.5 %	4.13	10.19	4.13±10.19
2016	15.76 Hm^3	46.5 %	3.72	12.04	3.72±12.04
2017	9.85 Hm^3	25.3 %	2.19	7.66	2.19±7.66
2018	33.07 Hm^3	82.5 %	11.41	21.66	11.41±21.66

Finally, in this "proof of concept", a certain relationship between the reliability of the predictions and the average value of the runoff has been observed (22,689 Hm^3, see Table IV.A1). In the case of annual runoffs lower than the average but close to it (predictive models for the years 2015 and 2016, 14.322 and 15.759 Hm^3 respectively; see Table IV.A1) the reliability of both models was practically 50% (46.5 %). This value was increased to 82.5 % for the 2018 model in which the recorded annual runoff was higher than the average (33.071 vs. 22.689 Hm^3, see Table IV.A1). However, when the annual runoff was significantly lower than the average (2017 model year, 9.853 vs. 22.689 Hm^3) the reliability achieved was 25.3%.

IV.5 Discussion and conclusions

Bayesian Causality has demonstrated an adequate and promising performance for modelling and forecasting water resources in river basins with clearly independent temporal behaviour.

Regarding temporal modelling, the revealed logical structure of interdependence allowed to advance in its knowledge by characterising in detail the regions of highest and lowest gradient of dependence mitigation. In this sense, the DMGs provided clear temporal horizons of dependence as well as the definition of a Symmetry Index. This novel index makes possible to assess temporal dependence from a quantitative perspective. Furthermore, the fact of summarizing this behaviour in an innovative dependence matrix allowed a better knowledge of the temporally conditioned fractions (TCR and TNCR), which highlighted a distinctive and differentiated "dependence signal" of each sub-basin. In this respect, the maintenance of this “signal” over time would suggest a persistence in the temporal behaviour of water resources that could condition their availability in the short and medium term.

At the same time, the study of the temporal dependence on the water resources of a basin based on the fractions TCR and TNCR may be an effective indicator to assess the suitability and reliability of a basin to meet certain demands. Both fractions can positively contribute to improve the water resources management of a river basin through their integration into Decision Support Systems. In this sense, the higher or lower influence of TNCR can be decisive on the total annual runoff, due to this fraction (uninfluenced by time) it may be considered as a source of uncertainty, relevant, provided that its percentage is significant.

On the other side, predictive models have shown the Bayesian Causality discovery capacity. From a minimum “dependence signal” provided through the dependence matrix reliable predictive models in basins with clearly independent temporal behaviour have been generated. Furthermore, in these predictive models, the fraction with the highest influence is the one that shows the lowest slope in its probability distribution function. This fact is consistent with that observed in basins of high temporal dependence, such as that shown in Molina et al., (2019). This reinforces the applicability of Bayesian Causality to basins with opposite temporal behaviour. Furthermore, the MAE and RMSE values are not significant. However, a certain relationship has been observed between the reliability of the prediction and the average value of the runoff.

Future research would advance the characterization of the Symmetry Index as a general indicator of the temporal behavior of water resources in a basin. This index could adequately represent the evolution of resource behavior considering different time periods.

Finally, this “proof of concept”, addressed by Causality Bayesian, has highlighted the usefulness of knowing information from the past to advance in the reliable of the future.

IV.6 Appendix 1

Table IV.A1: Historical annual runoff data available.

Year	Annual runoff (Hm^3)	
	Becerril reservoir	Serones reservoir
2003	41.131	45.045
2004	36.980	27.400
2005	8.041	6.100
2006	23.054	17.155
2007	6.001	22.446
2008	4.893	17.743
2009	2.827	23.838
2010	3.131	62.668
2011	3.782	19.820
2012	1.778	3.925
2013	5.180	20.922
2014	4.545	22.953
2015	3.626	14.322
2016	5.868	15.759
2017	6.182	9.853
2018	1.490	33.071
Average value:	9.907	22.689

CAPÍTULO V

Discusión, conclusiones y líneas futuras de investigación

V.1 Discusión general

En la actualidad es más que evidente el cambio en los patrones de comportamiento espacio-temporal de los recursos hídricos, lo que incrementa su incertidumbre, dificulta su predicción, y provoca sobre éstos una mayor presión. Para su sostenibilidad y disponibilidad futura esta situación supone un escenario complejo, especialmente en el caso de los recursos superficiales; siendo necesario avanzar en el conocimiento de las estructuras de dependencia espacio-temporal que definen su comportamiento. No obstante, esta situación también supone un reto para la investigación, donde la Causalidad tiene mucho que aportar, como esta Tesis Doctoral ha puesto de manifiesto.

Desde la perspectiva del descubrimiento de estructuras causales en datos observacionales y la cuantificación de su incertidumbre, la aplicación de la Inteligencia Artificial, y el consecuente desarrollo de las técnicas de aprendizaje automático, ha supuesto una revolución en la forma de abordar y entender la causalidad en hidrología. El avance ha sido significativo desde los enfoques de Granger (1969) hasta los modelos gráficos (Pearl, 1988; Spirtes, 2010), avanzando de la correlación (asociación) a la causalidad (cambio; Pearl, 2009; Pearl et al., 2016; Spirtes et al., 2000), incluso en el caso de datos incompletos (Pearl et al., 2016), considerando la incertidumbre (Korb y Nicholson, 2010) y mejorando la representatividad de los sistemas físicos, generando modelos más interpretables y parsimoniosos (Runge et al., 2019; Reichstein et al., 2019). Destacan especialmente los avances sobre redes neuronales artificiales (desde los enfoques clásicos a otros más complejos como las de Memoria a Largo-Corto plazo o las Convolucionales), y en menor medida sobre redes bayesianas. Frente al mayor desarrollo de las primeras, las Hipótesis de Trabajo (Punto I.4) e investigaciones que componen esta Tesis Doctoral (Capítulos II, III y IV) se han centrado en "explorar" la capacidad de la Causalidad, basada en el razonamiento causal mediante redes bayesianas, para "explicar", detectar y cuantificar las relaciones de dependencia espacio-temporales y temporales, entre las variables que simulan las aportaciones de una o varias cuencas, modelando y representado explícitamente la incertidumbre (Cain 2001).

Los Capítulos II, III y IV muestran una coherencia conceptual y metodológica, incidiendo en la necesidad de comprender los mecanismos que determinan el comportamiento espacio-temporal y temporal de los recursos hídricos superficiales, por sus implicaciones para su sostenibilidad y disponibilidad futura. El diseño metodológico es consistente con Pearl (1988) y Pearl et al., (2016), donde una variable ***X*** es la causa de otra variable ***Y*** si el valor de ***Y*** depende de ***X*** en cualquier circunstancia; lo que implica que el estado (valor) de una variable (efecto) depende del estado de otra (causa). Además, el análisis de la señal de dependencia existente en las series temporales hidrológicas ha puesto de manifiesto la estructura lógica de interdependencia que subyace en éstas, y que define el comportamiento espacio-temporal de los recursos hídricos superficiales en cuencas adyacentes o individuales. Asimismo, la maximización de la evidencia estadísticas entre las variables de las redes bayesianas, para la propagación de la dependencia, se inspiraría en la "Escalera de causalidad" (Ladder of causation; "Nivel 1 Observación"), de Pearl et al., (2016) y Pearl y Mackenzie (2018). Al mismo tiempo, este análisis de la dependencia se lleva a cabo sobre un conjunto de variables causalmente relacionadas mediante un grafo acíclico dirigido (DAG por sus siglas en inglés). Este planteamiento está en línea con los principios expuestos en Spirtes (2010), donde los datos observacionales (raw data) se consideran una forma válida de evidencia empírica a partir de la que se pueden inferir relaciones causales, bajo los supuestos[21] de "Hipótesis causal de Markov" y "Fidelidad causal". La utilización de las propiedades estadísticas de los datos observacionales como fuente para descubrir relaciones causales (Spirtes, 2010) representa un cambio en el paradigma de la predicción, al considerase las relaciones causa-efecto, en línea con lo indicado por Pearl (2009). En este enfoque, los DAGs son el elemento matemático esencial del modelado causal, ya que representan el conocimiento formal causal (Spirtes, 2010). Esta estructura lógica causal ha sido la base para el desarrollo de modelos predictivos, aplicables incluso al caso de sistemas de embalses caracterizados por una limitada disponibilidad de registros y un comportamiento claramente independiente de sus aportaciones.

Por otro lado, los procesos hidrológicos, por su propia naturaleza, son inherentemente distribuidos en el espacio con evolución temporal. Aunque los modelos actuales hidrológicos distribuidos (por ejemplo, SWAT, Soil and Water Assessment Tool) simulan procesos físicos en el espacio y en el tiempo, por lo general requieren de una gran cantidad de datos de entrada, a los que son sensibles (Rasheed et al., 2024) , así como de una importante labor de calibración (Tan et al., 2021). Además, la modelización y predicción hidrológica se ha caracterizado por la aplicación de técnicas estadísticas y de aprendizaje automático para identificar patrones y correlaciones en los datos (por

[21] De acuerdo con Spirtes (2010):

Hipótesis causal de Markov (Causal Markov Assumption): Cada variable es independiente de sus no-descendientes, dados sus padres en el grafo causal.

Fidelidad causal (Faithfulness): Todas las independencias estadísticas observadas en los datos reflejan la estructura causal del grafo, y viceversa.

ejemplo, redes neuronales o modelos de regresión, entre otras). Aunque estos modelos pueden alcanzar una elevada precisión presentan una limitada capacidad para “explicar” los mecanismos que en ellos subyacen, esenciales para la predicción basada en la causalidad (Spirtes et al., 2000; Spirtes, 2010), o incluso para predecir el impacto de intervenciones externas (Pearl, 2009). Por esta razón hay una creciente demanda de modelos "transparentes" e "interpretables", que no solo predigan, sino que también expliquen el "por qué" (Rudin, 2019), frente a los modelos de "caja negra" existentes en hidrología y otras ciencias ambientales. Las investigaciones de esta Tesis Doctoral responden a esta necesidad al proporcionar enfoques metodológicos capaces de capturar las interdependencias espaciales y temporales de los sistemas hidrológicos que permiten explicar su comportamiento, en línea con Holmström et al., (2015) y Runge et al., (2019). Áreas como la epidemiología (Hernan y Robins, 2020) también están adoptando marcos conceptuales similares.

Bajo estas premisas, las investigaciones desarrolladas adoptan el enfoque de los DAGs para representar las relaciones de dependencia causal y probabilística entre las variables hidrológicas, a través de un enfoque híbrido entre el conocimiento experto y el aprendizaje automático de la estructura basado en restricciones (Steck, 2001; Vogel et al., 2018).

Macian-Sorribes et al., (2020) identifica y caracteriza las relaciones causales (direccionalidad) mediante un triple análisis conjunto espacial, temporal y espacio-temporal de las series temporales de aportaciones a embalses en dos cuencas adyacentes. Esto supone una alternativa basada en datos frente a los modelos hidrológicos distribuidos. A su vez, es una innovación a enfoques centrados en correlaciones basados en redes neuronales, menos explícitos desde el punto de la vista de la inferencia causal (Akkala et al., 2025). Asimismo, en esta investigación resulta esencial la interpretación causal de las dependencias, lo que permite identificar qué variables (causa; cuencas) influyen directamente (efecto) unas en otras, es decir, permite identificar la dirección de las relaciones, y en qué condiciones se produce. Esto tiene importantes consecuencias, por ejemplo, a la hora de decidir actuaciones orientadas a reducir la incertidumbre (adquisición de información, o mejora en la calidad de los datos). La novedad de esta investigación implicó acudir a un análisis basado en la entropía, la entropía condicionada y la información mutua (Teoría de la Información) para su validación. Si bien se observaron ciertas diferencias, existe una adecuada concordancia entre los principales patrones presentes en los datos y en las alteraciones producidas durante un año seco. En este sentido, los cambios detectados mediante el modelo causal bayesiano al inicio del periodo seco abren la posibilidad de predicción de sequías a partir del seguimiento de las dependencias espacio-temporales. Asimismo, la ausencia de dependencia espacial entre las subcuencas de Alarcón y Contreras podría servir de indicador adelantado de escasez hídrica.

En este contexto, todavía son escasas las investigaciones, y las existentes se enmarcan en el ámbito metodológico. Santos-Fernandez et al., (2022) emplea un DAG bayesiano aplicado al análisis espacio-temporal de la calidad del agua en cursos fluviales. Por su parte Ossandón et al., (2022) propone un marco de modelado jerárquico bayesiano espacio-temporal para la predicción de caudales máximos estacionales en ríos. Al igual que en Macian-Sorribes et al., (2020), estos estudios ponen de manifiesto cómo el conocimiento en detalle de la conectividad espacial influye positivamente en el conocimiento temporal, en especial para la predicción.

Por su parte, Zazo et al., (2022) aplica la causalidad bayesiana para robustecer más el proceso de modelado causal en series temporales de aportaciones en ríos mediante un nuevo marco de estabilidad. El planteamiento metodológico es consistente con los principios formales de la inferencia causal expuestos, además de con la necesidad de que el aprendizaje automático garantice modelos no solo precisos, sino también robustos y fiables en entornos dinámicos (Arjovsky et al., 2019). En este sentido, la capacidad del modelado causal bayesiano para incorporar no solo el conocimiento previo sino también cuantificar la incertidumbre de manera probabilística, resultan fundamentales a la hora de modelar el comportamiento exclusivamente temporal (cuencas individuales), y establecer las relaciones causa-efecto entre las variables en sistemas complejos naturales como los hidrológicos.

En la situación actual, caracterizada por un creciente dinamismo en los datos, la fiabilidad de la inferencia causal está ligada a la estabilidad de los resultados (Peters et al., 2017), y la cuantificación de la incertidumbre para mejorar las predicciones (Fan, 2019). Ante este reto, Zazo et al., (2022) propone un novedoso marco metodológico para robustecer, mucho más, el modelado causal bayesiano mediante un innovador enfoque bi-objetivo recursivo que permite la optimización de los factores claves implicados en el proceso de aprendizaje-entrenamiento de los modelos (número de series sintéticas e intervalos de distribuciones discretas de probabilidad). Factores no estudiados en detalle todavía en la investigación hidrológica bayesiana causal. Asimismo, se han desarrollado dos nuevos indicadores, el primero “Índice de similitud”, que permite un análisis más en detalle de la propagación de la dependencia basado en el gráfico de mitigación de la dependencia (DMG, por sus siglas en inglés), y el segundo “Índice de estabilidad”, que evalúa el proceso general de la modelización causal. La combinación óptima de estos factores permitirá incrementar el conocimiento de la propagación de la evidencia estadística entre las variables, lo que abre la puerta a predicciones más robustas del comportamiento temporal de los recursos hídricos y, potencialmente espacio-temporal. Del mismo modo que en la investigación anterior, el marco de estabilidad de Zazo et al., (2022) continúa siendo una novedad.

Investigaciones recientes con enfoques afines refuerzan la conveniencia del modelado causal bayesiano, destacando su aplicabilidad a entornos no estacionarios y su potencial para mejorar la predicción, por ejemplo, Molina y García-Aróstegui, (2023) y Zhang et al., (2024) sobre redes bayesianas dinámicas. También basado en la teoría de grafos y las relaciones de dependencia condicional, Javidian et al., (2020) aunque sobre Gráficos de Cadena (Chain Graph)[22] conceptualmente coincide en el planteamiento de Zazo et al., (2022); si bien centrado en la estabilidad de los algoritmos de aprendizaje de la estructura. Esta vinculación pone de manifiesto la necesidad de unir teoría y aplicación en la inferencia causal para avanzar en la comprensión de sistemas complejos.

En cuanto a Zazo et al., (2023), el razonamiento causal bayesiano se aplica a la predicción de las aportaciones a embalses en cuencas con un comportamiento temporal claramente independiente, bajo la hipótesis de limitada disponibilidad de datos, una realidad en muchas cuencas a nivel global. La triple combinación de condiciones (predicción / datos limitados / independencia temporal) supone que no solo sean significativos los resultados alcanzados, sino también la singularidad de la investigación. En ésta se analiza la estructura temporal oculta de las series de aportaciones, y a partir de la “matriz de dependencia” (Molina y Zazo, 2018), se identifican las dos fracciones temporales condicionadas existentes en cualquier aportación (temporalmente condicionada y no condicionada; TCR y TNCR por sus siglas en inglés); la primera debida al tiempo y la segunda independiente. Ambas son la base para la generación de modelos predictivos de cada fracción desde un enfoque autorregresivo.

[22] Generalización de los DAGs (Javidian et al., 2020).

Conceptualmente se basa en Molina et al., (2019), donde se aplica la causalidad bayesiana al caso de cuencas con alta dependencia temporal sin limitación de datos (longitud de la serie temporal 69 registros). Ambos estudios coinciden en realizar el análisis sobre series anuales, y en ambos se pone de manifiesto la influencia en la aportación de la fracción con menor pendiente en la distribución acumulada de probabilidad de los modelos predictivos. En este sentido, los resultados obtenidos son coherentes con la investigación en la que se basa. Sin embargo, hay que destacar que en ambos se profundiza en el conocimiento sobre qué hace predecible la aportación, más que solo predecirlo de forma precisa.

Por otro lado, la mejora en la definición de la dependencia temporal gracias a las regiones de dependencia asociadas al gradiente de su mitigación y la propuesta de un "Índice de simetría" para evaluar cuantitativamente la dependencia en DMGs, son innovaciones que Zazo et al., (2023) propone. Asimismo, es reseñable la caracterización de las fracciones TCR y TNCR a partir de una mínima señal de dependencia presente (descubierta) en las series temporales. Esta señal y su vinculación con las fracciones, podría sugerir la persistencia de un comportamiento temporal de las aportaciones a los embalses, que podría condicionar la disponibilidad de recursos a corto y medio plazo. En este sentido, el estudio de la dependencia temporal de los recursos hídricos de una cuenca, basado en estas fracciones, constituiría un indicador novedoso para evaluar la idoneidad y fiabilidad de una cuenca. Ambas fracciones tienen el potencial de contribuir positivamente a mejorar la gestión de los recursos hídricos de una cuenca fluvial, especialmente al integrarse en Sistemas de Apoyo a la Decisión. Además, la influencia de TNCR, al no estar afectado por el tiempo, puede ser un factor determinante que condicione la aportación anual, por lo que puede considerarse una fuente relevante de incertidumbre, sobre todo si su porcentaje es significativo.

Aunque no bajo un marco explícito causal, Noorbeh et al., (2020) aplica redes bayesianas a la predicción de aportaciones anuales y mensuales al caso de embalses. Las métricas de evaluación de rendimiento presentan valores altos (anual: R^2 de 0,62; mensual: R^2 de 0,71), con rangos de precisión entre el 75% y el 83%. Este estudio viene a reforzar la idoneidad del enfoque bayesiano aplicado a la predicción. Esto queda patente en Vasheghani Farahani et al., (2024), donde basándose en Redes Neuronales Bayesianas se predicen caudales mensuales, mejorando los resultados en la modelización y predicción, frente a los planteamientos basados en Redes Neuronales Artificiales.

Esta Tesis Doctoral, confirma las ventajas expuestas en Vogel et al., (2014) a través de 6 propiedades, además de la idoneidad de las redes bayesianas para el análisis de dependencias y el aprendizaje estructural no supervisado. A su vez, las investigaciones expuestas, sobre casos de estudio diferentes con características y objetivos distintos, refuerzan la validez de los resultados obtenidos.

Por otro lado, aunque la disponibilidad y longitud de las series temporales puedan considerarse una debilidad, Zazo et al., (2023) ha evidenciado que ésta es no intrínseca. Aun así, es posible superar esta aparente limitación mediante procesos y modelos estocásticos, tal como indica Molina et al., (2016), o por medio de modelos hidrológicos de acuerdo con Zazo et al., (2020) ya que es posible mantener las tendencias y comportamientos de los DMGs.

Asimismo, otro de los retos abordados por esta Tesis Doctoral ha sido la implementación de los propios modelos causales, considerando aspectos de diseño estructural y de viabilidad computacional. Éstos, desde los exclusivamente temporales, más sencillos, hasta los espacio-temporales totalmente conectados (relacionados) más complejos, han supuesto un incremento de su dimensionalidad y de la densidad de los DAGs; puesto de manifiesto a través del número de (in)dependencias causales. Este aspecto puede influir en la estabilidad y robustez del proceso de aprendizaje estructural, sin embargo, en este caso no ha sido un obstáculo. En relación con la viabilidad, la complejidad computacional del algoritmo NPC empleado es similar a la del algoritmo PC, estimada en $O(n^k)$[23] (Kalisch y Bühlmann, 2007; Spirtes et al., 2000), siendo gestionable en el caso de modelos de hasta 50 variables (Kalisch y Bühlmann, 2007), mediante requerimientos típicos de hardware de un usuario estándar[24]. No obstante, ha sido posible escalar el razonamiento causal bayesiano y evaluar su capacidad bajo distintos niveles de conectividad y complejidad estructural. En este sentido, el marco metodológico definido se ha demostrado robusto para garantizar la consistencia del

[23] El coste computacional del algoritmo NPC se estima en $O(n^k)$, siendo “n” el número de variables y “k” el tamaño máximo del conjunto condicionante (Kalisch y Bühlmann, 2007; Spirtes et al., 2000).

La escalabilidad del algoritmo NPC, al igual que otros métodos de aprendizaje estructural basados en pruebas de independencia condicional (como el algoritmo PC), está condicionada por los parámetros “n” y “k”. Kalisch y Bühlmann, (2007) demuestra que esta complejidad es manejable en modelos pequeños o moderados ($n < 50$, $k \leq 3$), pero se incrementa de forma no lineal en redes densamente conectadas o con un elevado número de nodos, lo que compromete su aplicabilidad práctica sin técnicas de reducción dimensional o restricciones adicionales (Kalisch y Bühlmann, 2007).

[24] Molina et al., (2019) implementa un modelo causal bayesiano temporal, a escala anual, con 69 variables sin problemas computacionales.

aprendizaje causal bajo restricciones estructurales, lo que demuestra que el modelado causal bayesiano puede escalarse con éxito a sistemas hidrológicos complejos.

En definitiva, esta Tesis Doctoral, ha logrado cumplir tanto el objetivo general como los específicos definidos, a partir de las hipótesis planteadas, permitiendo profundizar intrínsecamente en el conocimiento y predicción de estos sistemas en base a datos puramente observaciones.

V.2 Conclusiones generales y Principales aportaciones

El objetivo general de esta Tesis Doctoral ha sido evaluar el potencial que la modelización causal bayesiana ofrece para mejorar el conocimiento espacio-temporal de los recursos hídricos superficiales, y su aplicación a la predicción hidrológica.

Para aplicar el Razonamiento Causal, mediante Redes Bayesianas, al descubrimiento de estructuras causales en series temporales hidrológicas, se ha desarrollado un marco metodológico robusto y fiable. Este marco ha permitido poner de manifiesto la estructura lógica de interdependencia temporal (individual de una cuenca), y/o espacio-temporal (entre cuencas adyacentes) característica de los recursos hídricos superficiales, y que define su comportamiento. Igualmente, esta estructura lógica característica revelada, descubierta u oculta (latentemente) en las series temporales de registros hidrológicos, ha posibilitado evaluar la capacidad de modelado y predicción de la Causalidad Bayesiana desde una triple perspectiva temporal, espacial y espacio-temporal.

Asimismo, la modelización causal bayesiana ha puesto en valor cómo el análisis de la información del pasado proporciona un conocimiento previo del futuro, especialmente útil para la planificación y gestión de los recursos hídricos superficiales de las cuencas.

Por otro lado, de acuerdo con el Objetivo General, se puede concluir:

- La adaptación del marco general a los casos de estudio seleccionados ha permitido evaluar su idoneidad y potencial para realizar análisis de la dependencia espacio-temporal de series hidrológicas.
- La metodología desarrollada en esta tesis identifica eficazmente las relaciones claves espacio-temporales entre variables, cómo influyen sus cambios omnidireccionalmente y su evolución.

- Las investigaciones realizadas han puesto de manifiesto el potencial analítico que la modelización causal bayesiana ofrece para captar, modelar, cuantificar y predecir las dependencias entre las variables de aportaciones, temporal (a nivel estacional y anual en cuencas de forma conjunta y/o individual); espacial y espacio-temporal (entre subcuencas adyacentes), de forma dinámica y estocástica.
- Los análisis llevados a cabo han demostrado la capacidad de la modelización causal bayesiana para gestionar procesos naturales, caracterizados por una inherente variabilidad y aleatoriedad, como la escorrentía superficial (aportación).

En cuanto a los Objetivos Específicos planteados:

- OE-1. Avanzar en el conocimiento espacio-temporal de las aportaciones:
    - Se ha comprobado que la técnica empleada es una potente metodología de análisis y predicción de los recursos hídricos superficiales en cuencas no reguladas, destacando su rendimiento en casos con comportamiento temporal independiente.
    - La innovación que suponen las matrices de dependencia y las fracciones temporalmente condicionadas de las aportaciones (TCR y TNCR) de una cuenca, ofrecen una nueva forma de analizar el comportamiento (respuesta) general de una cuenca a través de una "señal de dependencia" característica y diferenciada. Esta señal, junto con las dos fracciones anteriores, son un innovador indicador que contribuye a mejorar la evaluación preliminar sobre la idoneidad y fiabilidad de una cuenca.
    - La metodología empleada ha demostrado un alto rendimiento predictivo a partir de una mínima señal de dependencia y en series de reducida longitud.
    - La capacidad de identificar las relaciones clave espacio-temporales, omnidireccionalmente, ha demostrado un alto potencial de aplicación en la planificación y gestión de recursos hídricos y la gestión y predicción de sequías.

- OE-2. Proponer un marco metodológico para optimizar los factores claves implicados en el proceso de aprendizaje-entrenamiento de los modelos causales bayesianos:

  - Se ha presentado un marco metodológico para el proceso de aprendizaje-entrenamiento de los modelos causales bayesianos que optimiza los factores claves implicados (número de series sintéticas e intervalos las distribuciones discretas de probabilidad de los datos sintéticos para alimentar los modelos causales).

  - El nuevo marco de estabilidad propuesto robustece más aún el proceso de modelado causal en series temporales de aportaciones en ríos.

- OE-3. Proponer un nuevo indicador dinámico del comportamiento temporal en series hidrológicas de aportaciones.

  Las investigaciones desarrolladas han puesto de manifiestos avances significativos en la evaluación del comportamiento temporal de los recursos hídricos de una cuenca, cualitativa y cuantitativamente.

  Cualitativamente:

  - La estimación de la simetría/asimetría entre las funciones de mitigación de la dependencia temporal (W-MAX y W-MIN), permite una evaluación preliminar más detallada, del comportamiento de la cuenca, proporcionando horizontes definidos de dependencia temporal frente a los enfoques clásicos del correlograma.

  - La evolución de la mitigación/propagación de la dependencia temporal, a través de los gráficos DMGs, ofrece la posibilidad de definir regiones de mayor y/o menor (in)dependencia temporal.

  Cuantitativamente:

  - El "Índice de simetría" definido a partir del gráfico DMG.

  - El "Índice de dependencia temporal (I-DT)", como innovación del "Índice de simetría", y que evalúa en un único indicador, de dos componentes, la dependencia temporal (influencia del pasado) y su fuerza.

El análisis de la evolución de las componentes del índice I-DT, mediante ventanas temporales de una serie de mayor longitud, ofrece la posibilidad de estudios detallados del comportamiento y evolución temporal de los recursos hídricos superficiales de una cuenca. Esta característica tiene importantes implicaciones a la hora de la planificación, gestión y predicción de los recursos hídricos.

- OE-4. Validar el marco metodológico desarrollado y el nuevo índice dinámico de comportamiento temporal propuesto.
    - La aplicación conjunta de diferentes técnicas estadística y la Teoría de la Información ha permitido validar, tanto el marco metodológico general y específico diseñado, como los índices desarrollados y propuestos en esta Tesis Doctoral.

V.3 Líneas futuras de investigación

Como consecuencia de esta Tesis se han identificado las siguientes líneas de investigación para avanzar y profundizar.

Planificación y gestión hidrológica

- Integración de la causalidad bayesiana en los modelos de gestión de recursos hídricos y reglas de operación de embalses, mediante el uso de las relaciones causales espacio-temporales para la predicción de aportaciones.
- Aplicación al análisis y predicción espacial de sequías en un contexto de predicción de daños.
- Integración de las fracciones temporalmente condicionadas (TCR y TNCR) en los Sistemas de Apoyo a la Decisión.
- Implementación a escala mensual.

Modelización temporal

- Incorporación de bandas de incertidumbre en los gráficos DMG y caracterización de las regiones de dependencia del gráfico a partir del "Índice de simetría".
- Definición de umbrales del impacto en los recursos hídricos de una cuenca a través del "índice de dependencia temporal (I-DT).

En análisis espacial

- Aplicación de la causalidad bayesiana a la evaluación de las relaciones espaciales entre cuencas basada en el "Índice de similaridad".
- Clasificación de tramos fluviales en función del comportamiento y la interacción de las fracciones temporalmente condicionadas.
- Mapas dinámicos de evolución de la dependencia a escala de cuenca.

Modelos probabilísticos gráficos (Probabilistic Graphical Models, PGMs)

- Aplicación del marco metodológico desarrollado al campo de la clasificación en PGMs bayesianos.

REFERENCIAS

Ahmadi, A., Moridi, A., Han, D. 2015. Uncertainty Assessment in Environmental Risk through Bayesian Networks. *Journal of Environmental Informatics*, 25, 46-59.

Akaike, H., 1974. A New Look at the Statistical Model Identification. *IEEE Trans. Autom. Control*. 19, 716–723. doi: 10.1109/TAC.1974.1100705.

Akkala, A., Boubrahimi, S.F., Hamdi, S.M., Hosseinzadeh, P., Nassar, A. 2025. Spatio-Temporal Graph Neural Networks for Streamflow Prediction in the Upper Colorado Basin. *Hydrology*, 12(3), 60.

Ali, E., Cramer, W., Carnicer, J., Georgopoulou, E., Hilmi, N., Le Cozannet, G., Lionello, P. Cross-Chapter Paper 4: Mediterranean Region. In Climate Change 2022. Impacts, Adaptation and Vulnerability. Contribution of Working Group II to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. Pörtner, H.-O., Roberts, D.C., Tignor, M., Poloczanska, E.S., Mintenbeck, K., Alegría, A., Craig, M., Langsdorf, S., Löschke, S., Möller, V., et al., Eds.; Cambridge University Press: Cambridge, UK; New York, NY, USA, 2022; pp. 2233–2272.

Allan, R.P., and Soden, B.J. 2008. Atmospheric Warming and the Amplification of Precipitation Extremes. *Science*, 321(5895), 1481–1484.

Álvarez, S. 1992. Notas sobre la causalidad probabilista. Universidad de Salamanca.

Ancell Trueba, R. 2009. Aportaciones de las Redes Bayesianas en Meteorología. Predicción Probabilística de Precipitación. Ph.D. Thesis, University of Cantabria, Santander, Spain, 228 pp.

Aqil M., Kita I., Yano A., Nishiyama S. 2007. A comparative study of artificial neural networks and neuro-fuzzy in continuous modeling of the daily and hourly behaviour of runoff. *Journal of Hydrology*, 337: 22-34.

Arjovsky, M. 2020. Out of distribution generalization in machine learning. Ph.D. Thesis, University of New York, New York, U.S.A., 120 pp.

Balakrishnan, N., and Lai, C. (2009). Continuous bivariate distributions, Springer Science & Business Media, New York.

Barber, C., Lamontagne, J.R., Vogel, R.M. 2020. Improved estimators of correlation and R^2 for skewed hydrologic data. *Hydrological Sciences Journal*, 65(1), 87-101.

Battistelli, F., Messina, A., Tomassetti, L., Montiroli, C., Manzo, E., Torre, M., ... Petracchini, F. 2023. Assessment of Energy, Mobility, Waste, and Water Management on Italian Small Islands. *Sustainability*, 15(15), 11490.

Bayes, T. 1763. An Essay towards solving a Problem in the Doctrine of Chances. *Philosophical Transactions of the Royal Society of London*, 53, 370–418.

Bermejo Mancera, M.Á. 2011. Métodos estadísticos en series temporales no lineales, con aplicación a la predicción de energía eólica. Ph.D. Thesis, University Carlos III, Madrid, Spain, 159 pp.

Borgomeo, E., Farmer, C.L., Hall, J.W. 2015. Numerical rivers: A synthetic streamflow generator for water resources vulnerability assessments. *Water Resources Research*. 51 (7), 5382–5405.

Boulariah, O., Mikhailov, P.A., Longobardi, A., Elizariev, A.N., and Aksenov, S.G., 2021. Assessment of prediction performances of stochastic models: Monthly groundwater level prediction in Southern Italy. *Journal of Groundwater Science and Engineering* 9.2: 161-170.

Box, G.E., and Jenkins, G.M. 1976. Time series analysis: Forecasting and Control. USA, Holden-Day, pp 575.

Bradley, A.A., Habib, M., Schwartz, S.S. 2015. Climate index weighting of ensemble streamflow forecasts using a simple Bayesian approach. *Water Resources Research*, 51(9), 7382-7400.

Bras, R.L., Rodrıguez-Iturbe, I. 1985. Random Functions and Hydrology. Addison-Wesley, Massachusetts.

Cabañas de Paz, R. 2017. New Methods and Data Structures for Evaluating Influence Diagrams. Ph.D. Thesis, University of Granada, Granada, Spain, 360 pp.

Cain, J. 2001. Guidelines for using Bayesian Networks to support the planning and management of development programmes in the water sector and beyond. Centre for Ecology & Hydrology Wallingford, Wallingford, UK.

Carmona, G., Varela-Ortega, C., Bromley, J. 2011. The Use of Participatory Object-Oriented Bayesian Networks and Agro-Economic Models for Groundwater Management in Spain. *Water Resour.Manage*. 25, 1509-1524.

Castelletti, A., and Soncini-Sessa, R. 2007. Bayesian Networks and participatory modelling in water resource management. *Environmental Modelling & Software*. 22, 1075-1088.

CEDEX. 2017. Centro de Estudios y Experimentación de Obras Públicas, Ministerio de Fomento. Informe Técnico: Evaluación del impacto del cambio climático en los recursos hídricos y sequías en España. Madrid, Spain, pp. 15–19. Disponible en: https://www.miteco.gob.es/es/cambio-climatico/temas/impactos-vulnerabilidad-y-adaptacion/plan-nacional-adaptacion-cambio-climatico/agua-rrhh.html (Consultado: 30 diciembre 2021).

Chang, B., Guan, J., and Aral, M.M. 2015. Scientific Discourse: Climate Change and Sea-Level Rise. *Journal of Hydrologic Engineering*, 20(1), A4014003.

Chang, J., Bai, Y., Xue, J., Gong, L., Zeng, F., Sun, H., ... Ma, Y. 2023. Dynamic Bayesian networks with application in environmental modeling and management: A review. *Environmental Modelling & Software*, 105835.

Chanapathi, T., Thatikonda, S. 2020. Evaluation of sustainability of river Krishna under present and future climate scenarios. *Science of the Total Environment*, 738, 140322.

Charniak, E. 1991. Bayesian networks without tears. *AI magazine*, 12(4), 50-50.

CHD. 2015. Plan Hidrológico de la parte española de la Demarcación Hidrográfica del Duero. Disponible en: https://www.chduero.es (Consultado: 10 enero 2022).

Chenoweth, T., Hubata, R., St. Louis, R.D. 2000. Automatic ARMA identification using neural networks and the extended samples autocorrelation function: A reevaluation. *J. Decis. Support Syst.*, 29(1), 21–30.

Chiverton, A., Hannaford, J., Holman, I. P., Corstanje, R., Prudhomme, C., Hess, T. M., Bloomfield, J.P. 2015. Using variograms to detect and attribute hydrological change. *Hydrology and Earth System Sciences*, 19(5), 2395-2408.

CHJ. 2006. Mapa piezométrico general de la confederación hidrográfica del Júcar. In Comprobación y evaluación en la Cuenca Piloto del río Júcar de las Guías desarrolladas en el marco de la Estrategia común para la implementación de la Directiva Marco del Agua (in S. Valencia).

CHJ. 2007. Plan Especial de Alerta y Eventual Sequia en la Confederación Hidrográfica del Júcar (in Spanish). Valencia.

CHJ. 2015. Plan Hidrológico de la Demarcación Hidrográfica del Júcar. Valencia.

CHJ. 2020. Sistema de Información del Agua (SIA) de la Confederación Hidrográfica del Júcar. Red Piezométrica Operativa.

Croitoru, A., and Minea, I. 2015. The impact of climate changes on rivers discharge in Eastern Romania. *Theoretical and Applied Climatology*, 120: 563-573.

Darwiche, A. 2009. Modeling and Reasoning with Bayesian Networks. Cambridge University Press, Cambridge, UK.

Dechter, R. 2013. Reasoning with probabilistic and deterministic graphical models: Exact algorithms. Synthesis Lectures on Artificial Intelligence and Machine Learning, 7(3), 1–191.

De Michele, C., and Salvadori, G. 2003. A Generalized Pareto intensity-duration model of storm rainfall exploiting 2-Copulas. *Journal of Geophysical Research-Atmospheres*. 108, 4067.

Diaz, V., Perez, G.A.C., Van Lanen, H.A., Solomatine, D., Varouchakis, E.A. 2020. An approach to characterise spatio-temporal drought dynamics. *Advances in Water Resources*, 137, 103512.

Diez, F.J., Luque, M., Bermejo, I. 2018. Decision analysis networks. *International Journal of Approximate Reasoning*. 96, 1-17.

Donat, M.G., Lowry, A. L., Alexander, L.V., O'Gorman, P.A., and Maher, N. 2016. More Extreme Precipitation in the World's Dry and Wet Regions. *Nature Climate Change*, 6(5), 508–513.

Efron, B., and Tibshirani, R.J. 1993. An introduction to the bootstrap. Monographs on statistics and applied probability. Chapman and Hall/CRC.

Engelke, S., and Hitz, A.S., 2020. Graphical models for extremes. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*. 82, 871-932.

Estrela, M.J., Peñarrocha, D., and Millán, M. 2000. Multi-annual drought episodes in the Mediterranean (Valencia region) from 1950-1996. A spatio-temporal analysis. *International Journal of Climatology*, John Wiley & Sons, Ltd., 20(13), 1599–1618.

Eythorsson, D. and Clark, M. 2025. Toward Automated Scientific Discovery in Hydrology: The Opportunities and Dangers of AI Augmented Research Frameworks. *Hydrological Processes*, 39(1), e70065.

Fan, Y. 2019. Uncertainty quantification in hydrologic predictions: A brief review. *J. Environ. Inform. Lett*, 2, 48-56.

Fang, J., Yang, L., Wen, X., Li, W., Yu, H., Zhou, T. 2024. A deep learning-based hybrid approach for multi-time-ahead streamflow prediction in an arid region of Northwest China. *Hydrology Research*, 55(2), 180-204.

Feroz, R.M.A., Javed, A., Syed, A.H., Kazmi, S.A.A., and Uddin, E., 2020. Wind speed and power forecasting of a utility-scale wind farm with inter-farm wake interference and seasonal variation. *Sustainable Energy Technologies and Assessments* 42: 100882.

Foran Quinn, D., Murphy, C., Wilby, R.L., Matthews, T., Broderick, C., Golian, S., Donegan, S., and Harrigan, S., 2021. Benchmarking seasonal forecasting skill using river flow persistence in Irish catchments. *Hydrological Sciences Journal*, 66(4), 672-688.

Freire-González, J., Decker, C., and Hall, J. W. 2017. The Economic Impacts of Droughts: A Framework for Analysis. *Ecological Economics*, 132, 196–204.

Garrote, L., de Lama, B., and Martín-Carrasco, F., 2007. Previsiones para España según los últimos estudios de Cambio Climático. El Cambio Climático en España y sus consecuencias en el Sector del Agua. Universidad Rey Juan Carlos: Madrid, Spain, pp. 3–15.

Gil, M., Garrido, A., and Gómez-Ramos, A. 2011. Economic analysis of drought risk: An application for irrigated agriculture in Spain. *Agricultural Water Management*, 98(5), 823–833.

Giné-Garriga, R., Requejo, D., Molina, J.L., Pérez-Foguet, A. 2018. A novel planning approach for the water, sanitation and hygiene (WaSH) sector: The use of object-oriented bayesian networks. *Environmental modelling & software*, 103, 1-15.

Giuliani, M., Zaniolo, M., Castelletti, A., Davoli, G., and Block, P., 2019. Detecting the state of the climate system via artificial intelligence to improve seasonal forecasts and inform reservoir operations. *Water Resources Research*, 55(11), 9133-9147.

Giupponi, C., and Sgobbi, A. 2013. Decision Support Systems for Water Resources Management in Developing Countries: Learning from Experiences in Africa. *Water*, 5: 798-818.

González Casimiro, P. 2009. Análisis de series temporales: Modelos ARIMA. Facultad de Ciencias Económicas y Empresariales. Universidad del País Vasco. Vizcaya, España, pp. 1. ISBN: 978-84-692-3814-1.

Granger, C.W. 1969. Investigating causal relations by econometric models and cross-spectral methods. *Econometrica: Journal of the Econometric Society*, 37(3), 424-438.

Guinard, K., Mailhot, A., and Caya, D., 2015. Projected changes in characteristics of precipitation spatial structures over North America. *International Journal of Climatology*, 35(4), 596-612.

Gutiérrez, J.M., Cano, R., Sordo, C. 2004. Redes probabilísticas y neuronales en las ciencias atmosféricas. Ministerio de Medio Ambiente, Secretaría General Técnica, Madrid, España.

Hao, Z., and Singh, V. P. 2016. Review of Dependence Modeling in Hydrology and Water Resources. *Progress in Physical Geography*, 40(4), 549–578.

He, L., Shi, L., Song, W., Shen, J., Wang, L., Hu, X., Zha, Y. 2024. Synergizing Intuitive Physics and Big Data in Deep Learning: Can We Obtain Process Insights While Maintaining State-Of-The-Art Hydrological Prediction Capability? *Water Resources Research*, 60(12), e2024WR037582.

Hejazi, M.I., and Cai, X. 2011. Building more realistic reservoir optimization models using data mining - A case study of Shelbyville Reservoir. *Advances in Water Resources*, 34(6), 701–717.

Hernan, M.A., and Robins, J.M. 2020. Causal Inference: What If Chapman Hall/CRC, Boca Raton, Florida, USA.

Hipel, K.W., and McLeod, A.I. 1994. Time Series Modelling of Water Resources and Environmental Systems. Elsevier, Amsterdam, The Netherlands.

Holmström, L., Ilvonen, L., Seppä, H., and Veski, S. 2015. A Bayesian spatiotemporal model for reconstructing climate from multiple pollen records. *Institute of Mathematical Statistics in The Annals of Applied Statistics*, 9(3), 1194–1225.

Hosseini, M. and Kerachian, R., 2019. Improving the reliability of groundwater monitoring networks using combined numerical, geostatistical and neural network-based simulation models. *Hydrological Sciences Journal*, 64(15), 1803-1823.

HUGIN. 2021. http://data.biotracer.hugin.com/htmlhelp/index.html.

Hurst, H.E. 1951. Long-term storage capacity of reservoirs. *Transactions of Amer.Soc.Civil Eng. (ASCE)*. 116, 770-808.

IDEDuero. 2022. Duero River Basin Authority. Disponible en: http://www.mirame.chduero.es/ (Consultado: 10 enero 2022).

IDEE. 2023. Infraestructura de datos espaciales de España. Disponible en: https://www.idee.es/visualizador/ (Consultado: 16 octubre 2023).

IGME. 2020a. Map of Permeabilities of Spain scale 1/1000.000. https://igme.maps.arcgis.com/home/webmap/viewer.html?webmap=da8eb570845b41bbb5548c8266eaed0d (Consultado: 1 marzo 2020).

IGME. 2020b. Hydrogeological map of Spain scale 1/1000.000. https://igme.maps.arcgis.com/home/item.html?id=036292dc5b8946bd979a7dc47d2f8561 (Consultado: 1 marzo 2020).

IGME. 2022a. Hydrogeological map of Spain scale 1/1.000.000. Web Map Service (WMS). Disponible en: https://igme.maps.arcgis.com/home/webmap/viewer.html?webmap=036292dc5b8946bd979a7dc47d2f8561 (Consultado: 1 diciembre 2022).

IGME. 2022b. Map of Permeabilities of Spain scale 1/200.000. Web Map Service (WMS). Disponible en: https://www.arcgis.com/home/webmap/viewer.html?webmap=28aed6c672b046b68904ae0ffa9de802 (Consultado: 1 diciembre 2022).

IGN. 2022. Spatial Data Infrastructure. Web Map Service (WMS). Disponible: https://www.ign.es/wms-inspire/ign-base (Consultado: 1 febrero 2022).

Ilich N, and Despotovic J. 2008. A simple method for effective multi-site generation of stochastic hydrologic time series. *Stochastic Environmental Research and Risk Assessment*, 22: 265-279.

IPCC. 2023. Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. Disponible en: https://www.ipcc.ch/report/ar6/syr/downloads/report/IPCC_AR6_SYR_FullVolume.pdf (Consultado: 10 diciembre 2023).

Jain, A., and Kumar, A.M. 2007. Hybrid neural network models for hydrologic time series forecasting. *Applied Soft Computing*. 7, 585-592.

Javidian, M.A., Valtorta, M., Jamshidi, P. 2020. AMP chain graphs: Minimal separators and structure learning algorithms. *Journal of Artificial Intelligence Research*, 69, 419-470.

Jayakrishnan, R., Srinivasan, R., Santhi, C., Arnold, J.G. 2005. Advances in the application of the SWAT model for water resources management. *Hydrological Processes*, 19: 749-762.

Jiménez Álvarez, A., 2016. Desarrollo de Metodologías para mejorar la estimación de los Hidrogramas de Diseño para el cálculo de los órganos de desagüe de las presas. Thesis (PhD). Polytechnical University of Madrid, Madrid, Spain, 329 pp.

Jimeno Sáez, P. 2018. Simulación de procesos hidrológicos utilizando técnicas de machine learning y modelos hidrológicos. Ph.D. Thesis, Catholic University of Murcia, Murcia, Spain, 250 pp.

Jona Lasinio, G., Sahu, S. K., and Mardia, K. V. 2005. Modeling rainfall data using a Bayesian Kriged-Kalman model. Southhampton, UK.

Jyrkama, M.I., and Sykes, J. F. 2007. The Impact of Climate Change on Spatially Varying Groundwater Recharge in the Grand River Watershed (Ontario). *Journal of Hydrology*, 338(3–4), 237–250.

Kahil, M.T., Dinar, A., and Albiac, J. 2015. Modeling water scarcity and droughts for policy adaptation to climate change in arid and semiarid regions. *Journal of Hydrology*, 522, 95–109.

Kalisch, M., and Bühlman, P. 2007. Estimating high-dimensional directed acyclic graphs with the PC-algorithm. *Journal of Machine Learning Research*, 8(3).

Kalra, A., Li, L., and Ahmad, S. 2013. Improving Streamflow Forecast Lead Time using Oceanic-Atmospheric Oscillations for Kaidu River Basin, Xinjiang, China. *Journal of Hydrologic Engineering*, 18(8), 1031–1040.

Kendall, M.G. 1955. Rank correlations methods. 2^{th} ed. New York: Hafner.

Kim, S., Parhi, P., Jun, H., Lee, J. 2018. Evaluation of drought severity with a Bayesian network analysis of multiple drought indices. *Journal of Water Resources Planning and Management*, 144(1), 05017016.

Koller, D., and Friedman, N. 2009. Probabilistic Graphical Models: Principles and Techniques. The MIT Press, Cambridge, Massachusetts, USA.

Korb, K.B., and Nicholson, A.E. 2010. Bayesian artificial intelligence. CRC press.

Kousari, M.R., Hosseini, M.E., Ahani, H., and Hakimelahi, H. 2017. Introducing an Operational Method to Forecast Long-Term Regional Drought Based on the Application of Artificial Intelligence Capabilities. *Theoretical and Applied Climatology*, 127(1–2), 361–380.

Koutroumanidis, T., Sylaios, G., Zafeiriou, E., Tsihrintzis, V.A. 2009. Genetic modeling for the optimal forecasting of hydrologic time-series: Application in Nestos River. *Journal of Hydrology* 368: 156-164.

Kretschmer, M., Coumou, D., Donges, J. F., Runge, J. 2016. Using causal effect networks to analyze different Arctic drivers of midlatitude winter circulation. *Journal of climate*, 29(11), 4069-4081.

Kumar, P., Pattanaik, D.R., and Alone, A., 2022. Bias-Corrected Extended-Range Forecast Over India for Hydrological Applications During Monsoon 2020. *Pure and Applied Geophysics*, 1-15.

Lappenschaar, M., Hommersom, A., Lucas, P.J.F. 2012. Qualitative chain graphs and their use in medicine. Proceedings of the Sixth European Workshop on Probabilistic Graphical Models. Proceedings of the Sixth European Workshop on Probabilistic Graphical Models, Granada, Spain, 2012, 179-185.

Le, T.D., Hoang, T., Li, J., Liu, L., Liu, H., Hu, S. 2016. A fast PC algorithm for high dimensional causal discovery with multi-core PCs. *IEEE/ACM Transactions on computational biology and bioinformatics*, 16(5), 1483-1495.

Lehikoinen, A., Olsson, J., Bergström, L., Bergström, U., Bryhn, A., Fredriksson, R., Uusitaloc, L. 2019. Evaluating complex relationships between ecological indicators and environmental factors in the Baltic Sea: A machine learning approach. *Ecol.Ind*. 101, 117-125.

Lima, A.R., Cannon, A., and Hsieh, W. W. 2016. Forecasting Daily Streamflow using Online Sequential Extreme Learning Machines. *Journal of Hydrology*, 537, 431–443.

Lionello, P., and Scarascia, L. 2018. The relation between climate change in the Mediterranean region and global warming. *Regional Environmental Change*, 18 (5), 1481–1493.

Liu, D., Tian, F., Lin, M., Sivapalan, M. 2015. A conceptual socio-hydrological model of the co-evolution of humans and water: case study of the Tarim River basin, western China. *Hydrology and Earth System Sciences*, 19: 1035-1054.

Lopez-Nicolas, A., Pulido-Velazquez, M., and Macian-Sorribes, H. 2017. Economic risk assessment of drought impacts on irrigated agriculture. *Journal of Hydrology*, 550, 580–589.

Luo, Y., Zhou, Y., Chen, H., Xiong, L., Guo, S., Chang, F.J. 2024. Exploring a spatiotemporal hetero graph-based long short-term memory model for multi-step-ahead flood forecasting. *Journal of Hydrology*, 633, 130937.

Ma, Y., Zhong, P.A., Xu, B., Zhu, F., Yang, L., Wang, H., Lu, Q. 2022. Stochastic generation of runoff series for multiple reservoirs based on generative adversarial networks. *Journal of Hydrology*, 605, 127326.

Macian-Sorribes, H., and Pulido-Velazquez, M. 2017. Integrating Historical Operating Decisions and Expert Criteria into a DSS for the Management of a Multireservoir System. *Journal of Water Resources Planning and Management*, American Society of Civil Engineers, 143(1).

Macián-Sorribes, H. 2017. Design of optimal reservoir operating rules in large water resources systems combining stochastic programming, fuzzy logic and expert criteria. Ph.D. Thesis, Universitat Politècnica de València, Valencia, Spain, 254 pp.

Macian-Sorribes, H., Molina, J.L., Zazo, S., Pulido-Velázquez, M. 2020. Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling. *Journal of Hydrology*, 597, 125722.

Macian-Sorribes, H., and Pulido-Velazquez, M. 2020. Inferring efficient operating rules in multireservoir water resource systems: A review. *Wiley Interdisciplinary Reviews: Water*, 7(1), e1400.

Mackie, J.L. 1965. Causes and conditions. *American Philosophical Quarterly*, 2(4), 245-264.

Madsen, A.L., Lang, M., Kjaerulff, U.B., Jensen, F. 2003. The Hugin Tool for learning Bayesian networks. Symbolic and Quantitative Approaches to Reasoning with Uncertainty, Proceeding. ECSQARU 2003. Lecture Notes in Computer Science, vol 2711, 594-605. Springer, Berlin, Heidelberg.

Madsen, H., Lawrence, D., Lang, M., Martinkova, M., Kjeldsen, T.R. 2014. Review of trend analysis and climate change projections of extreme precipitation and floods in Europe. *Journal of Hydrology*, 519, 3634-3650.

Malekmohammadi, B., Kerachian, R., Zahraie, B. 2009. Developing monthly operating rules for a cascade system of reservoirs: Application of Bayesian Networks. *Environmental Modelling & Software*. 24, 1420-1432.

Malone, B., and Yuan, C. 2012. A Bounded Error, Anytime, Parallel Algorithm for Exact Bayesian Network Structure Learning (Contributed Paper). Proceedings of the Sixth European Workshop on Probabilistic Graphical Models, Granada, Spain, 235-242.

Mamitimin, Y., Feike, T., Doluschitz, R. (2015). Bayesian Network Modeling to Improve Water Pricing Practices in Northwest China. *Water*. 7, 5617-5637.

Marcos, P., Lopez-Nicolas, A., Pulido-Velazquez, M. 2017. Analysis of climate change impact on meteorological and hydrological droughts through relative standardized indices. In EGU General Assembly Conference Abstracts (p. 1391).

Marcos-Garcia, P., Lopez-Nicolas, A., Pulido-Velazquez, M. 2017. Combined use of relative drought indices to analyze climate change impact on meteorological and hydrological droughts in a Mediterranean basin. *Journal of Hydrology*. 554, 292-305.

Marotzke, J., Jakob, C., Bony, S., Dirmeyer, P. A., O'Gorman, P. A., Hawkins, E., ... Tuma, M. 2017. Climate research must sharpen its view. *Nature Climate Change*, 7(2), 89-91.

Martín Vide, F.J. 1994. Diez características de la pluviometría española decisivas en el control de la demanda y el uso del agua. Boletín de la Asociación de Geógrafos Españoles, 18: 9-16.

McGrayne, S.B. 2011. The Theory that Would Not Die: How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines, & Emerged Triumphant from Two Centuries of Controversy, Yale University Press, Yale.

Mediero, L., Garrote, L. and Martin-Carrasco, F., 2007. A probabilistic model to support reservoir operation decisions during flash floods. *Hydrological Sciences Journal*, 52(3), 523-537.

Mediero, L., Santillán, D., Garrote, L., Granados, A. 2014. Detection and attribution of trends in magnitude, frequency and timing of floods in Spain. *Journal of Hydrology*, 517, 1072-1088.

Mishra, A.K., and Desai, V.R. 2005. Drought forecasting using stochastic models. *Stochastic Environmental Research and Risk Assessment*, 19(5), 326–339.

Mishra, A.K., and Singh, V.P. 2010. A review of drought concepts. *Journal of Hydrology*, 391(1–2), 202–216.

Mishra, A.K., and Singh, V.P. 2011. Drought modeling - A review. *Journal of Hydrology*, 403(1–2), 157–175.

MITECO. 2021. Ministerio Para la Transición Ecológica. Gobierno de España. https://sig.mapama.gob.es/redes-seguimiento/ (Consultado: 10 marzo 2021).

MITECO. 2022. Ministerio Para la Transición Ecológica. Gobierno de España. Disponible en: https://sig.mapama.gob.es/geoportal/ (Consultado: 10 enero 2022).

MITECO. 2024. Ministerio Para la Transición Ecológica. Gobierno de España. https://www.miteco.gob.es/es/agua/temas/seguridad-de-presas-y-embalses/desarrollo.html (Consultado: 10 enero 2024).

Moghaddam, H.K., Moghaddam, H.K., Kivi, Z.R., Bahreinimotlagh, M., Alizadeh, M.J. (2019). Developing comparative mathematic models, BN and ANN for forecasting groundwater levels. *Groundwater for Sustainable Development*, 9, 100237.

Mohammadi, K., Eslami, H.R., Kahawita, R. 2006. Parameter Estimation of an ARMA Model for River Flow Forecasting using Goal Programming. *J. Hydrol.,* 331, 293–299.

Molina J.L. 2009. Análisis integrado y estrategias de gestión de acuíferos en zonas semiáridas.Aplicación al caso de estudio del Altiplano (Murcia, SE España). Ph.D. Thesis, University of Granada - Geological and Mining Institute of Spain, Granada, Spain, 303 pp.

Molina, J.L., Bromley, J., García-Aróstegui, J.L., Sullivan, C., and Benavente, J. 2010. Integrated water resources management of overexploited hydrogeological systems using Object-Oriented Bayesian Networks. *Environmental Modelling & Software*, 25(4), 383–397.

Molina, J.L., Pulido-Velazquez, D., Luis Garcia-Arostegui, J., Pulido-Velazquez, M. 2013. Dynamic Bayesian Networks as a Decision Support tool for assessing Climate Change impacts on highly stressed groundwater systems. *Journal of Hydrology*. 479, 113-129.

Molina, J.L., Zazo, S., Rodríguez-Gonzálvez, P., and González-Aguilera, D. 2016. Innovative Analysis of Runoff Temporal Behavior through Bayesian Networks. *Water*, 8(11), 484.

Molina, J.L., and Zazo, S. 2017. Causal Reasoning for the Analysis of Rivers Runoff Temporal Behavior. *Water Resour.Manage.*, 1-13.

Molina, J.L., and Zazo, S. 2018. Assessment of Temporally Conditioned Runoff Fractions in Unregulated Rivers. *J.Hydrol.Eng*. 23, 04018015.

Molina, J.L., Zazo, S., Martín-Casado, A.M. 2019. Causal Reasoning: Towards Dynamic Predictive Models for Runoff Temporal Behavior of High Dependence Rivers. *Water*. 11, 877.

Molina, J.L., Zazo, S., Martín-Casado, A., Patino-Alonso, M. 2020. Rivers' Temporal Sustainability through the Evaluation of Predictive Runoff Methods. *Sustainability*. 12, 1720.

Molina, J.L., Patino-Alonso, C., Zazo, S. 2021. Hybrid Causal Multivariate Linear Modelling (H_CMLM) method for the analysis of temporal rivers runoff. *Journal of Hydrology*. 126501.

Molina, J.L., Espejo, F., Zazo, S., Molina, M. C., Hamitouche, M., García-Aróstegui, J.L. 2022. HydroPredicT_Extreme: A probabilistic method for the prediction of extremal high-flow hydrological events. *Journal of Hydrology*, 610, 127929.

Molina, J.L., García-Aróstegui, J.L. 2023. Water table prediction through causal reasoning modelling. *Science of the Total Environment*, 867, 161492.

Nelsen, R. (2006). An introduction to copula, Springer, New York.

Nourani, V., Kisi, O., Komasi, M. 2011. Two hybrid Artificial Intelligence approaches for modeling rainfall-runoff process. *Journal of Hydrology*. 402, 41-59.

Noorbeh, P., Roozbahani, A., Kardan Moghaddam, H. 2020. Annual and monthly dam inflow prediction using Bayesian networks. *Water Resources Management*, 34, 29

Ochoa-Rivera, J.C. 2002. Modelo estocástico de redes neuronales para la síntesis de caudales aplicados a la gestión probabilística de sequías. Ph.D. Thesis, Universitat Politècnica de València, Valencia, Spain, 225 pp.

Ochoa-Rivera, J.C., Andreu, J., García-Bartual, R. 2007. Influence of inflows modeling on management simulation of water resources system. *Journal of Water Resources Planning and Management*, 133(2), 106-116.

Ochoa-Rivera, J.C. 2008. Prospecting droughts with stochastic artificial neural networks. *Journal of Hydrology*. 352, 174-180.

O'Gorman, P.A., 2015. Precipitation extremes under climate change. *Current climate change reports*, 1(2), 49-59.

Ombadi, M., Nguyen, P., Sorooshian, S., Hsu, K. L. 2020. Evaluation of methods for causal discovery in hydrometeorological systems. *Water Resources Research*, 56(7), e2020WR027251.

Ossandón, Á., Brunner, M.I., Rajagopalan, B., Kleiber, W. 2022. A space–time Bayesian hierarchical modeling framework for projection of seasonal maximum streamflow. *Hydrology and Earth System Sciences*, 26(1), 149-166.

Ouma, Y.O., Cheruyot, R., Wachera, A.N. 2021. Rainfall and runoff time-series trend analysis using LSTM recurrent neural network and wavelet neural network with satellite-based meteorological data: case study of Nzoia hydrologic basin. *Complex & Intelligent Systems*, 1-24.

Papacharalampous, G., Tyralis, H. and Koutsoyiannis, D., 2019. Comparison of Stochastic and Machine Learning Methods for Multi-Step Ahead Forecasting of Hydrological Processes. *Stoch. Environ. Res. Risk Assess*, 19, 33, 481–514.

Pearl, J. 1985. Bayesian networks: A model of self-activated memory for evidential reasoning. In Proceedings of the 7th conference of the Cognitive Science Society. 1985, August, University of California, Irvine, CA, USA (pp. 15-17).

Pearl, J. 1988. Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference. Morgan Kaufmann, San Francisco, USA.

Pearl, J. 1995. Causal diagrams for empirical research. *Biometrika*, 82(4), 669–688.

Pearl, J. 2009. Causality: models, reasoning and inference. Cambridge University Press, New York City, NY, USA.

Pearl, J. 2014. Graphical Models for Probabilistic and Causal Reasoning. Computing Handbook, Third Edition: Computer Science and Software Engineering, T. Gonzalez, J. Diaz-Herrera, and A. Tucker, eds., Chapman & Hall / CRC, Boca Raton, Florida, USA.

Pearl, J., Glymour, M., N.P. Jewell. 2016. Causal Inference in Statistics: A primer, John Wiley & Sons Ltd, West Sussex, U.K. ISBN: 978-1119186847.

Pearl, J., and Mackenzie, D. 2018. The book of why: The new science of cause and effect. Basic books.

Pearson, K. 1896. Mathematical contributions to the theory of evolution III. Regression, heredity and panmixia. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 187, 253–318.

Peng, T., Zhou, J., Zhang, C., Fu, W., 2017. Streamflow Forecasting Using Empirical Wavelet Transform and Artificial Neural Networks. *Water*, 9, 406.

Peters, J., Janzing, D., Schölkopf, B. 2017. Elements of causal inference: foundations and learning algorithms, p. 288. The MIT Press.

Pfahl, S., O'Gorman, P. and Fischer, E., 2017. Understanding the regional pattern of projected future changes in extreme precipitation. *Nature Clim Change*, 7, 423–427.

Pham, H.V., Sperotto, A., Furlan, E., Torresan, S., Marcomini, A., Critto, A. 2021. Integrating Bayesian Networks into ecosystem services assessment to support water management at the river basin scale. *Ecosystem Services*, 50, 101300.

Pulido-Velazquez, M.A. 2004. Optimización económica de la gestión del uso conjunto de aguas superficiales y subterráneas en un sistema de recursos hídricos. Contribución al análisis económico propuesto en la directiva marco europea del agua. Ph.D. Thesis, Universitat Politècnica de València, Valencia, Spain, ISBN: 0-493-5874.

Ramos Fernández, J.M. 2018. Implementación de los modelos gráficos probabilísticos bayesianos en la ayuda al manejo clínico de la bronquiolitis aguda del lactante. Ph.D. Thesis, University of Malaga, 137 pp.

Rasheed, N.J., Al-Khafaji, M.S., Alwan, I.A., Al-Suwaiyan, M.S., Doost, Z.H., Yaseen, Z.M. 2024. Survey on the resolution and accuracy of input data validity for SWAT-based hydrological models. *Heliyon*, 10(19).

Recio Villa, I., Martínez Rodríguez, J.B., Molina, J.L., and Pino Tarragó, J.C., 2018. Multiobjective optimization modeling approach for multipurpose single reservoir operation. *Water*, 10(4), 427.

Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., Carvalhais, N., Prabhat, F. 2019. Deep learning and process understanding for data-driven Earth system science. *Nature*, 566(7743), 195-204.

Rodríguez, D., Dolado, J. 2007. Capítulo 10: Redes bayesianas en la ingeniería del software. En NETBIBLO (Eds.), Técnicas cuantitativas para la gestión en la ingeniería del software (pp. 220). A Coruña, España. ISBN: 978-84-9745-204-5.

Rodriguez-Iturbe, I., Mejia, J. M., Dawdy, D. R. 1972. Streamflow simulation: 1. A new look at Markovian models, fractional Gaussian noise, and crossing theory. *Water Resources Research*, 8(4), 921-930.

Rolnick, D., Donti, P.L., Kaack, L.H., Kochanski, K., Lacoste, A., Sankaran, K., ... Bengio, Y. 2022. Tackling climate change with machine learning. *ACM Computing Surveys (CSUR)*, 55(2), 1-96.

Romano, E., Del Bon, A., Petrangeli, A.B., Preziosi, E. 2013. Generating synthetic time series of springs discharge in relation to standardized precipitation indices. Case study in Central Italy. *Journal of Hydrology*, 507: 86-99.

Rubio-Martin, A., Pulido-Velazquez, M., Macian-Sorribes, H., and Garcia-Prats, A. 2020. System dynamics modeling for supporting drought-oriented management of the Jucar river system, Spain. *Water*, 12(5), 1407.

Rubio-Martin, A., Llario, F., Garcia-Prats, A., Macian-Sorribes, H., Macian, J., Pulido-Velazquez, M. 2023. Climate services for water utilities: Lessons learnt from the case of the urban water supply to Valencia, Spain. *Climate Services*, 29, 100338.

Rudin, C. 2019. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature machine intelligence*, 1(5), 206-215.

Runge, J., Bathiany, S., Bollt, E., Camps-Valls, G., Coumou, D., Deyle, E., Glymour, C., Kretschmer, M., Mahecha, M.D., Muñoz-Mari, J., van Nes, E.H., Peters, J., Quax, R., Reichstein, M., Scheffer, M., Schoelkopf, B., Spirtes, P., Sugihara, G., Sun, J., Zhang, K., and Zscheischler, J. 2019. Inferring causation from time series in Earth system sciences. *Nature communications*, 10(1), 2553.

Said, A. 2006. The implementation of a Bayesian network for watershed management decisions. *Water Resour.Manage*. 20, 591-605.

Salas, J.D., Delleur, J.W., Yevjevich, V.M., and Lane, W.L. 1980. Applied Modeling of Hydrologic Time Series. Water Resources Publications, Littleton, Colorado, USA.

Salas, J.D., Saada, N., Chung, C.H., Lane, W.L., Frevert, D.K. 2000. Stochastic analysis, modeling, and simulation (SAMS), Version 2000—User's manual. Computing Hydrology Laboratory, Water Resources, Hydrologic and Environmental Research Center, Technical Report, (10).

Sanchez-Matos, J., Andrade, E. P., Vázquez-Rowe, I. 2023. Revising regionalized water scarcity characterization factors for selected watersheds along the hyper-arid Peruvian coast using the AWARE method. *The International Journal of Life Cycle Assessment*, 28(11), 1447-1465.

Santos-Fernandez, E., Ver Hoef, J.M., Peterson, E.E., McGree, J., Isaak, D.J., Mengersen, K. 2022. Bayesian spatio-temporal models for stream networks. *Computational Statistics & Data Analysis*, 170, 107446.

Sarabia-Alzaga, J., and Gómez-Déniz, E. 2008. Construction of multivariate distributions: a review of some recent results. *Statistics and Operations Research Transactions*. 32, 3-36.

Schroeter, K., Kreibich, H., Vogel, K., Riggelsen, C., Scherbaum, F., Merz, B. 2014. "How useful are complex flood damage models?" *Water Resour.Res*. 50, 3378-3395.

Schwarz, G. 1978. Estimating the dimension of a model. *The annals of statistics*, 461-464.

Scutari, M., Graafland, C. E., Gutiérrez, J.M. 2019. Who learns better Bayesian network structures: Accuracy and speed of structure learning algorithms. *International Journal of Approximate Reasoning*, 115, 235-253.

See, L., and Openshaw, S. 2000. A hybrid multi-model approach to river level forecasting. *Hydrological Sciences Journal-Journal Des Sciences Hydrologiques*. 45, 523-536.

Sendrowski, A., Passalacqua, P. 2017. Process connectivity in a naturally prograding river delta. *Water Resources Research*, 53(3), 1841-1863.

SEPREM. 2022. Spanish association of dams and reservoirs. Disponible en: http://www.seprem.es/ (Consultado: 10 enero 2022).

Shiau, J.T., and Hsu, H.T. 2016. Suitability of ANN-based daily streamflow extension models: a case study of Gaoping River basin, Taiwan. *Water resources management*, 30, 1499-1513.

Shin, J.Y., Kwon, H., Lee, J.H., Kim, T. 2019. Probabilistic long-term hydrological drought forecast using Bayesian networks and drought propagation. *Meteorol.Appl.* 27(1), e1827.

Singh, V.P. 2011. Hydrologic Synthesis using Entropy Theory: Review. *Journal of Hydrologic Engineering*, 16(5), 421–433.

Singh, A., Imtiyaz, M., Isaac, R.K., Denis, D.M. 2012. Comparison of soil and water assessment tool (SWAT) and multilayer perceptron (MLP) artificial neural network for predicting sediment yield in the Nagwa agricultural watershed in Jharkhand, India. *Agricultural Water Management*, 104, 113-120.

Solana Dueso, J. El Agua como el primer principio: Las Razones de Tales de Mileto. CONVIVIUM, Núm. 22, 2009, p. 5-23.

Solans, M.A., Macian-Sorribes, H., Martínez-Capel, F., Pulido-Velazquez, M. 2023. Vulnerability assessment for climate adaptation planning in a Mediterranean basin. *Hydrological Sciences Journal*, 69:1, 21-45.

Spearman, C. 1904. The proof and measurement of association between two things. *The American Journal of Psychology*, 15, 72–101.

Sperotto, A., Molina, J.L., Torresan, S., Critto, A., and Marcomini, A. 2017. Reviewing Bayesian Networks potentials for climate change impacts assessment and management: A multi-risk perspective. *Journal of Environmental Management, Academic Press*, 202, 320–331.

Spirtes, P., Glymour, C., Scheines, R. 2000. Causation, Prediction, and Search. Adaptive Computation and Machine Learning. (2nd edition). MIT Press, Cambridge, Massachusetts, USA.

Spirtes, P. 2010. Introduction to Causal Inference. *Journal of Machine Learning Research*. 11, 1643-1662.

Srinivas, V.V., and Srinivasan, K. 2006. Hybrid matched-block bootstrap for stochastic simulation of multiseason streamflows. *Journal of Hydrology*. 329 (1–2), 1–15.

Srivastav, R.K., Srinivasan, K., Sudheer, K.P. 2011. Simulation-optimization framework for multi-season hybrid stochastic models. *Journal of Hydrology*, 404: 209-225.

Steck, H. 2001. Constraint-based structural learning in Bayesian networks using finite data sets. Ph.D. Thesis, Technische Universität München, Germany, 171 pp.

Stone, L. 2020. Causal inference in statistics: A primer. Perspectives on Information Fusion, 3(1), 27-35.

Suárez-Almiñana, S. 2021. Incorporación de las predicciones meteorológicas y climáticas en la planificación y gestión de las sequías. Aplicación a la Cuenca del Júcar. Ph.D. Thesis, Universitat Politècnica de València, Spain, 309 pp.

Suppes, P. 1970. A Probabilistic Theory of Causality. New York, NY, USA.

Sun, A.Y., Jiang, P., Mudunuru, M.K., Chen, X. 2021. Explore spatio-temporal learning of large sample hydrology using graph neural networks. *Water Resources Research*, 57(12), e2021WR030394.

Tan, M.L., Gassman, P.W., Liang, J., Haywood, J.M. 2021. A review of alternative climate products for SWAT modelling: Sources, assessment and future directions. *Science of the Total Environment*, 795, 148915.

TRASERO, 2015. Tratamiento y Gestión de Series Temporales Hidrológicas. Diputación Provincial de Alicante-Departamento de Ciclo Hídrico. Alicante, Spain, pp. 28–30. ISBN 978-84-15327-28-8.

Trenberth, K. 2011. Changes in Precipitation with Climate Change. *Climate Research*, 47(1–2), 123–138.

Tripathy, K.P. and Mishra, A.K. 2024. Deep learning in hydrology and water resources disciplines: Concepts, methods, applications, and research directions. *Journal of Hydrology*, 628, 130458.

Tyralis, H. and Koutsoyiannis, D., 2014. A Bayesian Statistical Model for Deriving the Predictive Distribution of Hydroclimatic Variables. *Clim. Dyn.* 42, 2867–2883. doi: 10.1007/s00382-013-1804.

UNFCCC, 2021. United Nations Framework Convention on Climate Change. Disponible: https://unfccc.int/sites/default/files/resource/2021%20-%20Comunicacion%20Adaptacion%20Espa%C3%B1a.pdf (Consultado: 10 diciembre 2023).

Valipour, M., Banihabib, M.E., Behbahani, S.M.R. 2012. Parameters Estimate of Autoregressive Moving Average and Autoregressive Integrated Moving Average Models and Compare their Ability for Inflow Forecasting. *J. Math. Stat.*, 8, 330–338.

Vasheghani Farahani, E., Massah Bavani, A. R., Roozbahani, A. 2025. Enhancing reservoir inflow forecasting precision through Bayesian Neural Network modeling and atmospheric teleconnection pattern analysis. *Stochastic Environmental Research and Risk Assessment*, 39(1), 205-229.

Vázquez-Fernández, M, López-Pérez, E. 1998. Mecánica para Ingenieros, estática y dinámica. 7th edn. Noela Publications, Madrid, Spain. ISBN 978-84-88012-04-3.

Venna, S.R., Katragadda, S., Raghavan, V., Gottumukkala, R. 2021. River stage forecasting using enhanced partial correlation graph. *Water Resources Management*, 35(12), 4111-4126.

Verma, T., and Pearl, J. 1991. Equivalence and synthesis of causal models. In Proceedings of the Sixth UAI Conference, UAI '90, pages 255–270, 1991.

Verma, T., and Pearl, J. 1992. An algorithm for deciding if a set of observed independencies has a causal explanation. In Uncertainty in artificial intelligence (pp. 323-330). Morgan Kaufmann.

Versini, P.A., Pouget, L., McEnnis, S., Custodio, E., Escaler, I. 2016. Climate change impact on water resources availability: case study of the Llobregat River basin (Spain). *Hydrological Sciences Journal*, 61(14), 2496-2508.

Vicente-Serrano, S.M., González-Hidalgo, J.C., de Luis, M., and Ravents, J. 2004. Drought patterns in the Mediterranean area. *Climate Research*, Inter-Research Science Center, 26(1), 5–15.

Vicente-Serrano, S.M., and Cuadrat-Prats, J.M. 2007. Trends in drought intensity and variability in the middle Ebro valley (NE of the Iberian peninsula) during the second half of the twentieth century. *Theoretical and Applied Climatology*, 88(3), 247–258.

Vogel, K., Riggelsen, C., Merz, B., Kreibich, H., and Scherbaum, F. 2012. Flood damage and influencing factors: A Bayesian network perspective. In Proceedings of the 6th European workshop on probabilistic graphical models (PGM 2012), University of Granada, 625, Granada, Spain, pp. 347-354.

Vogel, K., Riggelsen, C., Scherbaum, F., Schröter, K., Kreibich, H., and Merz, B. 2013. Challenges for Bayesian network learning in a flood damage assessment application. In G. Deodatis, B. R. Ellingwood, and D. M. Frangopol (Eds.), Safety, reliability, risk and life-cycle performance of structures and infrastructures. London: CRC Press, pp. 3123-3130.

Vogel, K., Riggelsen, C., Korup, O., and Scherbaum, F. 2014. Bayesian network learning for natural hazard analyses. *Natural Hazards and Earth System Science*, 14(9), 2605-2626. https://doi.org/10.5194/nhess-14-2605-2014.

Vogel, K., Weise, L., Schröeter, K., and Thieken, A.H. 2018. Identifying Driving Factors in Flood-Damaging Processes Using Graphical Models. *Water Resour.Res*. 54, 8864-8889.

Wang, W., Chau, K., Cheng, C., and Qiu, L. 2009. A Comparison of Performance of several Artificial Intelligence Methods for Forecasting Monthly Discharge Time Series. *Journal of Hydrology*, 374(3–4), 294–306.

Wang, Y., Yang, J., Chen, Y., De Maeyer, P., Li, Z., Duan, W. 2018. Detecting the causal effect of soil moisture on precipitation using convergent cross mapping. *Scientific reports*, 8(1), 12171.

Wasko, C., and Sharma, A. 2015. Steeper Temporal Distribution of Rain Intensity at Higher Temperatures within Australian Storms. *Nature Geoscience*, 8(7), 527-U166.

Wei, S., Zuo, D., Song, J. 2012. Improving prediction accuracy of river discharge time series using a Wavelet-NAR artificial neural network. *J.Hydroinf.* 14, 974-991.

Wikle, C. K., Berliner, L. M., and Cressie, N. 1998. Hierarchical Bayesian space-time models. *Environmental and Ecological Statistics*, 5, 117–154.

Wu, F., Zhan, J., Su, H., Yan, H., and Ma, E. 2015. Scenario-Based Impact Assessment of Land use/Cover and Climate Changes on Watershed Hydrology in Heihe River Basin of Northwest China. *Advances in Meteorology*, 410198.

Xue, J., Gui, D., Lei, J., Zeng, F., Mao, D., Zhang, Z. 2017. Model development of a participatory Bayesian network for coupling ecosystem services into integrated water resources management. *Journal of Hydrology*. 554, 50-65.

Yang, T., Gao, X., Sorooshian, S., and Li, X. 2016. Simulating California reservoir operation using the classification and regression-tree algorithm combined with a shuffled cross-validation scheme. *Water Resources Research*, 52(3), 1626–1651.

Yang, T., Asanjan, A.A., Faridzad, M., Hayatbini, N., Gao, X., and Sorooshian, S. 2017a. An Enhanced Artificial Neural Network with a Shuffled Complex Evolutionary Global Optimization with Principal Component Analysis. *Information Sciences*, 418, 302–316.

Yang, T., Asanjan, A.A., Welles, E., Gao, X., Sorooshian, S., and Liu, X. 2017b. Developing Reservoir Monthly Inflow Forecasts using Artificial Intelligence and Climate Phenomenon Information. *Water Resources Research*, 53(4), 2786–2812.

Zazo, S. 2017. Analysis of the Hydrodynamic Fluvial Behaviour through Causal Reasoning and Artificial Vision. Ph.D. Thesis, University of Salamanca, Ávila, Spain, 159 pp.

Zazo, S., Macian-Sorribes, H., Sena-Fael, C.M., Martín-Casado, A.M., Molina, J.L. and Pulido-Velazquez, M. 2019. Qualitative approach for assessing runoff temporal dependence through geometrical symmetry. (Contributed Paper). Proceedings Internacional Congress on Engineering. Engineering for Evolution (ICEUBI2019). 27 - 29 November 2019, Covilhã, Portugal.

Zazo, S., Molina, J.L., Ruiz-Ortiz, V., Vélez-Nicolás, M., García-López, S. 2020. Modeling River Runoff Temporal Behavior through a Hybrid Causal–Hydrological (HCH) Method. *Water*, 12, 3137.

Zazo, S., Molina, J.L., Macian-Sorribes, H. and Pulido-Velazquez, M. 2021a. Analysis of predictability of uncertain inflows to reservoirs. (Contributed Paper). Workshop ICSH STAHY 2021. International Association of Hydrological Sciences (IAHS) and the Research Institute of Water and Environmental Engineering (IIAMA) of the Universitat Politècnica de València. 16 - 17 September 2021, Valencia, Spain.

Zazo, S., Molina, J.L., Macian-Sorribes, H. and Pulido-Velazquez, M. 2021b. Advances in the analysis of the spatio-temporal properties of multivariate hydrological time series based on Information Theory. (Contributed Paper). Workshop ICSH STAHY 2021. International Association of Hydrological Sciences (IAHS) and the Research Institute of Water and Environmental Engineering (IIAMA) of the Universitat Politècnica de València. 16 - 17 September 2021, Valencia, Spain.

Zazo, S., Martín-Casado, A.M., Molina, J.L., Macian-Sorribes, H., and Pulido-Velazquez, M., 2022. Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework. *Journal of Hydrology*, 610 127832.

Zazo, S., Molina, J.L., Macian-Sorribes, H., Pulido-Velazquez, M. 2023. Assessment of the predictability of inflow to reservoirs through Bayesian Causality. *Hydrological Sciences Journal*, 68:10, 1323-1337.

Zhang, H., Wang, B., Li Liu, D., Zhang, M., Feng, P., Cheng, L., Eamus, D. 2019. Impacts of future climate change on water resource availability of eastern Australia: A case study of the Manning River basin. *Journal of Hydrology*, 573, 49-59.

Zhang, W., Liu, G., Chiaka, J.C., Yang, Z. 2023. Flood risk cascade analysis and vulnerability assessment of watershed based on Bayesian network. *Journal of Hydrology*, 626, 130144.

Zhang, W., Xu, P., Liu, C., Fang, H., Qiu, J., Zhang, C. 2024. Dynamic bayesian-network-based approach to enhance the performance of monthly streamflow prediction considering nonstationarity. *Water*, 16(7), 1064.

Zounemat-Kermani, and M., Teshnehlab, M. 2008. Using adaptive neuro-fuzzy inference system for hydrological time series prediction. *Applied soft computing*, 8(2), 928-936.

APÉNDICE I.
Índice de dependencia temporal (I-DT). Formulación

A partir de los resultados de la investigación Zazo et al., (2023), en este Apéndice se detallan los fundamentos matemáticos en los que se basa la formulación del "Índice de Dependencia Temporal (I-DT) " que se propone.

I-DT supone una innovación del "Índice de simetría" expuesto en Zazo et al., (2023), y al igual que éste, se obtiene a partir del Gráfico de Mitigación de la Dependencia (Dependece Mitigation Graph; DMG). Como se ha indicado anteriormente, este gráfico resume la propagación de la fuerza de la dependencia a lo largo del tiempo a través de toda la red bayesiana definida.

El hecho de que la propagación se lleve a cabo para cada una de las variables de decisión consideradas, gracias a la maximización del mayor intervalo *a priori* de la distribución de probabilidad discreta, permite disponer de una curva de mitigación de la dependencia temporal única para cada variable. Esta curva relaciona la dependencia temporal (variable independiente: "tiempo" expresado en forma de desfase temporal "lags"), con la fuerza de esa dependencia (variable dependiente: medida a través del "porcentaje relativo de cambio" producido en una variable "hija" conectada con otra "padre"; Molina et al., 2016). Este conjunto de curvas es sintetizado en el DMG por medio de las envolventes de propagación positiva (W-MAX) y negativa (W-MIN), envolventes que posteriormente son ajustadas a funciones matemáticas. Ambas funciones conjuntamente (su área total) definen la relación distintiva de la serie temporal en cuanto a su dependencia temporal y fuerza de esa relación, lo que constituye el comportamiento temporal general de los recursos hídricos en el punto analizado (Zazo et al., 2022,2023).

Aplicando el concepto de "centro de gravedad" al área total del DMG es posible definir un indicador de represente todas las "fuerzas de dependencia" que subyacen en la serie temporal analizada. Esta característica es la base para la definición del I-DT, y que permite resumir tanto la dependencia temporal como la fuerza de esa relación de dependencia de una serie temporal en un único indicador de dos componentes.

Basado en Vázquez-Fernández y López-Pérez (1998), y a partir de la definición del "Índice de simetría" de la investigación Zazo et al., (2023), el I-DT se expresa matemáticamente como:

$$A_{W-MAX} = \int_{0}^{TH_{W-MAX}} W - MAX \;;\; A_{W-MIN} = \int_{0}^{TH_{W-MIN}} W - MIN$$

$$A = A_{W-MAX} + |\, A_{W-MIN}|$$

$$X_{W-MAX} = \frac{1}{A_{W-MAX}} \int_{0}^{TH_{W-MAX}} W - MAX$$

$$Y_{W-MAX} = \frac{1}{2 \cdot A_{W-MAX}} \int_{0}^{TH_{W-MAX}} [W - MAX]^2$$

$$X_{W-MIN} = \frac{1}{A_{W-MIN}} \int_{0}^{TH_{W-MIN}} W - MIN$$

$$Y_{W-MIN} = \frac{1}{2 \cdot A_{W-MIN}} \int_{0}^{TH_{W-MIN}} [W - MIN]^2$$

$$X_{I-DT} = \frac{(X_{W-MAX} \cdot A_{W-MAX}) - (X_{W-MIN} \cdot A_{W-MIN})}{A}$$

$$Y_{I-DT} = \frac{(Y_{W-MAX} \cdot A_{W-MAX}) - (Y_{W-MIN} \cdot A_{W-MIN})}{A}$$

donde $A_{W\text{-}MAX}$ y $A_{W\text{-}MIN}$ son respectivamente las áreas positiva y negativa de las funciones W-MAX y W-MIN, $TH_{W\text{-}MAX}$ y $TH_{W\text{-}MIN}$ son los horizontes temporales de ambas funciones matemáticas (ver Zazo et al., 2023), A el área total del DMG, $X_{W\text{-}MAX}$, $Y_{W\text{-}MAX}$, $X_{W\text{-}MIN}$, $Y_{W\text{-}MIN}$ son las coordenadas del centro de gravedad de las áreas positiva y negativa $A_{W\text{-}MAX}$ y $A_{W\text{-}MIN}$, y finalmente $X_{I\text{-}DT}$ e $Y_{I\text{-}DT}$ los valores del índice propuesto. $X_{I\text{-}DT}$ indica la dependencia temporal de la serie, expresado en tiempo (escala anual y sub-anual), e $Y_{I\text{-}DT}$ representa la "fuerza" de la relación de dependencia expresada como "porcentaje relativo de cambio".

La interpretación del índice I-DT de una serie temporal sería la siguiente:

- Cuanto más se aleje la componente $X_{I\text{-}DT}$ del eje Y, mayor es la dependencia temporal de la serie analizada.
- Cuanto más próximo esté la componente $Y_{I\text{-}DT}$ del eje X, menor será la fuerza de la dependencia temporal en la serie considerada.

El análisis continuo que ofrece el DMG, gracias a la Causalidad Bayesiana, frente a los enfoques clásicos discretos, permite un mayor grado de detalle en la evolución de la dependencia temporal. Este hecho se pone de manifiesto en la disponibilidad de valores a escala temporal sub-anual. La Figura AI.1 muestra los valores de las componentes del I-DT basado en los resultados de la investigación Zazo et al., (2023).

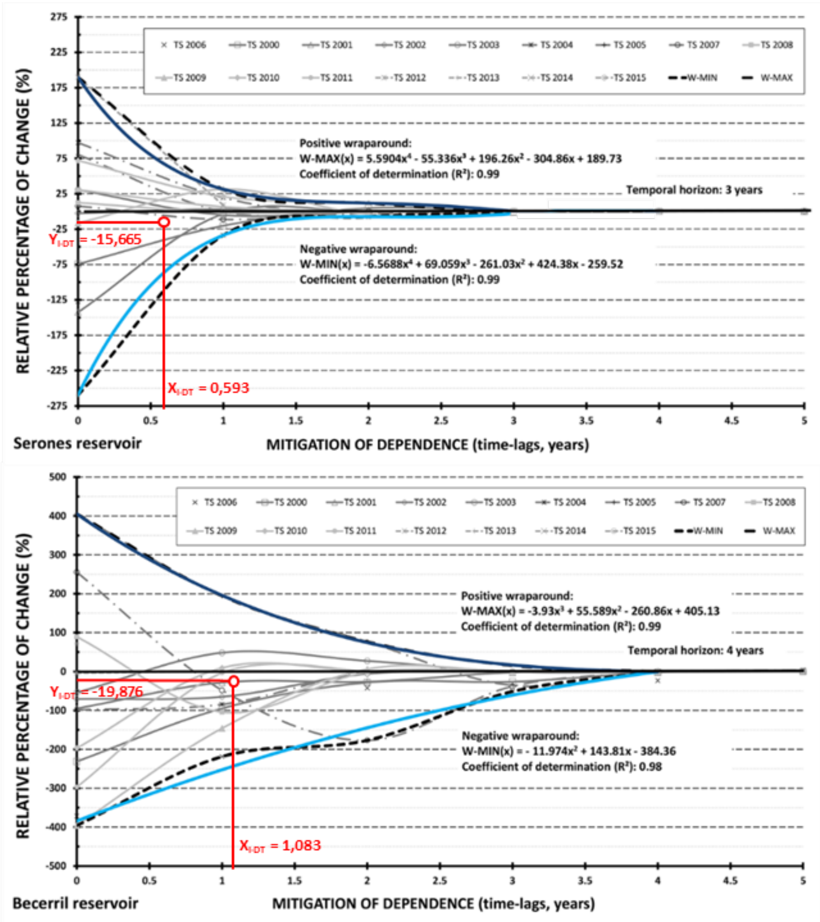


Figura AI.1: I-DT valores. Superior: Embalse de Serones. Inferior: Embalse de Becerril. Fuente de los gráficos DMG Zazo et al., (2023).

Para la validación del índice I-DT, dada su novedad, se acude a un análisis comparativo del orden temporal de las series analizadas mediante enfoques clásicos como el correlograma, y los métodos y criterios para la selección de modelos (Molina et al., 2016).

La Tabla AI.1 resume los resultados de la selección de modelos ARMA, basados en el criterio de información de Akaike, y llevado a cabo con el apoyo de la aplicación informática TRASERO ® (versión 2.3.0). Por su parte en la Tabla AI.2 se muestran los resultados del análisis comparativo de idoneidad de orden temporal de las series.

Tabla AI.1: Selección de modelos ARMA.

Casos de estudio	Modelo ARMA	Criterio de información de Akaike
Embalse de Serones	$p = 1$, $q = 0$	-5,359105
	$p = 1$, $q = 1$	-5,358764
	$p = 1$, $q = 2$	-5,358423
	$p = 1$, $q = 3$	-5,358082
	$p = 2$, $q = 0$	-5.358765
	$p = 2$, $q = 1$	-5,358423
	$p = 2$, $q = 2$	-5,358082
	$p = 2$, $q = 3$	-5,357741
	$p = 3$, $q = 0$	-5,358424
	$p = 3$, $q = 1$	-5,358082
	$p = 3$, $q = 2$	-5,357740
	$p = 3$, $q = 3$	-5,357399
Embalse de Becerril	$p = 1$, $q = 0$	-6,391680
	$p = 1$, $q = 1$	-6,391338
	$p = 1$, $q = 2$	-6,390996
	$p = 1$, $q = 3$	-6,390653
	$p = 2$, $q = 0$	-6,391338
	$p = 2$, $q = 1$	-6,390996
	$p = 2$, $q = 2$	-6,390655
	$p = 2$, $q = 3$	-6,390312
	$p = 3$, $q = 0$	-6,390997
	$p = 3$, $q = 1$	-6,390655
	$p = 3$, $q = 2$	-6,390314
	$p = 3$, $q = 3$	-6,389971

Tabla AI.2: Comparación de los análisis del orden temporal. Fuente: Figura IV.3 y Tabla IV.3 Zazo et al., (2023).

Casos de estudio	Correlograma	Selección de modelos	$X_{I\text{-}DT}$
Embalse de Serones	Independiente (0)	AR(*1*)	0,592
Embalse de Becerril	Lags 1 a 3 dependientes	AR(*1*) y AR(*2*)	1,083

Los valores obtenidos son concordantes, destacando la independencia del correlograma (0) para el caso del embalse de Serones y el valor de la componente X_{I-DT} de 0,592. En el caso del embalse de Becerril, los valores de los coeficientes de correlación r_1 a r_3 muestran valores semejantes y fuera de la zona de independencia del correlograma (ver Figura IV.3), lo que sería consistente tanto con la selección de modelos como con el valor de la componente X_{I-DT} de 1,083.

APÉNDICE II.
Índices de calidad de las revistas científicas

ÍNDICES DE CALIDAD DE LAS REVISTAS CIENTÍFICAS

Journal of Hydrology (Netherlands)

- Editorial: Elsevier.
- ISSN: 0022-1694.
- URL: https://www.sciencedirect.com/journal/journal-of-hydrology
- 5-year Impact Factor: 6.6.
- Impact Factor (2022): 6.4.
- Source Normalized Impact per Paper (SNIP-2022): 1.715.
- SCImago Journal Rank (SJR-2022): 1.670.
- H Index: 274.
- CiteScore (SCOPUS-2022): 10.4.
- Quartile (Journal Citation Reports-2022):

  Rank: 9/103 (Q1, First decile) Water Resources.
  13/139 (Q1) Engineering, Civil.
  15/202 (Q1, First decile) Geosciences, Multidisciplinary.
- Quartile (SCImago Journal Rank-2022):

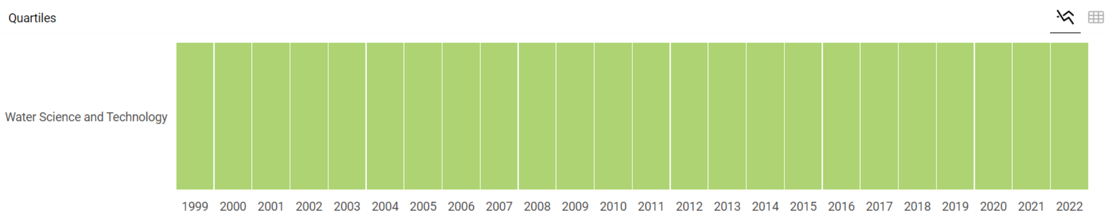
  Rank: (Q1) Water Science and Technology.
- Quartile (SCOPUS-2022):

  Rank: 14/248 (Q1, First decile) Water Science and Technology.
- Impact Factor (2021): 6.708.
- Source Normalized Impact per Paper (SNIP-2021): 1.83.
- SCImago Journal Rank (SJR-2021): 1.611.
- CiteScore (SCOPUS-2021): 9.1.
- Quartile (Journal Citation Reports-2021):

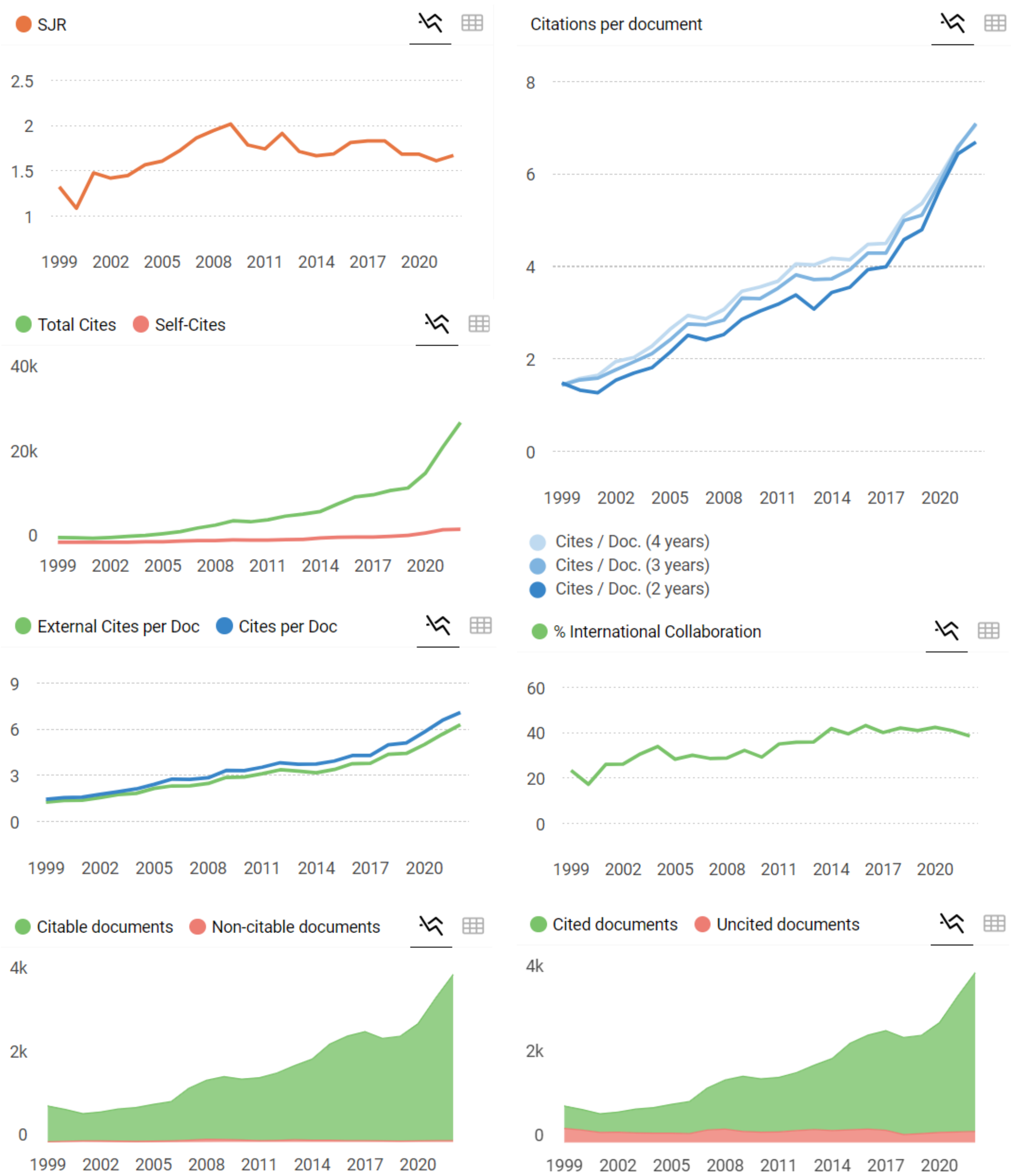
  Rank: 9/100 (Q1, First decile) Water Resources.
  11/138 (Q1) Engineering, Civil.
  13/202 (Q1, First decile) Geosciences, Multidisciplinary.
- Quartile (SCImago Journal Rank-2021):

  Rank: (Q1) Water Science and Technology.
- Quartile (SCOPUS-2021):

  Rank: 13/237 (Q1, First decile) Water Science and Technology.



Q1 (green). Q2 (yellow). Q3 (orange). Q4 (red).



Scimago Journal & Country Rank (http://www.scimagojr.com)
Note: "*k*" is expressed in thousands of documents or citations

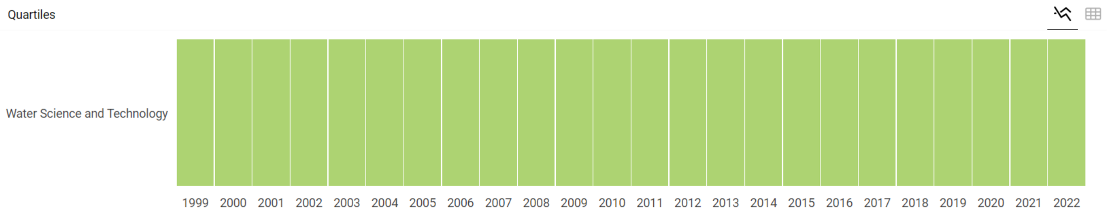
Hydrological Sciences Journal (England)

- Editorial: Taylor Francis Ltd.
- ISSN: 0262-6667.
- URL: https://www.tandfonline.com/journals/thsj20
- 5-year Impact Factor: 3.9.
- Impact Factor (2023): 2.8.
- Source Normalized Impact per Paper (SNIP-2023): 0.905.
- SCImago Journal Rank (SJR-2023): 0.778.
- H Index: 118.
- CiteScore (SCOPUS-2023): 6.6
- Quartile (Journal Citation Reports-2023):

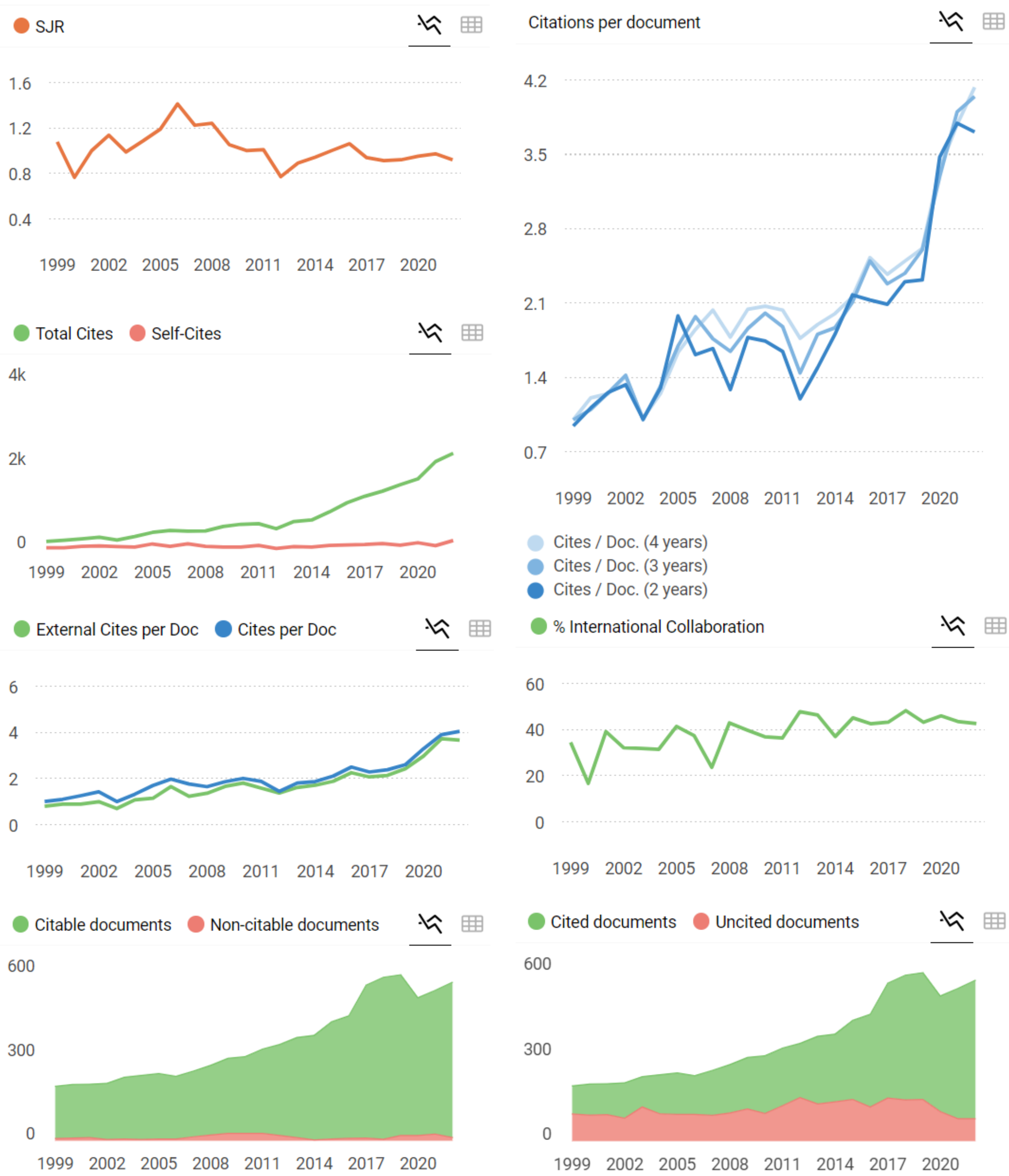
  Rank: 38/127 (Q2) Water Resources.
- Quartile (SCImago Journal Rank-2023):

  Rank: (Q1) Water Science and Technology.
- Quartile (SCOPUS-2023):

  Rank: 48/261 (Q1) Water Science and Technology.



Q1 (green). Q2 (yellow). Q3 (orange). Q4 (red).



Scimago Journal & Country Rank (http://www.scimagojr.com)
Note: “*k*” is expressed in thousands of documents or citations

APÉNDICE III.
Repercusión de las investigaciones

A continuación, se detalla el historial de los artículos científicos que constituyen esta Tesis Doctoral, y su repercusión científica internacional, hasta 31 de julio de 2025.

Publicación científica I

Analysis of spatio-temporal dependence of inflow time series through Bayesian causal modelling

HISTORIAL DEL ARTÍCULO

- Publicación: Journal of Hydrology. Enviado/aceptado 16 de agosto de 2020 / 29 de octubre de 2020. Publicación en línea: 5 de noviembre de 2020.
- Indexación Web of Science (WOS): 10 de junio de 2021.
  - Total, de citas recibidas / autocitas: 14 / 5.

INVESTIGACIONES DONDE SE HA CITADO LA PUBLICACIÓN

Chen, T., Zou, L., Xia, J., Liu, H., Wang, F. 2022. Decomposing the impacts of climate change and human activities on runoff changes in the Yangtze River Basin: Insights from regional differences and spatial correlations of multiple factors. *Journal of Hydrology*, 615, 128649.

Kang, M., Chen, D., Meng, N., Yan, G., Yu, W. 2024. Identifying Unique Spatial-Temporal Bayesian Network without Markov Equivalence. *IEEE Transactions on Artificial Intelligence*.

Minea, I., Albulescu, A.C. 2025. Drought Over Time: an Investigation of the Impact of Meteorological Drought on Groundwater and Surface Water in the East of Romania. *Earth Systems and Environment*, 1-23.

Molina, J.L., Patino-Alonso, C., Zazo, S. 2021. Hybrid Causal Multivariate Linear Modelling (H_CMLM) method for the analysis of temporal rivers runoff. *Journal of Hydrology*. 126501.

Molina, J.L., Espejo, F., Zazo, S., Molina, M. C., Hamitouche, M., García-Aróstegui, J.L. 2022. HydroPredicT_Extreme: A probabilistic method for the prediction of extremal high-flow hydrological events. *Journal of Hydrology*, 610, 127929.

Molina, J.L., García-Aróstegui, J. L. 2023. Water table prediction through causal reasoning modelling. *Science of the Total Environment*, 867, 161492.

Molina, J.L., Zazo, S., Espejo, F. 2025. Meta-water-modelling (Meta-WaM): A new framework for increasing applicability of digital water modelling. *Knowledge-Based Systems*, 318, 113543.

Ren, D., Hu, Q., Zhang, T. 2024. EKLT: Kolmogorov-Arnold attention-driven LSTM with transformer model for river water level prediction. Journal of Hydrology, 132430.

Sun, Q., Zheng, T., Zheng, X., Cao, M., Zhang, B., Jiang, S. 2023. Causal interpretation for groundwater exploitation strategy in a coastal aquifer. *Science of the Total Environment*, 867, 161443.

Wang, F., Bian, J., Zheng, G., Li, M., Sun, X., Zhang, C. 2023. A modelling approach to the efficient evaluation and analysis of water quality risks in cold zone lakes: a case study of Chagan Lake in Northeast China. *Environmental Science and Pollution Research*, 30(12), 34255-34269.

Wang, R., Ma, L., Ren, Y., Zhao, H., Zhou, L., Luo, L., ... He, G. 2025. Compact Temporal Causal Algorithm for Modeling Prediction in the Green Ammonia Production Process. *Chemical Engineering & Technology*, 48(5), e70016.

Zazo, S., Martín-Casado, A.M., Molina, J.L., Macian-Sorribes, H., and Pulido-Velazquez, M., 2022. Performance assessment of Bayesian Causal Modelling for runoff temporal behaviour through a novel stability framework. *Journal of Hydrology*, 610 127832.

Zazo, S., Molina, J.L., Macian-Sorribes, H., Pulido-Velazquez, M. 2023. Assessment of the predictability of inflow to reservoirs through Bayesian Causality. *Hydrological Sciences Journal*, 68:10, 1323-1337.

Zhu, Y., Yang, P., Xia, J., Huang, H., Chen, Y., Li, Z., ... Lu, X. 2024. Drought propagation and its driving forces in central Asia under climate change. *Journal of Hydrology*, 131260.

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INVESTIGACIONES DONDE SE HA CITADO LA PUBLICACIÓN

Beshavard, M., Adib, A., Ashrafi, S. M., Kisi, O. 2022. Establishing effective warning storage to derive optimal reservoir operation policy based on the drought condition. *Agricultural Water Management*, 274, 107948.

Molina, J.L., García-Aróstegui, J. L. 2023. Water table prediction through causal reasoning modelling. *Science of the Total Environment*, 867, 161492.

Zazo, S., Molina, J.L., Macian-Sorribes, H., Pulido-Velazquez, M. 2023. Assessment of the predictability of inflow to reservoirs through Bayesian Causality. *Hydrological Sciences Journal*, 68:10, 1323-1337.

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Molina, J.L., Zazo, S., Espejo, F., Patino-Alonso, C., Blanco-Gutiérrez, I., Zarzo, D. 2024. Risk Colored Snake (RCS): An Innovative Method for Evaluating Flooding Risk of Linear Hydraulic Infrastructures. *Water*, 16(3), 506.

Molina, J.L., Patino-Alonso, C., Espejo, F. 2025. Bayesian stochastic rainfall generator (BSRG): intelligent and digital tool for rainfall forecasting through bayesian causal modelling. *Water Resources Management*, 1-18.

Molina, J.L., Zazo, S., Espejo, F. 2025. Meta-water-modelling (Meta-WaM): A new framework for increasing applicability of digital water modelling. *Knowledge-Based Systems*, 318, 113543.