# Inverse Methods in Hydrogeology: Evolution and Recent Trends

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**Abstract**

Parameter identification is an essential step in constructing a groundwater model. The process of recognizing model parameter values by conditioning on observed data of the state variable is referred to as the inverse problem. A series of inverse methods has been proposed to solve the inverse problem, ranging from trial-and-error manual calibration to the current complex automatic data assimilation algorithms. This paper does not attempt to be another overview paper on inverse models, but rather to analyze and track the evolution of the inverse methods over the last decades, mostly within the realm of hydrogeology, revealing their transformation, motivation and recent trends. Issues confronted by the inverse problem, such as dealing with multiGaussianity and whether or not to preserve the prior statistics are discussed.
*Keywords:* Heterogeneity; parameter identification; data assimilation; uncertainty; groundwater modeling.

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## 1. Introduction

Mathematical modeling of subsurface flow and mass transport is needed, for instance, for groundwater resources management or for contaminant remediation. The forward model requires specification of a variety of parameters, such as, hydraulic conductivity, storativity and sources or sinks together with initial and boundary conditions. However, in practice, it is impossible to characterize the model exhaustively from sparse data because of the complex hydrogeological environment; for this reason, inverse modeling is a valuable tool to improve characterization. Inverse models are used to identify input parameters at unsampled locations by incorporating observed model responses, e.g., hydraulic conductivities are derived based on hydraulic head and/or solute concentration data. Deriving model parameters from model state observations is common in many other disciplines, such as petroleum engineering, meteorology and oceanography. This work mostly focuses on inverse methods used in hydrogeology.

### *1.1. The forward problem and the inverse problem*

The forward problem involves predicting model states, e.g., hydraulic head, drawdown and solute concentration, based on a prior model parameterization. Combining mass conservation and Darcy's laws, the forward groundwater flow model in an incompressible or slightly compressible saturated aquifer can be written as (Bear, 1972)

$$\nabla \cdot (K \nabla h) = S_s \frac{\partial h}{\partial t} + Q \tag{1}$$

subject to initial and boundary conditions, where $\nabla \cdot$ is the divergence operator $(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z})$, $\nabla$ is the gradient operator $(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})^T$, $K$ is hydraulic conductivity $[LT^{-1}]$, $h$ is hydraulic head $[L]$, $S_s$ is specific storage $[L^{-1}]$, $t$ is time $[T]$, and $Q$ is source or sink $[T^{-1}]$. The differential equation governing non-reactive transport in the subsurface is:

$$\phi \frac{\partial C}{\partial t} = -\nabla \cdot \big(qC\big) + \nabla \cdot \big(\phi \mathrm{D} \nabla C\big) \tag{2}$$

subject to initial and boundary conditions, where $C$ is the concentration of solute in the liquid phase $[ML^{-3}]$, $\phi$ is porosity [–], D is the local hydrodynamic dispersion tensor $[L^2T^{-1}]$ usually defined as $D_i = \alpha_i |q| + D_m$ where $\alpha_i$ refer to the longitudinal and transverse dispersivities $[L]$ and $D_m$ is the molecular diffusion coefficient $[L^2T^{-1}]$, and $q$ is the Darcy velocity $[LT^{-1}]$ given by Darcy's law as $q = -K\nabla h$.

The inverse problem aims at determining the unknown model parameters by making use of the observed state data. In the early days of groundwater modeling, it was common to start with a prior guess of the model parameters, run the forward model to obtain the simulated states, and then enter in a manual loop iteratively modifying the parameters, and then running the forward model, until observed and simulated values were close enough so as to accept the model parameter distribution as a good representation of the aquifer. This "trial and error" method falls into the scope of "indirect methods" as opposed to the "direct methods" which do not require multiple runs of the forward model to derive the model parameters (Neuman, 1973) as will be discussed below.

### *1.2. Why is the inverse problem necessary?*

Sagar et al. (1975) classified the inverse problem into five types according to the unknowns, i.e., model parameters, initial conditions, boundary conditions, sources or sinks and a mixture of the above. Most documented inverse methods fall into the first type, that is, they try to identify model parameters, which contribute largely to the model uncertainty due to the inherent heterogeneity of aquifer properties. Parameter identification is of importance considering the fact that no reliable predictions can be acquired without a good characterization of model parameters. Parameter identification is a broad concept here including not only the property values within facies but the facies distribution, or in other words, geologic features. The effect of geologic uncertainty in groundwater modeling is examined, for instance, by He et al. (2013) in a real case study. Furthermore, data scarcity deteriorates the characterization of the model parameters and raises the uncertainty. Besides estimating aquifer parameters, the inverse methods also play a critical role in assessment of uncertainty for the predictions. Furthermore, the inverse problem might be used as a guide for data collection and the design of an observation network. The reader is referred to Poeter and Hill (1997) who discussed the benefits of inverse modeling in depth. In this work we are mainly concerned with the uncertainty introduced by the unknown model parameters and thus the inverse methods that are used to characterize these parameters.

### *1.3. Why is the inverse problem difficult?*

A problem is properly posed if the solution exists uniquely and varies continuously as the input data changes smoothly. However, most of the inverse problems in hydrogeology are ill-posed and they cannot be solved unless certain assumptions and constraints are specified. Ill-posedness may give rise to three problems: non-uniqueness, non-existence and non-steadiness of the solutions, among which non-uniqueness is the most common. Non-uniqueness primarily stems from the fact that the number of parameters to be estimated exceeds that of the available observation data. Another reason is that the observations are sometimes not sensitive to the parameters to be identified; in other words, the information content of the observations is very limited. For instance, hydraulic heads close to the prescribed head boundaries are more influenced by the boundaries than by the nearby hydraulic conductivities (i.e., the hydraulic heads are not so sensitive to the conductivities), and on the contrary, the hydraulic heads close to the prescribed flux boundaries are determined to a large extent by the hydraulic conductivities nearby (Carrera and Neuman, 1986b).

A series of suggestions have been proposed to alleviate the ill-posedness:

1. Reduce the number of unknown parameters, e.g., using zonation, or collect more observation data so that the numbers of data and unknowns are balanced.
2. Consider the prior information or some other type of constraint to restrict the space within which parameters may vary.
3. Impose regularization terms to reduce fluctuations during the optimization iterations (Neuman, 1973).
4. Maximize the sensitivity of observations to model parameters, for instance, by designing properly the observation network.
5. Minimize the nonlinearity in the model equation. Carrera and Neuman (1986b) argued that working with the logarithm of hydraulic conductivity reduces the degree of non-convexity during optimization. An alternative is to infer hydraulic conductivity using fluxes rather than heads as done by Ferraresi et al. (1996), since the relationship between hydraulic conductivity and flux is linear (Darcy's law) while the relationship between hydraulic conductivity and head is nonlinear.

Detailed discussions on this subject can be found in Emsellem and De Marsily (1971), Neuman (1973), Carrera and Neuman (1986b) and McLaughlin and Townley (1996) among others.

Besides the ill-posedness problem, computational burden is the second main hurdle for inverse problems (Neuman, 2006). There are several reasons for the high CPU time requirement. Since many inverse models are iterative, the forward model has to be run many times until an acceptable parameter distribution is obtained. The time needed to run the forward model grows exponentially with the degree of discretization and the level of heterogeneity. When multiple realizations are sought, CPU demand grows with the number of realizations. For those methods that use gradient minimization, the sensitivity matrices of model variables on parameters are computed, which is very time consuming. A few measures to reduce computational demand have been proposed, for instance, (a) certain kernel techniques render it possible to select representative realizations from a large ensemble so that the size of the ensemble can be reduced (e.g., Scheidt and Caers, 2009; Ginsbourger et al., 2013); (b) upscaling can be performed prior to any forward simulation in order to reduce solution time (e.g., Tran et al., 2001; Li et al., 2012c; Myrseth et al., 2013); (c) use of parallel/distributed computing technologies (e.g., Tavakoli et al., 2013; Xu et al., 2013a); (d) use of efficient surrogate models to reduce the number of unknowns that must be computed at each time step, i.e., reduced-order flow modeling (e.g., He et al., 2012; Pau et al., 2013; Awotunde and Horne, 2011).

The problem of scales is the third difficulty to be confronted in the application of the inverse method. Measurements from boreholes (made in situ or in the laboratory), local pumping tests, and regional aquifer estimates are the three common scales (Dagan, 1986; Kitanidis and Vomvoris, 1983) at which information is handled in aquifer modeling. As Emsellem and De Marsily (1971) pointed out, "permeability is a parameter with no punctual value but with an average value in a region of a given size". The support of the permeability measured from the field is normally smaller than the cell size of the numerical model. In practice, permeability should be upscaled to a scale consistent with that of the numerical model discretization, otherwise the forward model would be computationally very expensive. A variety of approaches to calculate the upscaled permeability or hydraulic conductivity are available (e.g., Renard and Marsily, 1997; Sanchez-Vila et al., 2006; Wen and Gómez-Hernández, 1996; Zhou et al., 2010; Li et al., 2011). Besides, the scale inconsistency between field measurement support and numerical model discretization extends also to the observations, which can be obtained at different supports, too.

### *1.4. Outline of the paper*

Despite all sorts of difficulties, many inverse methods have been proposed to solve the inverse problem. In the present paper we do not intend to review all current inverse methods, since several others have reviewed the topic from different points of view (e.g., Carrera et al., 2005; De Marsily et al., 2000; McLaughlin and Townley, 1996; Oliver and Chen, 2010; Yeh, 1986). But rather, we would like to analyze the evolution of the inverse models, from the simple trial-and-error approaches of yesterday to the sophisticated ensemble Kalman filters of today, pointing out the incremental improvements that happened in the way.

In the remainder of this paper we mainly focus on seven key topics, as follows:

- Section 2.1 discusses the direct method. Then, in the following sections, we focus on the indirect approaches.
- Section 2.2 shows a linear inverse method in which the groundwater flow model is solved by linearizing the partial differential equation under certain assumptions. Its shortcoming motivates development of the nonlinear inverse methods in which the forward problem is solved numerically. The inverse methods in the remaining sections all belong to the nonlinear type.
- Section 2.3 highlights the importance of considering uncertainty and introduces the inverse method

based on Monte Carlo simulation in which multiple plausible realizations are used to represent the real system.

- Section 2.4 discusses sampling the posterior distribution rather than minimizing an objective function as the solution to the inverse problem.
- Section 2.5 focuses on integrating new observations sequentially without the need to reformulate the problem.
- Section 2.6 discusses whether the prior statistical structure of the model should be preserved through the inversion algorithm.
- Section 2.7 addresses the issue of multiGaussianity in inverse modeling and the difficulties to get away from it.

In each section, we will introduce a typical inverse method explaining its principle, implementation details, advantages and shortcomings. Recent trends of the inverse modeling are summarized in Section 3. The paper ends with some conclusions.

## 2. Evolution of inverse methods

Many approaches have been proposed to solve the inverse problem. Several comparison studies have been carried out to evaluate their performances, among them Zimmerman et al. (1998) and Hendricks Franssen et al. (2009) both compared seven different inverse methods. The former work focused on the transmissivity estimation and subsequent forecast of transport at the Waste Isolation Pilot Plant (WIPP). The latter used a different set of seven inverse methods to characterize well catchments by groundwater flow modeling. Some methods, such as the maximum likelihood method, the self-calibration method and the pilot point method were analyzed in both works. In this section we would like to track the evolution of inverse methods along with the objectives that cope with the pitfalls of the inverse methods.

### *2.1. Direct or indirect approach?*

Inverse methods fall into two groups: direct ones and indirect ones (Neuman, 1973). Nowadays, only indirect methods are considered; however, it was the direct method that, somehow, gave rise to the indirect one. The move from direct methods to indirect ones would be the first major evolution in solving the inverse problem, and for this reason we start this analysis by recalling the direct method and why it had to be discarded in favor of the indirect one.

The forward problem of groundwater flow can be expressed as $F(K) = h$, where $F(\cdot)$ is an equation such as Equation 1 relating the system parameters (e.g., hydraulic conductivity $K$) to the model responses (e.g., hydraulic head $h$). The forward problem requires that model parameters be known over the entire domain. In such a case, the inverse problem can be simply formulated as $K = F^{-1}(h)$, provided, that $h$ is known exhaustively. (The boundary conditions, source and sink terms could also be identified if necessary (Sagar et al., 1975).)

Although the theory is straightforward, it is virtually impossible to obtain a realistic solution by solving the algebraic equations resulting after the discretization of the inverse equation due to the serious ill-posedness and the singularity of the matrices involved in the numerical formulation (Sun, 1994). Some modifications were proposed to cope with these difficulties, such as, considering more equations than there are unknowns to build an over-determined system so that the effect of measurement errors is reduced (Ponzini and Lozej, 1982); or, imposing a constraint on the objective function, which converts the inverse problem into a linear programming problem (Kleinecke, 1971; Neuman, 1973) or a minimization problem (Navarro, 1977).

The main shortcoming of the direct method is that it requires that piezometer heads have been measured at all nodes of the discretized domain, and for it to yield stable results, head measurements are needed everywhere for several orthogonal boundary conditions in the sense explained by Ponzini and Lozej (1982).

It is worthwhile mentioning that, recently, Brouwer et al. (2008) proposed a direct approach called the "double constraint method" to determine permeability. Although it is not strictly a direct method, since it does not require having observations extensively over the entire domain, the final step of the method, computing the permeabilities, uses a direct approach. The method assumes that pairs of pressure/flow rates are available at a number of points in the domain. A guess of the spatial distribution of the permeabilities is made and two forward runs are performed, the first one considers the measured pressures as prescribed boundary conditions (disregarding the flow rate data), the second one uses the flow rates as prescribed boundary conditions (disregarding the pressure data), then the prior permeability guess is forgotten and new permeabilities are computed "directly" at each block interface using the pressure gradients derived from the first run and the flow rates derived from the second one. The process is repeated, and eventually the spatial distribution of permeabilities converges to a stable one. The method was compared in a synthetic example with the results obtained by the ensemble Kalman filter yielding good results. Another direct inverse method was proposed recently (Irsa and Zhang, 2012), in which the hydraulic conductivity is determined using steady-state flow measurements with unknown boundary conditions. In this method the groundwater flow equation is solved analytically using a Trefftz-based approximation, then a collocation technique enforces the global flow solution. The method is mainly applied on homogenous aquifers and also on heterogeneous aquifers with a known prior distribution of hydraulic conductivities.

The virtual impossibility of having state observation data over the entire domain gave rise to the indirect methods capable of handling limited numbers of observations. In the following, only indirect methods are discussed.

### *2.2. Linearization or not?*

Kitanidis and Vomvoris (1983) proposed the geostatistical approach (GA) as a very clever way to reduce the number of unknown values and subsequently mitigate the ill-posedness problem. Conductivities are not the subject of the identification problem, but rather the parameters of the variogram that describe the spatial correlation of the conductivities. Once the variogram has been identified, conductivities are interpolated by kriging onto the model cells.

The procedure of the GA can be summarized into two main parts: structure analysis and linear estimation. Structure analysis consists of three steps as follows:

1. Select a geostatistical model, e.g., decide a variogram function and whether the model is stationary or not. The model structure is selected based on all available information.
2. Estimate the parameters characterizing the model structure such as trend (if any), variance and correlation ranges. The joint probability function of log-permeability and head is assumed multiGaussian, and the hydraulic heads are expressed as a linear function of log-permeability, after linearizing Equation 1. Then, the parameters of the geostatistical model (generally no more than five) are estimated through maximum likelihood. The Gauss-Newton method is used to solve the iterative maximization of the likelihood function.
3. Examine the validity of model. The estimated structure is either accepted or modified during the test (i.e., the variogram function is changed, or anisotropy is introduced).

As soon as the geostatistical model is accepted, the log-permeability field is estimated by cokriging, a best linear unbiased estimation algorithm, which is capable of providing estimations with minimum error variance. Later, Dagan (1985) and Rubin and Dagan (1987) proposed an extension of the GA using Bayesian conditional probabilities.

The advantages of the GA reside in two main aspects. First, it reduces the number of the effective parameters to be estimated by introducing the concept of random function into the inverse problem. In this way, the ill-posedness is alleviated since (a) the number of unknown values is far less than the number of observations and (b) the estimated parameters are independent of grid discretization. Second, this method is computationally efficient arising from two facts: hydraulic head is obtained by a first-order approximation of the flow equation instead of numerically solving it; a linear estimation (cokriging) is applied as soon as the geostatistical structure is identified with no iterative optimization involved, saving CPU time to a large extent. The method was first verified on a one-dimensional test and found stable and well-behaved (Kitanidis and Vomvoris, 1983).

Despite the several advantages of this method, we have to mention some shortcomings. First, the approximation of the hydraulic head after linearizing the flow equation is only valid if the log-conductivity exhibits a small variance. Hoeksema and Kitanidis (1984) alleviated this problem by applying the method to a two-dimensional isotropic confined aquifer in which hydraulic heads are obtained by solving numerically the partial differential equation, and then Kitanidis (1995) further generalized it onto a quasi-linear approach, which was applied to condition on concentration data in a steady-state flow by Schwede and Cirpka (2009). Second, the final conductivity map is obtained by kriging, this has two implications: first, and most important, the final maps are smooth since they represent an ensemble expected value of the random function model, and therefore cannot represent a real aquifer, and second, since kriging only uses the covariances for the estimation, as soon as the heads cannot be approximated as a linear combination of the conductivities, the solution of the flow equation in the final conductivity maps will not honor the measured piezometric heads.

The need to apply the inverse model to hydraulic conductivity spatial distributions with large heterogeneity forced moving from the linearized approaches to other approaches in which this linearization is not necessary. The inverse methods involved in the following sections do not apply linearization of the forward problem.

### *2.3. Deterministic estimation or stochastic simulation?*

A typical example of nonlinear inverse approaches is the maximum likelihood method (MLM) developed by Carrera and Neuman (1986a). The method is able to estimate simultaneously such parameters as hydraulic conductivity, specific storage, porosity, dispersivity, recharge, leakage and boundary conditions by incorporating head and concentration measurements as well as prior information (Medina and Carrera, 1996). Zonation is employed to reduce the number of parameters to be estimated, that is, hydraulic conductivities are assumed constant or vary gradually over large patches of the aquifer, thus, the number of unknowns is proportional to the number of patches. Then, the groundwater problem (Equation 1, or 2 or both) is solved numerically subject to initial and boundary conditions. Let $x$ be a vector of all the unknown parameters, $y_i^{obs}$ be a vector of available measurements of type $i$ and $y^{obs}$ be a vector with all measurements of all types, a set of optimum parameter estimates is obtained by maximizing the likelihood $L(x \mid y^{obs})$. Under the hypothesis that all the data could be transformed to jointly follow a multiGaussian distribution, the likelihood function can be expressed as follows:

$$L(x \mid y^{obs}) \propto exp\{-\frac{1}{2}\sum_{i=1}^{N_m}(y_i - y_i^{obs})^T C_{y,i}^{-1}(y_i - y_i^{obs})\} \tag{3}$$

where $y_i$ is a vector of computed model states (e.g., head and concentration), $C_{y,i}$ is the corresponding covariance of observation errors and $N_m$ is the number of types of measurements. Maximizing $L(x \mid y^{obs})$ is equivalent to minimizing $-2\ln(L)$, and the optimization problem turns to minimizing the objective function:

$$J = \sum_{i=1}^{N_m}(y_i - y_i^{obs})^T C_{y,i}^{-1}(y_i - y_i^{obs}). \tag{4}$$

Iterative minimization algorithms are applied on the objective function until certain convergence criteria are met. The uncertainty of parameter estimates is evaluated by a lower bound of the covariance matrix. Note that a regularization term can be included in the objective function above in order to ensure stability of the optimization problem (Medina and Carrera, 1996). The objective function becomes then

$$J = \sum_{i=1}^{N_m}(y_i - y_i^{obs})^T C_{y,i}^{-1}(y_i - y_i^{obs}) + (x - x^{pri})^T C_x^{-1}(x - x^{pri}) \tag{5}$$

where $x^{pri}$ is the prior model parameter vector and $C_x$ is the covariance of $x$.

One of the important features of using zonation is that the number of unknown parameters is reduced significantly so that the potential ill-posedness problem is circumvented to some extent. Furthermore, the MLM might be used as a conceptual model identification tool, i.e., to identify the best model structure among several alternatives; in this respect, Carrera (1987) argued that the criterion KIC proposed by Kashyap (1982) is the most effective. Recently Riva et al. (2011) demonstrated the discriminatory power of KIC numerically concluding that the Bayesian model quality criterion KIC is well suited for the estimation of statistical data- and model-parameters in the context of nonlinear maximum-likelihood geostatistical inverse problems.

However, some limitations of the MLM are apparent. Although the zonation scheme does help to reduce the number of the unknowns, it causes over-smoothness, i.e., inherently heterogeneous geologic properties are represented by a few patches of homogeneous conductivities, and at the same time the zonation scheme may introduce unacceptable discontinuities between zones. Although it is also true that the maximum likelihood formulation could also be used to estimate a posterior covariance map that could be used, together with the estimated map to generated stochastic realizations. Furthermore, some zone discretizations may cause bias, depending on the number of zones and measurements (Kitanidis, 1996). Also, as stated earlier, the objective function is constructed under the assumption of a multinormal distribution, i.e., the prior residuals and estimates follow a multiGaussian distribution. The implications of this assumption will be discussed further in Section 2.7.

The MLM was probably the first widely successful inverse method, it could incorporate many types of observations, it included a regularization term to prevent wide fluctuations during the optimization phase, and, because it did not use any approximation for the relationship between the state variables and the aquifer parameters, it yielded a zoned map of hydraulic conductivities that reproduced very well the observed data. However, the MLM method produced a single map, too smooth to really describe the heterogeneity observed in nature.

Small scale variability had already being identified as one of the important factors controlling aquifer response. Recognizing this, De Marsily et al. (1984) developed the pilot point method (PiPM) as a procedure to introduce more variability into an aquifer model obtained by kriging interpolation. Starting from a kriging map of the hydraulic conductivities, smooth as all kriging estimation maps are, De Marsily et al. (1984) position a fictitious datum where no observation exists, and assigns to it a value so that when kriging is performed again with this new datum, the new kriging map provides a better approximation to the observed piezometric head data. New pilot points are introduced sequentially into the model until there is enough heterogeneity in the model so as to reproduce the observed head data. This procedure had several advantages: the aquifer could be discretized at any scale, since after each iteration, (block) kriging was performed on the entire aquifer; the heterogeneity was consistently treated throughout the process, since the same variogram model was used for all kriging estimations; and, because of the way the procedure is implemented, the fictitious data introduced at the pilot points were always within the local limits of variability of the variable as induced by the underlying random function model. The PiPM was successfully applied to model the Culebra formation overlying the Waste Isolation Pilot Plan (WIPP) (Cooley and Hill, 2000; LaVenue et al., 1995; RamaRao et al., 1995, 2000). The main problem of the PiPM was still that, at the end, there was only a single representation of the aquifer, a single kriging map that, although more heterogeneous than the kriging map computed from the conductivity data alone, still was too smooth.

Moreover, the PiPM has been criticized recently by Rubin et al. (2010) stating that first it uses prior as a constraint rather than a starting point of parameter identification; second, it causes instability and artifacts of the generated field. Alternatively Rubin et al. (2010) present the anchored distribution method, and subsequently Murakami et al. (2010) and Chen et al. (2012) applied this method for three-dimensional aquifer characterization at the Hanford 300 Area.

An estimated map, let it be obtained by kriging, maximum likelihood or Bayesian conditional probabilities, is an average map, and the average does not necessarily represent reality. The same way that the average outcome of throwing a dice (3.5) does not correspond to any of the dice face pips, the average of an ensemble of potential realizations, does not correspond with any realization. The smooth fields obtained by these methods fail to reflect the local spatial variability and will necessarily fail in properly predicting mass transport (e.g., Gómez-Hernández and Wen, 1994).

It is then when the self-calibrated method is proposed (SCM) and the concept of inverse stochastic modeling starts being considered. The idea is not to seek a single smooth representation of the spatial variability of hydraulic conductivity capable of reproducing the observed piezometric head and/or concentration data, but to generate multiple realizations, all of which display realistic patterns of short scale variability, all of which reproducing the observed piezometric head and/or concentration data. In the scope of the stochastic inverse methods, non-uniqueness is not anymore a problem but an advantage, since all alternative solutions to the inverse problem are considered likely realizations of the aquifer heterogeneity, and all solutions are treated as an ensemble of realizations that must be further analyzed to make uncertainty-qualified predictions.

The concept of the SCM was first outlined by Sahuquillo et al. (1992) and then elaborated by Gómez-Hernández et al. (1997) accompanied with two applications and an implementation program (Capilla et al., 1997, 1998; Wen et al., 1999). The SCM is based on the PiPM with the following rationale: instead of starting from a kriging map and introducing local perturbations by adding fictitious pilot points, let's start from multiple realizations generated by a conditional simulation algorithm; and instead of identifying the optimal location of the next pilot point and introducing them sequentially, locate what Gómez-Hernández et al. (1997) call "master points" all at once (as many as two or three per correlation length) and determine the values of the perturbations in a single optimization step. Master point locations can be randomly selected and vary at different iterations. To understand the SCM, one has to recall that a conditional realization is the sum of a conditional mean (kriging map) plus a correlated residual map (Journel, 1974), what SCM does is to apply the pilot point method with multiple points at once to modify the conditional mean with the objective that the new conditional mean plus the correlated residuals would match the observation data. By applying this optimization approach to all the realizations of an ensemble, the SCM is capable of generating multiple realizations, all of which are conditional to the state observation. Thus, it comes the term inverse stochastic modeling.

With such an ensemble of realizations, it was possible to make transport predictions in each of the realizations and collect all of these predictions to build a model of prediction uncertainty based on realistic realizations.

It was soon realized that the concept of the SCM could be implemented in the original PiPM, and it has been applied multiple times since then (e.g., Alcolea et al., 2006, 2008; Lavenue and De Marsily, 2001).

Gómez-Hernández et al. (2003) reviewed stochastic conditional inverse modeling showing the strengths of SCM. The SCM was extended to incorporate concentration data (Hendricks Franssen et al., 2003; Wen et al., 2002a) for the characterization of hydraulic conductivity, and also to incorporate breakthrough data of both reactive and nonreactive data to characterize the spatial variability of the sorption coefficient (Huang et al., 2004). Recently, genetic algorithms have been coupled with the SCM to search for the optimal locations of the master points as well as the optimal perturbation at these locations (Wen et al., 2005, 2006); Hendricks Franssen et al. (2008) applied SCM to integrate the pattern information from remote sensing images; Heidari et al. (2012) coupled SCM with ensemble Kalman filter to assimilate the dynamic data in real-time; Li et al. (2013a) applied the master points concept of the SCM into the ensemble pattern matching method that have a capability to preserve the geologic structures as well as the static and dynamic data (Li et al., 2013b).

The MLM, the PiPM and the SCM are closely related in that they follow a very similar perturbation and updating scheme. The update process for the PiPM is illustrated in "Figure 1" of RamaRao et al. (1995) and in "Figure 1" of Alcolea et al. (2006). For the sake of completeness and comparison, we graphically show a sketch of the updating algorithm for all the three methods (Figure 1). In the MLM, it is as if there is a pilot point in each zone, and the perturbation in the pilot point extends uniformly constant over the entire zone, in the PiPM, the pilot point perturbation dies out with the correlation length of the random function model, and in the SCM, the perturbation of the entire field is obtained by kriging the perturbations in each master point. All three methods seek finding those perturbations that added to the initial guess will result in a new field that is conditional to the observed state data.

It is worth to point out that the widely used program PEST (Doherty, 2004), a model-independent nonlinear parameter estimation program, which is also based on the minimization of an objective function, could be framed in the family of PiPM-based methods. In this approach, the regularized inversion is commonly used when the model has many different parameters or when a number of models are simultaneously simulated (e.g., Hunt et al., 2007; Fienen et al., 2009; Doherty and Hunt, 2010). In the pilot point implementation of the

PEST code, parameters are estimated at the predefined pilot point locations and then spatial interpolation is used to complete the field; then, a regularization term is included in the penalty function to control the stability and uniqueness of the solution of a highly parameterized model (Hunt et al., 2007). The truncated singular-value decomposition and Tikhonov regularization (i.e., hybrid subspace) schemes (Tonkin and Doherty, 2005) have been proposed and integrated into this approach, which was subsequently extended to account for the uncertainty of estimated parameter within a Monte Carlo framework in the so-called subspace Monte Carlo technique (Tonkin and Doherty, 2009; Yoon et al., 2013). Note that, Moore and Doherty (2005) and Moore and Doherty (2006) show that the regularized inversion method produces fields relatively smoother or simpler than the true conductivity field. Clearly, this regularized inversion method, like the PiPM, only optimizes a few parameters (simple model) in the groundwater flow model, which is commonly insufficient for transport predictions such as travel times that require a higher level of system detail, as demonstrated in the case study by Moore and Doherty (2005). As a consequence, optimization of the whole aquifer, with millions of degrees of freedom (complex model), in a stochastic framework is warranted. The issue of simplicity versus complexity in model conceptualization has already been subject of debate between hydrogeologists (e.g., Hunt and Zheng, 1999; Hunt et al., 2003; Gómez-Hernández, 2006; Hill, 2006; Haitjema, 2006; Hunt et al., 2007; Renard, 2007).

An alternative to the Monte Carlo approach within the framework of maximum likelihood is a moment equation based inverse algorithm as proposed by Hernandez et al. (2003, 2006). Optimum unbiased estimates of model states such as hydraulic head and flux are obtained by their first ensemble moments. Additionally the approach is able to provide the second order moments which can be used to measure the estimate uncertainty of model parameters and states. The moment equation inverse algorithm is applied at the Montalto Uffugo research site (Italy) by Janetti et al. (2010). The method has been extended from steady state flow to transient flow (Riva et al., 2009) and from model state prediction to model parameter identification (Riva et al., 2011). Compared with the SCM, the moment equation method is computationally efficient but it only provides a single smooth estimate of the random functions in that it utilizes the conditional mean as the estimate.

### *2.4. Minimization or sampling?*

Up to here all inverse methods discussed are based on the minimization of an objective function that measures the mismatch between the simulated state and the observed values. However, there are alternative ways to achieve the same results without resorting to an optimization problem, but rather to sampling a multivariate probability distribution.

Suppose that model parameter $x$ is characterized by a multiGaussian distribution with mean $\mu$ and variance $C_x$, $x \sim N(\mu, C_x)$, with a prior probability density given by

$$\pi(x) \propto exp\{-\frac{1}{2}(x-\mu)^T C_x^{-1}(x-\mu)\}. \tag{6}$$

Assuming that the discrepancies between observed state variables $y^{obs}$ and their corresponding model simulations $y^{sim} = F(x)$ is also multiGaussian with error covariance $C_y$, the joint probability distribution of $y^{obs}$ given $x$ is,

$$\pi(y^{obs} \mid x) \propto exp\{-\frac{1}{2}(y^{obs} - F(x))^T C_y^{-1}(y^{obs} - F(x))\}. \tag{7}$$

Using Bayes' theorem, the posterior distribution of $x$ given the observations $y^{obs}$ can be written as

$$\begin{aligned}\pi(x \mid y^{obs}) &= \frac{1}{c}\pi(x) \cdot \pi(y^{obs} \mid x) \\ &\propto exp\{-\frac{1}{2}(x-\mu)^T C_x^{-1}(x-\mu) - \frac{1}{2}(y^{obs} - F(x))^T C_y^{-1}(y^{obs} - F(x))\}\end{aligned} \tag{8}$$

with $c$ being a normalization constant. The Markov chain Monte Carlo method (McMC) (Hastings, 1970; Metropolis et al., 1953; Oliver et al., 1997) is suitable for drawing samples from the posterior conditional distribution $\pi(x \mid y^{obs})$. If a sufficiently large chain is generated following the procedure described below, the chain will converge so that its members will be drawn from the posterior conditional distribution. The procedure of McMC is the following (Robert and Casella, 2004)

1. Initialize the first realization $x$.
2. Update $x$ according to the Metropolis-Hastings rule:
   - Propose a candidate realization $x^*$ conditional on the last realization by drawing from the transition kernel $x^* \sim q(x^* \mid x)$.
   - Accept the candidate $x^*$ with probability $\min\{1, \alpha\}$ and

$$\alpha = \frac{\pi(x^* \mid y)}{\pi(x \mid y)} \cdot \frac{q(x \mid x^*)}{q(x^* \mid x)}. \tag{9}$$

3. Loop back to the second step.

The two critical points on the McMC method are the selection of the transition kernel $q(x^* \mid x)$ and how to compute the acceptance probability $\alpha$. The first attempt to apply the McMC in hydrogeology is by Oliver et al. (1997) who generated permeability realizations conditioned to variogram and pressure data using a local transition kernel. This local kernel only modifies a single cell in the realization of $x$ when making the transition from $x$ to $x^*$. Such a localized perturbation, specially if the aquifer discretization is large, makes the method quite slow, since after each proposal there is a need to evaluate the state equation (groundwater flow model) and to decide whether the proposal is accepted or not. If the transition kernel is global, producing a new realization which changes in every cell of the aquifer, the probability that the candidate is rejected is quite high. An alternative is to use a block kernel in which the proposed realizations differs from the previous one only over a certain region inside the aquifer (Fu and Gómez-Hernández, 2009b). The so-called blocking McMC gives better results than either the local or global transition kernels. If, in addition, the evaluation of the state of the system, for the purposes of computing the acceptance probability, is made on a coarse scale with the aid of upscaling, and only the high acceptance probability members are submitted to the fine scale evaluation, the convergence rate of the chain will be improved.

As mentioned, the McMC is not an optimization algorithm, it aims at generating multiple independent realizations by sampling from the posterior parameter distribution conditioned on the observations. It is also important to notice that, since the posterior distribution is built from the prior parameter distribution, the realizations generated are consistent with the prior model. We will return later to the issue of whether it is important or not to preserve the prior model structure throughout the inversion process in Section 2.6.

The original McMC is computationally demanding since each proposed realization is subject to forward simulation that involves solving a partial differential equation over a large domain and, possibly, a long time period. Furthermore, these proposed realizations are not necessarily accepted, which generally requires that a large number of candidate realizations have to be generated and evaluated. A lot of work has been devoted to increase the efficiency of McMC by means of increasing the acceptance rates or reducing the dimensionality of the forward simulation. A "limited-memory" algorithm has been used to accelerate sampling using low-dimensional jump distributions (Kuczera et al., 2010). A two-stage McMC has been proposed to improve the efficiency of McMC (Dostert et al., 2009; Efendiev et al., 2009), in which fine scale simulations are performed only if the proposal at the coarse scale is accepted. Another drawback of McMC is related with the low mixing speed of the chain, in other words, the McMC should sample from the entire posterior distribution, but it takes quite a long chain until this happens (Fu and Gómez-Hernández, 2009b,a; Romary, 2010).

### *2.5. Real time integration or not?*

The trajectory of inverse modeling up to here shows quite a large evolution from the initial methods. At this stage, there are still two main problems. The first, and most important one, is CPU requirements; the second is the need to reformulate the problem from the beginning if new data in space or time are collected.

Inverse stochastic modeling supposed a big leap in aquifer characterization, but, in essence, it was equivalent (from a computational point of view) to performing inverse modeling seeking a single best estimate, but as many times as realizations were needed. It was necessary to find an alternative capable of generating multiple conditioned realizations of conductivity in a more efficient manner. If this could be achieved, it would be interesting that as new data are collected, as it happens in any monitoring network, the newly collected piezometric heads or concentrations could be incorporated into the inverse model naturally without any modification of the algorithm. The ensemble Kalman filter (EnKF) is an example of such methods capable of it (Evensen, 1994; Burgers et al., 1998).

The EnKF is based on the Kalman filter, a data assimilation algorithm for systems in which the relation between model parameters and states is linear (Kalman, 1960). This linearity renders an exact propagation of the covariance with time. However, the equations depicting groundwater and solute transport model are nonlinear (Equations 1 and 2), which prevents the computation of the covariance evolution in time. As a solution to this problem, the extended Kalman filter was proposed, the nonlinear function is approximated linearly by a Taylor-series expansion and this linearization is used for covariance propagation. The problem with the extended Kalman filter is that the covariance approximation deteriorates as time passes, especially in highly heterogeneous fields for which the Taylor-series approximation is poor. The method is also very time-consuming when the aquifer is finely discretized (Evensen, 2003).

The EnKF circumvents the problem of covariance propagation in time by working with an ensemble of realizations. The forward problem is solved on each realization, and the ensemble of resulting states is used to compute the covariance explicitly. This is one of the reasons that the EnKF is computationally efficient. Another reason resides in that the EnKF is capable of incorporating the observations sequentially in time without the need to store all previous states nor the need to restart groundwater simulation from the very beginning.

The theory and numerical implementation of the EnKF is described extensively in Evensen (2003, 2007). Here we will only recall the basics of the EnKF. The EnKF deals with dynamic systems, for which observed data are obtained as a function of time and used to sequentially update the model. The joint state vector $x_i$, for realization $i$, including both the parameters controlling the transfer function and the state variables, is given by:

$$x_i = \begin{pmatrix} A \\ B \end{pmatrix}_i = \begin{pmatrix} (a_1, a_2, \ldots, a_N)^T \\ (b_1, b_2, \ldots, b_N)^T \end{pmatrix}_i \tag{10}$$

where $A$ is the vector of model parameters such as hydraulic conductivities and porosities, and $B$ is the vector with the state variables such as hydraulic heads and concentrations. The size of the state vector ensemble $\mathbf{x}$ is determined by the number of grid cells in which the domain has been discretized ($N$) and the number of realizations in the ensemble ($N_r$), i.e., $\mathbf{x} = (x_1, x_2, \ldots, x_{N_r})$. Note that the boldface indicates the vector ensemble.

The EnKF consists of two main steps: forecast and update. The forecast step involves the transition of the state vector from time $t-1$ to time $t$, i.e., $\mathbf{x}_t = F(\mathbf{x}_{t-1})$, where $F(\cdot)$ is the transfer function. Normally this transfer function leaves the model parameters unchanged and forecasts the state variables to the next time step using the groundwater model (Equations 1 and/or 2). After observation data are collected the state vector is updated by Kalman filtering:

$$\mathbf{x}_t^u = \mathbf{x}_t^f + \mathbf{G}_t(\mathbf{y}_t^{obs} + \varepsilon - \mathbf{H}\mathbf{x}_t^f), \tag{11}$$

where $\mathbf{x}_t^u$ is the joint vector ensemble with the updated states at time $t$ and $\mathbf{x}_t^f$ is the vector ensemble with the forecasted states; $\mathbf{y}_t^{obs}$ is the observation at time $t$; $\varepsilon$ is an observation error with zero mean and covariance $\mathbf{R}$; $\mathbf{G}_t$ is the Kalman gain, derived after the minimization of a posterior error covariance,

$$\mathbf{G}_t = \mathbf{P}_t^f\mathbf{H}^T(\mathbf{H}\mathbf{P}_t^f\mathbf{H}^T + \mathbf{R})^{-1}, \tag{12}$$

it multiplies the residuals between observed and forecasted values to provide an update to the latter; $\mathbf{H}$ is the observation matrix; $\mathbf{P}_t^f$ is the ensemble covariance matrix of the state $\mathbf{x}_t^f$ computed through

$$\mathbf{P}_t^f \approx \frac{1}{N_r - 1}(\mathbf{x}_t^f - \bar{\mathbf{x}}_t^f)(\mathbf{x}_t^f - \bar{\mathbf{x}}_t^f)^T, \tag{13}$$

where $\bar{\mathbf{x}}_t^f$ is the ensemble mean, $\bar{\mathbf{x}}_t^f \approx \frac{1}{N_r}\sum_{i=1}^{N_r} x_{t,i}^f$; and $x_{t,i}^f$ is a realization of the ensemble of state vectors. It is worth noting that we do not have to compute the whole covariance matrix explicitly because we can compute directly $\mathbf{P}_t^f\mathbf{H}^T$ and $\mathbf{H}\mathbf{P}_t^f\mathbf{H}^T$ taking advantage of the fact that most of the entries of $\mathbf{H}$ are zeroes.

Most inverse methods need to store the previous states when conditioning to new observed data, and the forward simulation has to be restarted from the initial time until the time when the new observation data are collected. On the contrary, the EnKF is able to assimilate the real time observation data storing only the latest state. Once the updating is done, the forward model is run from the last time step, and the assimilated observation data can be discarded. A new forecast is performed, new data collected, and updated repeated. This is one of the reasons why the EnKF is computationally efficient. The sequential data assimilation scheme of the EnKF is shown in Figure 2. The EnKF has been widely applied as a data assimilation tool in diverse disciplines such as oceanography, meteorology and hydrology (e.g., Bertino et al., 2003; Chen and Zhang, 2006; Houtekamer and Mitchell, 2001; Moradkhani et al., 2005; Nowak, 2009; Wen and Chen, 2006).

Notice that the EnKF is neither an optimization method nor a sampling one, it is a data assimilation filter based on the minimization of a posterior covariance. For this reason, the EnKF is optimal when parameter and states are linearly related and follow a multiGaussian distribution (Evensen and Leeuwen, 2000). However, in hydrogeology, hydraulic conductivity is likely not to be properly modeled as multiGaussian, and even if it were, the states (heads and concentrations) would never be linearly related to the parameters or propagate in time with a linear transfer function. Some work has been done attempting to circumvent the problem of nonGaussianity, but this issue will be discussed later in Section 2.7.

Besides the issue of multiGaussianity, some disadvantages related with the EnKF include: (a) underestimation of model variability, especially when the ensemble size is small and the parameter field is highly heterogeneous; (b) non-physical and spurious update of state vectors. These disadvantages can lead to filter inbreeding or divergence. To address this problem, several regularization strategies are proposed such as covariance inflation (Anderson, 2007), distance-based covariance localization (Chen and Oliver, 2010; Nan and Wu, 2011), adaptive localiztion with wavelets (Chen and Oliver, 2012), the use of damping factors (Hendricks Franssen and Kinzelbach, 2008) and the application of the confirming approach (Wen and Chen, 2006). Wen and Chen (2007) addressed some practical issues in applying EnKF, such as non-linearity via iteration, the selection of initial models, and non Gaussianity.

The EnKF has been successfully applied for building geological models conditioned on piezometric head data (e.g., Chen and Zhang, 2006; Hendricks Franssen and Kinzelbach, 2008; Hendricks Franssen and Kinzelbach, 2009; Kurtz et al., 2012; Panzeri et al., 2013; Xu et al., 2013a,b). With regard to conditioning on concentration data, Huang et al. (2009) applied the EnKF to update a conductivity field by assimilating both steady-state piezometric head and concentration data; Liu et al. (2008) simulated multiple parameters (e.g., hydraulic conductivity, dispersivities, mobile/immobile porosity) for the MADE site; Li et al. (2012a) applied EnKF to jointly calibrate hydraulic conductivity and porosity by conditioning on both piezometric head and concentration data in a fully transient flow; Schöniger et al. (2012) assimilated the normal-score transformed concentration data to calibrate conductivities. Jafarpour and Tarrahi (2011) assessed the performance of EnKF in subsurface characterization accounting for uncertainty in the variogram.

### 2.6. *Preserve prior structure or not?*

The inverse methods based on optimization attempt to minimize the deviation between predicted states and observation data, disregarding, sometimes, the prior model used to generate the initial guess fields from which the optimization starts. Kitanidis (2007) stated that "the degree of data reproduction is a poor indicator of the accuracy of estimates" questioning whether seeking the best reproduction of the observed data justifies any departure from the prior model. There has been some debate on whether the prior model structure should be preserved through the inverse modeling process, or, on the contrary, the optimization process may allow the final set of realizations to depart (drastically) from the original model as driven by the need to reproduce the observed states. The best option, probably, lies in between; the prior model should be taken into account and should be used as a regularization element, while the new data should allow to introduce some deviations on the prior model when this is the only way to approximate them. In this respect, Neuman (1973) proposed the multiple-objective algorithm in which the model parameters are constrained not only by the minimization of the reproduction error but also by a physical plausibility criterion. A similar strategy is used by Carrera and Neuman (1986a) and Medina and Carrera (1996) in the MLM method, in which prior information is combined into the likelihood functions, or by Alcolea et al. (2006) in the PiPM, in which a regularization term is added to the objective function.

There are methods which, by construction, will produce realizations consistent with the prior model structure, such as the McMC, in which the prior model is implicitly built into the definition of the posterior conditional probability distribution from which the chain of realizations is drawn.

There are two other methods that, by construction, will preserve the prior model during the inversion process, thus ensuring that the parameter distributions are physically plausible at the end of the inversion process: the gradual deformation method (GDM) and the probability perturbation method (PrPM).

The GDM method, as initially proposed by Hu (2000), is based in the successive linear combination of pairs of realizations. A single parameter controls this linear combination, the value of which is computed by a simple optimization procedure. The optimal value produces a linear combination that improves the reproduction of the observed state. In addition, if both realizations are multiGaussian with the same mean and covariance it is easy to show that, after the linear combination, the resulting realization will also be multiGaussian with the same mean and covariance. This pairwise combination is repeated until an acceptable match to the observed data is attained. This simple, but extremely effective, approach, which only worked for multiGaussian fields was soon extended to work with other random function fields in conjunction with sequential simulation algorithms. In sequential simulation algorithms, each node of the realization is visited sequentially, a random number is drawn and a nodal value is obtained from the local conditional distribution, which has been computed accordingly to the random function model. There are sequential simulation algorithms to generate multiGaussian realizations (e.g., Gómez-Hernández and Journel, 1993), realizations with arbitrary indicator covariance functions (e.g., Gómez-Hernández and Srivastava, 1990) or realizations based on the multiple-point patterns derived from a training image (e.g., Strebelle, 2002). In all cases, it all reduces to mapping a set of independent uniform random numbers into a realization of correlated values using as a transfer function the local conditional probabilities computed according to Bayes' rule. When the GDM is applied to generate realizations of independent uniform random numbers, the resulting realizations will always be consistent with the prior random function model, which was used to compute the local conditional probabilities.

The attractiveness of GDM is that each iteration is a simple optimization step, and that it preserves the prior spatial structure. The GDM algorithm can be summarized as follows:

1. Generate two independent Gaussian white noises, $z_1$ and $z_2$, with zero mean and unit variance. The two noises are combined to form a new Gaussian white noise vector $z$ with zero mean and unit variance according to

$$z = z_1 \sin(\rho\pi) + z_2 \cos(\rho\pi) \tag{14}$$

   where $\rho$ is a deformation parameter ranging from -1 to 1. If $\rho = 0$, $z$ is the same as $z_2$ and if $\rho = 1/2$, $z$ is the same as $z_1$. Note that more than two noises could be combined to increase the convergence rate (Ying and Gomez-Hernandez, 2000; Le Ravalec-Dupin and Noetinger, 2002).

2. The random vector $z$, is transformed into a uniform white noise vector $u = G^{-1}(z)$, with $G(\cdot)$ being the Gaussian cumulative distribution function, and $u$ is used with a geostatistical sequential simulation algorithm to yield a realization $x$, $x = S(z)$.

3. Run the forward model $F(\cdot)$ (e.g., Equation 1) on the generated property realization to obtain the simulated model responses, such as flow rates and hydraulic heads.

4. An objective function measuring the mismatch between the simulated model response and the observed data is built as

$$J(\rho) = \sum_{i=1}^{n} \omega_i (F(x(\rho))_i - F(x(\rho))_i^{obs})^2. \tag{15}$$

   where $\omega_i$ is a weight and $n$ is the number of observed data.

5. Minimize the objective function to obtain the optimal $\rho$, and update the random vector $z$.

6. The updated random vector $z$ will replace the previous $z_1$ and will be combined with a newly generated

vector $z_2$ to construct a new random vector. Then loop back to the second step until all the observed data are matched up to some tolerance.

The drawback of the GDM is related to the convergence rate. Le Ravalec-Dupin and Noetinger (2002) found that the convergence rate is strongly influenced by the number of realizations which are combined in each iteration. Caers (2003) proposed an efficient gradual deformation algorithm by coupling the traditional GDM, multiple point geostatistics and a fast streamline-based history matching method with the aim to reduce CPU demand for parameter identification in highly heterogeneous reservoir. Another criticism to GDM has been whether it generates realizations spanning the entire space of variability coherent with the observed data; in this respect, Liu and Oliver (2004) assessed the performance of the GDM through a one-dimensional experiment; after comparison of the GDM with other inverse methods, such as the McMC, they concluded that the GDM is able to produce reasonable distributions of permeability and porosity. Wen et al. (2002b) compared the SCM and a specific variant of GDM that they call geomorphing applied to a binary aquifer (sand/shale).

Another method that attempts to preserve the prior structural model is the probability perturbation method (Caers, 2003). The probability perturbation is also based on the sequential simulation algorithm, therefore, it will preserve the random function model that is implicit to the algorithm used. Given a fixed random path to visit the nodes of the aquifer, a fixed set of random numbers, and a fixed set of conditional probability distributions, the PrPM will freeze the random numbers and perturb the conditional probability distributions in order to achieve the match to the observed data. Recall that the GDM freezes the probability distributions and modifies the random numbers. The perturbation of the conditional probabilities is performed by means of a single parameter $r_D$ that is subject to optimization. This parameter can be interpreted as the degree of perturbation needed to apply to the seed realization in order to match the state data, if $r_D$ is close to zero, the actual realization gives a good reproduction of the state data and there is no need to change anything, if $r_D$ is close to one, the current realization is far from matching the observation data and there is a need to generate another realization independent of the previous one, any value in between would generate a realization that represents a transition between these two independent realizations. Caers (2007) compared the performances of the GDM and the PrPM in several simple examples from such aspects as preservation of prior structure and accuracy of posterior sampler.

The PrPM method has been extended to allow different perturbations in different geological zones of the aquifer, that is, $r_D$ is allowed to vary piecewise within the aquifer according to pre-defined zones (Hoffman and Caers, 2005). The PrPM was initially applied to categorical variables, and later it was extended to continuous ones (Hu, 2008). Hoffman et al. (2006) applied PrPM in a real oil field. The PrPM has been mostly used in petroleum engineering although recently it has been applied in groundwater modeling, e.g., combined with a multiple-point geostatistical method to locate high permeability zones in an aquifer (Ronayne et al., 2008).

Before Caers proposed the PrPM, the idea of perturbing probabilities had already been proposed by Capilla et al. (1999) although in a slightly different context. They used the concept of the SCM method, but instead of working with the conductivity values directly, they transformed these conductivity values onto cumulative probabilities using the local conditional probability distributions obtained by kriging (the probability field of Froidevaux (1993)). The type of kriging used could be indicator kriging and could incorporate soft conditioning data, and therefore, the spatial structure associated to such type of kriging would be preserved through the optimization process. Once the probabilities had been computed, the SCM method would be applied to seek the best spatial distribution of probabilities that when backtransformed onto conductivities would result in the best match to the observed state data. Later, to improve its efficiency, the optimization step of the probability fields was combined with the GDM by Capilla and Llopis-Albert (2009).

The problem associated to theses latter methods is: what if the prior model is not correct? What if the prior model implies an isotropic spatial correlation, but, in reality conductivities are highly anisotropic with channels of high permeability and quasi impermeable barriers? Some studies have analyzed the impact of a wrong a priori model choice, for instance, Kerrou et al. (2008) applied the SCM method on a fluvial sediment aquifer in a steady-state flow with a wrong prior model (i.e., multiGaussian instead of non-multiGaussian) and concluded that the channel structures cannot be retrieved, even when a large number of direct and indirect data are used for conditioning; Freni and Mannina (2010) analyzed the impact of different a priori hypotheses and found that improper assumptions could lead to very poor parameter estimations; Li et al. (2012b) and Xu et al. (2013b) assessed the performance of normal-score EnKF (NS-EnKF) in a transient flow in non-multiGaussian media and they argued that, if the monitoring net was designed properly, the localized NS-EnKF was able to identify the channel structure even when an erroneous prior random function model was used. A possible solution to account for the prior model uncertainty is to use multiple prior models as done by Suzuki and Caers (2008) although at a very large computational demand.

### *2.7. MultiGaussian or not?*

Ever since the publication of the seminal paper on stochastic hydrogeology by Freeze (1975), hydraulic conductivity has been assumed to follow a univariate lognormal distribution. His assumption was based on experimental data, and it was later corroborated by Hoeksema and Kitanidis (1985) who analyzed the histogram and covariance of hydraulic conductivity data from 31 regional aquifers to conclude that, indeed, hydraulic conductivity is best modeled by a logGaussian histogram. However, there are still many cases, such as aquifers in fluvial deposits, in which several highly contrasting facies coexist and in which conductivities are better characterized by a multimodal distribution. Multimodal distribution also applies when one lumps data in a single sample and tries to homogenize a composite medium (Winter et al., 2003). But, the most important issue is not whether the histogram of the conductivities is normal or not, after all, it is always possible to apply a normal-score transformation to the data so that the transformed data follows a Gaussian histogram; the most important issue is whether the best model to characterize the spatial continuity of hydraulic conductivity is the multiGaussian model or not. Applying a normal-score transform to the data will render them univariate normal, but it does not imply that the higher-order moments (the ones controlling the continuity of the extreme values, or the curvilinear arrangements of some conductivity values) should follow a multiGaussian model.

The nonGaussian models have been explored for some time (e.g., Rubin and Journel, 1991; Gómez-Hernández and Wen, 1998; Journel and Deutsch, 1993; Woodbury and Ulrych, 1993; Zinn and Harvey, 2003; Kerrou et al., 2008; Renard and Allard, 2011), and the dangers of using a multiGaussian model in aquifers with high continuity of extreme values were already exposed by Journel and Deutsch (1993) and Gómez-Hernández and Wen (1998).

Of all the methods discussed, all of those which are based on the minimization of the sum of square deviations have a tendency to generate multiGaussian realizations, even if the seed realizations prior to the start of the inverse procedure are nonGaussian. Basically, all methods that use only moments up to the order two (covariance) in their formulation will behave in this way as a consequence that the multiGaussian distribution is the only one fully characterized by a mean value and a two-point covariance function. This is the case of the GA, the SCM, the PiPM, or the MLM. Even the EnKF, which only uses the ensemble derived covariance to update the realizations after each data collection stage, will end up with realizations with a multiGaussian flavor even if the initial ensemble is not.

Some of the methods discussed can handle non-multiGaussian patterns of variability, such as the McMC, the GDM or the PrPM. It is apparent that those methods that can benefit from techniques such as multiple point geostatistical simulation, which can generate realizations of conductivity with realistic patterns according to a training image (Mariethoz, 2009), are very promising. There have been some attempts to modify the EnKF to handle non multiGaussian ensembles. For example, Zhou et al. (2011, 2012b) proposed to transform both the parameter and state variables from non-multiGaussian to Gaussian ones through normal-score transformation, and then perform the updating of transformed variables using EnKF; Sun et al. (2009) coupled EnKF with Gaussian mix models to handle the nonGaussian conductivity realizations; Sarma and Chen (2009) developed a kernel EnKF to handle the connectivity of conductivity based on multiple point statistics; Jafarpour and Khodabakhshi (2011) suggested to update the mean of ensemble conductivity realizations and then use this mean as soft data to regenerate the updated model using multiple point statistics; Hu et al. (2012) proposed to update the uniform-score random number that is used to draw the local conditional probability in the multiple point statistics, using the EnKF; Zhou et al. (2012a) and Li et al. (2013b) presented an ensemble pattern matching method, which is an update of EnKF method by using the multiple point statistics (i.e., pattern) to quantify the correlation between parameter and state variables instead of the two-point statistics (i.e., mean and covariance), and thus it has a capability to handle dynamic data integration in the complex formations such as the fluvial depositions; Li et al. (2013b) further improved the computational efficiency by coupling ensemble pattern matching method with the master points concept of SCM method.

### *2.8. Evolution of inverse approaches to date*

Table 1 summarizes the inverse methods discussed so far. As time has passed, inverse models have, sequentially, gotten away from the linearization of the state equation, become stochastic, attempted to preserve the prior structure (or at least introduce some controls which will give the prior structure information some weight during the inverse modeling process), and become capable of handling non-multiGaussian realizations. In our opinion the best inverse model should be the one that is stochastic, is capable to deal with multiple sources of state data governed by a complex state equation, is not limited to multiGaussian realizations, can weight in prior information, and can generate multiple realizations in an efficient manner. At the same time we have to mention that some preliminary methods in the evolution of the inverse modeling are revisited and modified to propose new approaches, for instance, a variant of the direct method (Irsa and Zhang, 2012) and a zonation-kriging method (Tsai, 2006).

## 3. Recent trends of inverse methods

The methods discussed so far have already been thoroughly tested and their advantages and pitfalls are well known. In the last few years, new issues have been brought into the inverse model formulation that we would like to mention next.

### *3.1. Integrating multiple sources of information*

Direct measurements of parameters of interest (usually known as "hard data") represent the first constraint that the model must meet. These data are easily handled by standard geostatistic methods (Deutsch and Journel, 1998). Then, there are soft data, that is, indirect measurements of the parameters. Recent developments in physical and geophysical techniques provide indirect measurements that are non-linearly related to the parameter of interest and that should be used also to constrain our aquifer model. Examples of these techniques are ground-penetrating radar (Dafflon et al., 2009; Kowalsky et al., 2004), time-lapse electrical resistivity (Irving and Singha, 2010), 4D-seismic (Le Ravalec-Dupin, 2010), spatial altimetry (Getirana, 2010), and remote sensing (Brunner et al., 2007; Hendricks Franssen et al., 2008). It is worth noting that certain techniques (e.g., remote sensing) are able to provide information over a large area rather than at quasi-point scale. Besides the hard and soft (geo)physical measurements, state data other than hydraulic heads or flow rates should be used to infer aquifer parameters, for instance peak concentration arrival times (Bellin and Rubin, 2004) or groundwater ages (Sanford, 2010).

Two other types of data have been used to identify aquifer structure, i.e., water table fluctuations due to tides, and connectivity data. Tidal induced water table fluctuations carry information about the aquifer properties in coastal aquifers. Head fluctuations have been used to identify possible preferential flow paths between the sea and the coastal aquifer (Alcolea et al., 2007; Park et al., 2011; Slooten et al., 2010). The other rarely applied constraint is connectivity, which is found to play a critical role in transport modeling. In a synthetic example, Zinn and Harvey (2003) demonstrated how the same conductivity values when rearranged in space to induce different connectivity patterns have very different flow and transport behavior. Some indicators has been proposed to measure the connectivity (e.g., Knudby and Carrera, 2005, 2006; Le Goc et al., 2010), and some attempts to include connectivity information in inverse modeling have been carried out (Alcolea and Renard, 2010; Renard et al., 2011).

### *3.2. Combining high order moments*

To include curvilinear features in the spatial distribution of the hydraulic conductivities amounts to go beyond the two point covariance (a second-order moment) and to account for high order moments. A possible approach is with multiple point geostatistics (Guardiano and Srivastava, 1993; Strebelle, 2002). We have already discussed how the GDM and the PrPM take advantage of the sequential simulation methods based on multiple point geostatistics to generate inverse conditional realizations following the patterns extracted from a training image (such as the one in Figure 3). An alternative avenue is the use of spatial cumulants

(Mustapha and Dimitrakopoulos, 2010). Other examples include those by Alcolea and Renard (2010) who proposed a block moving window algorithm taking advantage of multiple point simulations, Mariethoz et al. (2010) who proposed an iterative resampling algorithm, and Zhou et al. (2012a) and Li et al. (2013b) who presented an ensemble pattern matching inverse method.

### *3.3. Handling multiscale problem*

Observation data may be available at different support scales. If the aquifer model is discretized very fine to characterize the extreme heterogeneity of the geological parameters, it can be computationally impossible to solve a stochastic inverse problem as we stated in the Section 1.3. On the contrary if the model discretization is coarse in order to integrate the coarse scale observation data, it might lose some small scale but important features of the aquifer. A scale balance must be reached. Some authors have combined upscaling and inverse modeling to address the scale problem. For instance, upscaling is introduced into the McMC and forms a block McMC method (Fu and Gómez-Hernández, 2009b; Fu et al., 2010); upscaling is combined with EnKF to assimilation coarse scale observations and at the same time honor the small scale properties (Li et al., 2012c; Li and Ren, 2010); a multiresolution algorithm is proposed by applying regression in the space of wavelet transformation (Awotunde and Horne, 2011).

### *3.4. Parameterizing the conductivity field*

Reducing the number of unknowns of a heterogeneous conductivity field (i.e., parametrization) remains an active research area in inverse modeling. This approach usually consists of two steps: (a) reconstruct the hydraulic conductivity field using a relatively small number of parameters, (b) and then apply an optimization method in the new parameterized space. The purpose of parameterizing the conductivity field is apparent: to mitigate the ill-posedness in the inverse modeling.

The covariance-based principal component analysis (PCA) or the Karhunen-Loeve expansion are commonly used to represent the geological model in a reduced space for the multiGaussian media, (e.g., Oliver, 1996; He et al., 2012). Jafarpour and McLaughlin (2009) introduced a discrete cosine transformation to parameterize the conductivity field. Sarma et al. (2008) developed a kernel PCA to parameterize, not the covariance, but multiple point statistics of the conductivity field. In this approach, the high-dimensional data is transformed into a feature space by defining a kernel transformation function, and the parametrization is accomplished in the corresponding kernel feature space; a model is obtained by transforming back from the feature space to the model space (i.e., pre-image problem), which raises another non-linear optimization problem in this process (e.g., Borg and Groenen, 2005; Scheidt et al., 2011; Park, 2011). Li and Jafarpour

(2010) proposed to use discrete wavelet transform to reconstruct the conductivity field. Bhark et al. (2011) developed a generalized grid-connectivity based parametrization method to integrate dynamic data into geological models. More recently, there is a set of papers dealing with the reconstruction of conductivity field by using sparse representatives and dictionaries (e.g., Khaninezhad et al., 2012a,b; Elsheikh et al., 2013).

### *3.5. Assessing the uncertainty of prediction*

Ensemble based inverse methods have a capability to assist assessing the uncertainty of prediction that is routinely required by the decision maker. Any method based on Bayes' theorem definitely is able to model a posterior probability. Examples of this method include traditional reject sampling (Von Neumann, 1951), iterative spatial resampling (Mariethoz et al., 2010) and McMC-based methods (Oliver et al., 1997; Fu and Gómez-Hernández, 2009b; Alcolea and Renard, 2010). All the methods mentioned above could be formulated as resampling methods and are extremely computational expensive due to the iterative evaluation of the forward simulation on thousands of conductivity realizations. On the contrary, minimization-based methods, such as the EnKF and the pattern-search based method (e.g., Zhou et al., 2012a; Li et al., 2013b) are computational efficient and are able to assess the uncertainty of predictions using updated ensemble conductivities. However, both methods work with ensembles of realizations what implies that a large ensemble size is commonly required, resulting in a high computational cost, too.

## 4. Conclusions

We have given an overview of the evolution of inverse methods in hydrogeology, i.e., how the algorithms have evolved during the last decades to solve the inverse problem, from direct solutions to indirect methods, from linearization to non-linearization of the transfer function, and from single estimate to stochastic Monte Carlo simulation. Furthermore, we consider a few issues involved in solving the inverse problem, e.g., whether the multiGaussian assumption is appropriate and whether the prior structure should be honored. Inverse models have gone a long way since their inception, and they keep evolving with the aim of improving aquifer characterization while, at the same time, respecting all the information and data available.

Overall, the development of inverse methods shows some features:

- The goal of inverse problem is not just parameter identification, but also improved predictions.
- Stochastic inverse methods are becoming the trend for the generation of multiple realizations, which will serve to build a model of uncertainty on both parameters and states.

- There is a need for methods that are capable to generate geological models as diverse as possible while matching observed data to ensure that the uncertainty in the predictions is properly captured.
- Multiple sources of observations are integrated in the inverse modeling, multiple scale problems are handled and multiple new algorithms are introduced into the inverse modeling, for instance, multiple point geostatistics and wavelet transform.

**Acknowledgements.** The authors gratefully acknowledge the financial support by the Spanish Ministry of Science and Innovation through project CGL2011-23295. We would like to thank Dr. Alberto Guadagnini (Politecnico di Milano, Italy) for his comments during the reviewing process, which helped improving the final paper.

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Table 1: Details of the inverse methods mentioned in the paper. The attributes of each inverse method are reported based on its most popular implementation.

| | Linearization | Stochastic | Structure preservation | Gaussian assumption | M or S[1] | References[2] |
|---|---|---|---|---|---|---|
| Direct method | | | | | | |
| | Yes | No | No | - | M | Navarro (1977) |
| Indirect method | | | | | | |
| GA | Yes | No | No | Yes | M | Kitanidis and Vomvoris (1983); Kitanidis (1995) |
| MLM | No | No | No | Yes | M | Carrera and Neuman (1986a) |
| PiPM | No | No[3] | No | -[4] | M | De Marsily et al. (1984); RamaRao et al. (1995); Alcolea et al. (2006) |
| SCM | No | Yes | No | -[4] | M | Gómez-Hernández et al. (1997); Hendricks Franssen (2001) |
| McMC | No | Yes | Yes | No | S | Oliver et al. (1997) |
| GDM | No | Yes | Yes | No | M | Hu (2000) |
| PrPM | No | Yes | Yes | No | M | Caers (2002); Hoffman and Caers (2005) |
| EnKF | No | Yes | No | Yes | - | Evensen (1994, 2007) |

1: Minimization of an objective function (M) or Sampling from a distribution (S).
2: References of original work and to main improvements
3: In its inception PiPM pursued a single aquifer map, but it was later converted onto a stochastic approach.
4: Although implicitly there is no multiGaussian assumption in its formulation, the final realizations tend to become multiGaussian given the way the optimization model is formulated

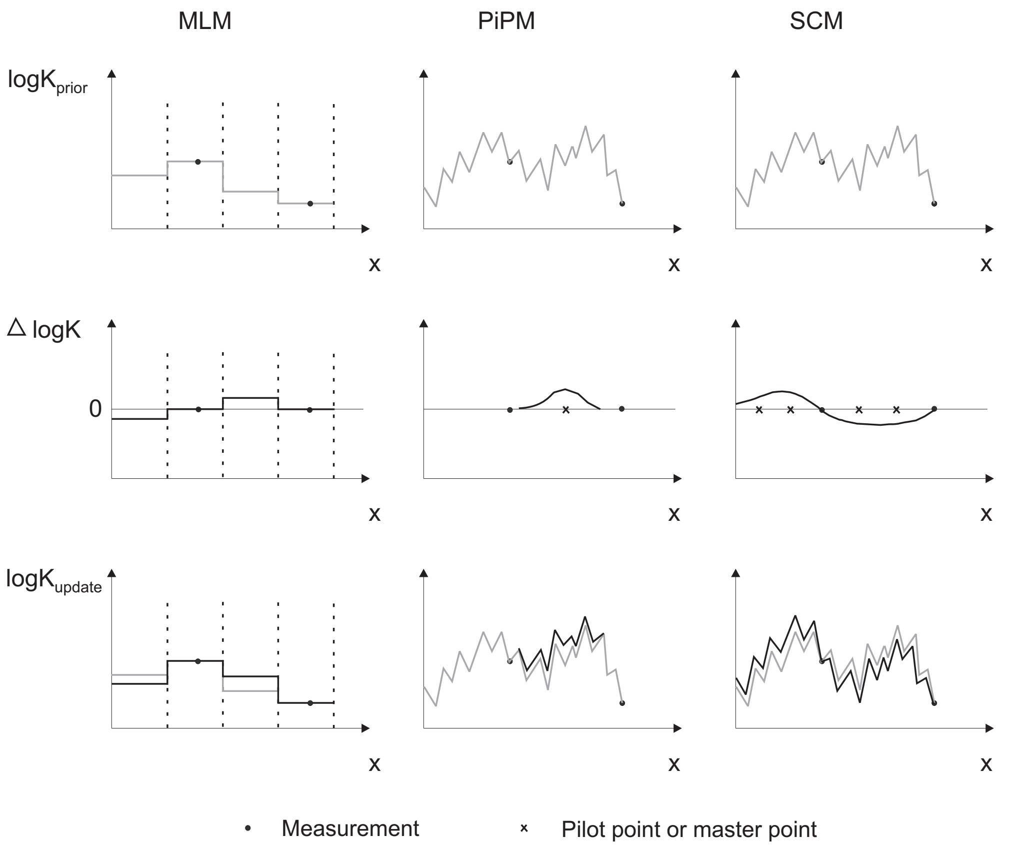


Figure 1: Schematic illustration of MLM, PiPM and SCM. Suppose the parameter to be estimated is the log hydraulic conductivity. The prior guess is updated by adding a perturbation, $\mathrm{logK_{update}} = \mathrm{logK_{prior}} + \Delta\mathrm{logK}$. The PiPM adds a perturbation around each pilot point sequentially. A seed logK field of the realization ensemble is shown for the SCM, which is modified by adding a perturbation that is computed by interpolating the perturbations at the master points.

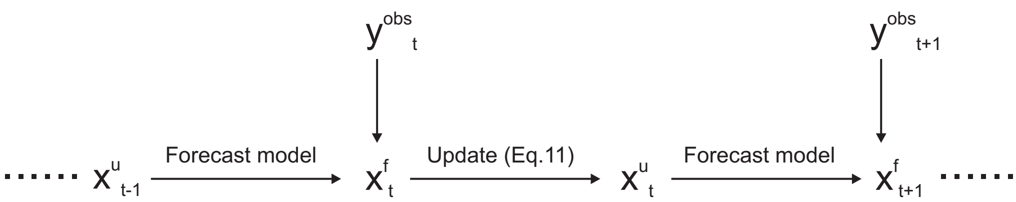


Figure 2: Workflow of the EnKF.

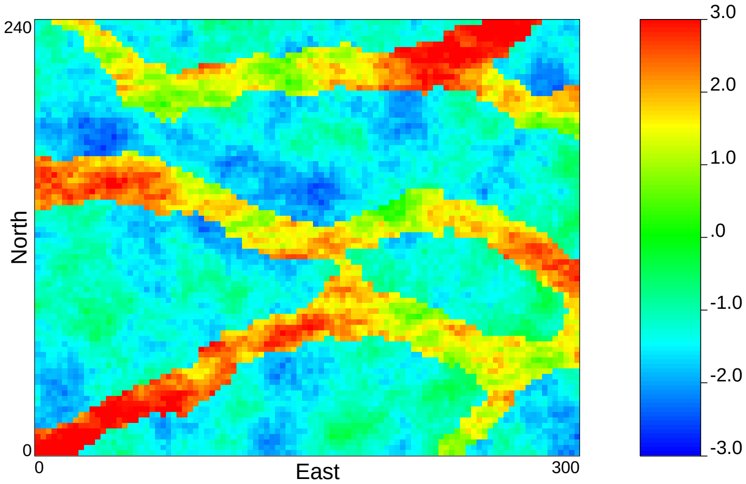


Figure 3: Conceptual model of a fluvial deposited aquifer used as a training image by the multiple point based simulation algorithms.