

Essay

Some Remarks About Forward and Inverse Modelling in Hydrology, Within a General Conceptual Framework

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Abstract: The solution to inverse problems is crucial for model calibration and to provide a good basis for model results to be reliable. This paper is based on a recently proposed conceptual framework for the development and application of mathematical models that require the solution of forward and inverse problems. The focus of this paper is on the discussion of some terminology related to the results of forward problems and their reanalysis, on the use of the proposed framework to revise and generalise some methods of solutions of the inverse problem, and to provide a non-standard insight in some aspects about the Bayesian approach to model calibration.

Keywords: forward problems; inverse problems; mathematical modelling; groundwater hydrology; rainfall–runoff modelling; catchment hydrology

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1. Introduction

Since several decades ago, mathematical modelling has been common practice in hydrology, not only by researchers but also by practitioners. This approach is natural in the framework of modern science, especially in physics, which has been based on systematic experimentation and mathematical abstraction since the XVII century. Mathematical models should provide a mathematical twin of the real world. Analytical models, based on closed-form solutions of the physico-mathematical equations, are very useful for interpreting laboratory or field data, or to provide fast assessment of different alternatives during planning and design activities, but they are based on quite restrictive assumptions. In particular, they can be rarely applied to model complex systems, especially in the presence of non-linearity and heterogeneity. Numerical models for geophysics and environmental physics can handle these complex situations. Such models can be considered as mathematical tools to simulate the behaviour of a real system with a virtual representation of the natural system itself.

The results of a physical-based, discrete (or numerical) model are reliable and useful only if the following conditions are met: the physics is properly described, i.e., the phenomenological laws that are applied [1] are appropriate to describe physical phenomena at the relevant scale; the numerical methods are accurate and properly respect conservation principles (the basic principles of conservation of mass, energy, linear momentum, etc.); the parameters used in the model are correct, i.e., the model is properly calibrated and validated.

However, “appropriate”, “accurate”, and “correct” are qualitative adjectives: scientists and engineers seek to express them in a quantitative way. This is not always easy and straightforward. In fact, the phenomenological laws and the corresponding relevant parameters could depend on the time and space scales that are considered in the specific application. Moreover, the required accuracy in the simulation of the natural system depends on the goals of the model, on the extent and the quality of the available data set,

on the scale at which processes are simulated, and on the relationship of model scale with measurement scale.

This paper is focused on numerical models in hydrology, but it is not a review of mathematical modelling and of the theory and application of inverse problems. Several books are devoted to the discussion of the discrete inverse problem (DIP) (see, e.g., [2–8] for an extensive introduction to this topic).

Following the seminal papers by Nelson [9,10], several researchers dealt with several applications and with different approaches in groundwater hydrology [11–39] and soil physics [40–43]. The relevance of model calibration and of inverse problems to simulate groundwater dynamics in global models of the water cycle has been recently recognised [44]. The application of automatic calibration has been widespread also in the field of surface hydrology, at least from the '70s of the XX century [45–51] and more extensively in the following decades (see, e.g., [52–66] as a largely incomplete list of the vast literature on this subject). These works considered the parameter fitting for different kinds of models [67], ranging from lumped to distributed models, empirical models based on a small number of parameters, conceptual models based on a simple structure, and physical-based distributed models. Interesting examples of model calibration for integrated surface/subsurface models [68,69] can be found in the scientific literature, as well as reviews of inverse problems in other sub-fields of geophysics [70].

The discussion proposed here is based on the conceptual framework to cast forward and inverse problems in geophysics proposed by the author with some of his coworkers [71]. The specific goals of this work are the following:

1. The introduction of a proper terminology, focused on the use of mathematical models in geophysics and environmental physics;
2. The discussion of some properties of the DIP by making use of a paradigmatic example of a non-linear model;
3. Some methods of solution to the DIP, which belong to the family of the so-called “direct” methods, are embedded in the abovementioned conceptual framework;
4. The Bayesian approach is also embedded in the abovementioned conceptual approach in order to discuss a couple of aspects that can be relevant.

The structure of this paper is as follows: Section 2 introduces a paradigmatic example useful to discuss the basic concepts about forward and inverse problems in hydrology. Section 3 is devoted to the introduction of the forward problem and to point 1 above (Section 3.3). In Section 4, the DIP is stated and its properties are discussed. Section 5 is focused on points 3 and 4 above. Finally, Section 6 is devoted to a discussion of some conclusive remarks.

2. A Paradigmatic Problem

Diffusive processes are very common in any sub-field of hydrology (catchment hydrology, rainfall–runoff, river hydraulics, groundwater hydrology, etc.). They are modelled with partial differential equations that are based on physical conservation principles (e.g., mass, energy, and linear momentum) and on phenomenological laws (Fick’s, Fourier’s, Darcy’s, etc.), are complemented with boundary and initial conditions (BICs), and most often assume the general form:

$$b \cdot D_t u = \operatorname{div}(a \operatorname{grad} u) + f, \quad (1)$$

where u is the “potential” (e.g., hydraulic head for groundwater flow, solute concentration for contaminant transport, or temperature for heat flow), D_t is the Lagrangian derivative [72–74], f is the source/sink term, and a and b are two phenomenological coefficients. Namely, a is a conductivity, diffusivity, or transmissivity that quantifies the ability of the medium to transfer the physical quantity under examination; b is a capacity that quantifies the ability of the system to store or release the physical quantity in response to variations of the potential.

Equation (1) can assume specific forms when applied to the different transport phenomena considered in groundwater hydrology, e.g., groundwater flow, solute transport, and heat transfer. In surface hydrology, the continuity equation (mass conservation) and Navier–Stokes equation (linear momentum conservation) can be further modified by introducing proper approximations, like those used to derive the classical Saint–Venant equation [75] or other models (see, e.g., [76]).

In the simplest case of a 1D, purely diffusive (i.e., convective terms are neglected), stationary process, (1) reduces to

$$\frac{d}{dx} \left(a \frac{du}{dx} \right) = -f. \quad (2)$$

For this example, a conservative finite-difference approximation can be synthetically written as

$$a_{i-1/2} \frac{u_{i-1} - u_i}{\Delta x_{i-1/2}} + a_{i+1/2} \frac{u_{i+1} - u_i}{\Delta x_{i+1/2}} = \varphi_i, \quad i = 1, \dots, N-1, \quad (3)$$

where $i \in \{0, \dots, N\}$ is the index used to identify a node that is the centre of one of the $N+1$ non-overlapping cells that cover the whole domain (see the geometry in Figure 1); $a_{i-1/2}$ represents the phenomenological coefficient (e.g., internode or interblock conductance, given by the product of internode or interblock conductivity times the surface separating two adjacent blocks); u_i is the potential at node i ; $\Delta x_{i-1/2}$ is the spacing between adjacent nodes; and φ_i is the sum of the source terms (expressed as a flow rate of the considered quantity per unit surface) in the cell i . Each of the terms on the left-hand side of (3) represents the specific flux per unit surface of the considered quantity (e.g., mass and energy) entering the cell i through the surface separating two adjacent cells. This is shown graphically through the grey arrows in Figure 1.

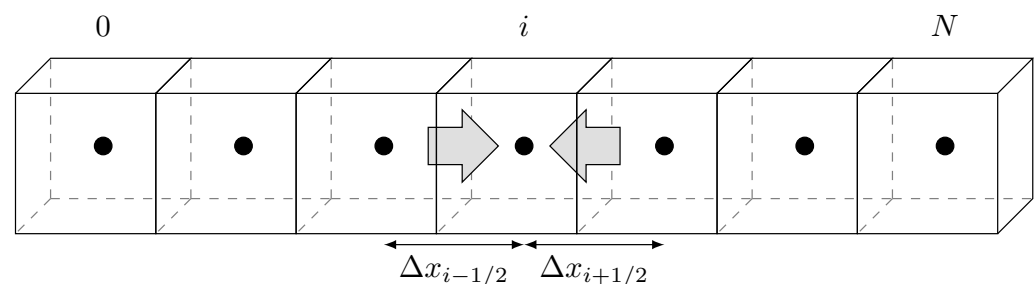


Figure 1. Discretisation grid for the paradigmatic example. Nodes are denoted as black dots; arrows show the incoming fluxes through the borders of the cell i , appearing on the left-hand side of (3).

Dirichlet boundary conditions (BCs) are easily introduced by setting u_0 or u_N equal to the prescribed value. Neumann BCs can be introduced by substituting $a_{1/2}(u_0 - u_1)/\Delta x_{1/2}$ with the prescribed value $q_{1/2}$; the term $a_{N-1/2}(u_N - u_{N-1})/\Delta x_{N-1/2}$ can be substituted with its prescribed value $q_{N-1/2}$, analogously. Neumann BCs permit to write (3) also for $i = 0$ or $i = N$.

3. Forward Modelling

The goals of mathematical models in hydrology can be very widespread and differentiated, as they may include the following:

1. Comparison of the model outcomes with the results of laboratory and field experiments in order to test the validity of physical theories;
2. Interpretation of field data for the determination of physical properties of natural systems (e.g., interpretation of well tests);
3. Simulation of the impact of management and exploitation of water resources on the natural systems;
4. Simulation of the effects of remediation actions to support risk analysis concerning the pollution of water resources and the environment;

5. Simulations of the impacts of land use programs on water resources for strategic environmental assessment and for environmental impact assessment;
6. Simulation of the impacts of natural stressors (e.g., climate change) to support risk analysis related to hydro-meteorological intense events;
7. Support to the optimal design and setup of monitoring networks or laboratory and field experiments, including sampling frequency, precision of the instruments, and of the measuring procedures and gauges resolution.

3.1. Statement of the Forward Problem

A numerical mathematical model can be represented by a set of equations that describe the state of the physical system under study as a function of model parameters. The model parameters are included in an array $\mathbf{p}$, whereas an array $\mathbf{s}$ includes the quantities that describe the state of the system. It is important to stress that the term “array”, rather than vector, is used here to denote mathematical structures that can play different roles. In fact, in this work, arrays denote a collection of physical quantities and parameters that will be considered either as a column vector, in order to apply standard methods of linear algebra, or as a finite set of elements. A discrete model can be written as the following system of equations:

$$\mathbf{f}(\mathbf{p}, \mathbf{s}) = 0, \quad (4)$$

where the function $\mathbf{f}$ may assume different forms for different problems and may refer to time-evolving systems, for which $\mathbf{s}$ is split into sub-arrays corresponding to the state of the system at different time steps.

For the paradigmatic example considered in this work, the state of the system is the potential at the nodes, i.e., $\mathbf{s} = \{u_i, i = 0, \dots, N\}$, and (2) can be written as

$$\mathbf{f}(\mathbf{p}, \mathbf{s}) = \mathbf{A}(\mathbf{p})\mathbf{s} - \mathbf{b}(\mathbf{p}) = 0, \quad (5)$$

where $\mathbf{A}$ is a square matrix and $\mathbf{b}$ is used to model both the source terms and the BCs. The forward problem aims at solving (3) with respect to u_i , if $a_{i-1/2}$ and φ_i are known, whereas the inverse problem aims at identifying the best values of the phenomenological parameters $a_{i-1/2}$, $i = 1, \dots, N$.

Equation (5) is a prototype also for the following:

1. Two-dimensional or three-dimensional problems;
2. Transient conditions, recalling the remark in the line after (4);
3. Different methods of numerical solution of the partial differential equations (e.g., finite elements and spectral methods);
4. Non-linear processes, for which $\mathbf{A}$ and $\mathbf{b}$ depend on $\mathbf{s}$.

The abovementioned applications include different approaches for numerical integration of the mass and linear momentum equations in catchment hydrology, e.g., with a Muskingum–Cunge approach [77]. The general form given by (4) applies in a relatively easy way also to input–output models such as the advection–diffusion approach (e.g., [76,78]), the classical unit hydrograph concept (which goes back to Dooge’s work in the 1950s [79]) and similar approaches (e.g., [80]), or the curve number method ([81], see the remarks at the end of Section 4.2).

From a formal and general point of view, one can introduce the forward problem as follows:

Problem 1 (Forward problem—FP). *Let $\mathbf{p} \in \mathcal{P} \subseteq \mathbb{R}^{N(\mathbf{p})}$ be known, where $\mathcal{P}$ is the subset of $\mathbb{R}^{N(\mathbf{p})}$ that takes into account any possible constraint on the model parameters (e.g., conductivity must be positive); then, the FP is stated as finding $\mathbf{s} \in \mathcal{S} \subseteq \mathbb{R}^{N(\mathbf{s})}$ such that (4) is satisfied.*

If a unique solution of the FP can be found, it can be expressed in an explicit, possibly non-linear form as

$$\mathbf{s} = \mathbf{g}(\mathbf{p}). \quad (6)$$

For the sake of simplicity, in this paper, it is assumed that the FP is well-posed, i.e., a solution exists; is unique; and depends with continuity on $\mathbf{p}$. However, this is not always the case [82].

3.2. Data and Parameters

Array $\mathbf{p}$ includes any model parameter, comprising those describing the geometry of the discretisation grid (e.g., the spacing of the grid or the time step for time-evolving processes). Therefore, some of these parameters are fixed before the application of the model; their values will depend on the available data, which are the elements of $\mathbf{d}$. Then, the fixed parameters can be grouped in a “sub-array” $\mathbf{p}^{(\text{fix})}$, whose dimension is $N_{(\text{p})}$ and which depends on the data: $\mathbf{p}^{(\text{fix})}(\mathbf{d})$.

For the paradigmatic example, $\mathbf{d}$ includes the following:

1. The position of the points where potential is measured;
2. The measured values of potential;
3. Other measurements necessary to estimate the values of the source terms or the BICs.

On the other hand, for rainfall–runoff models, $\mathbf{d}$ could include the following:

1. Time series of water level or discharge measured at stream gauging stations;
2. Time series of rainfall rate monitored at meteorological stations in the drainage basin;
3. Topographic data or a digital elevation model of the drainage basin.

For the paradigmatic example, $\mathbf{p}^{(\text{fix})}$ includes the values of $\Delta x_{i-1/2}$, $i \in \{1, \dots, N\}$, and possibly the source terms and the values of the BCs, e.g., u_0 and u_N in the case of Dirichlet BCs.

Array $\mathbf{p}^{(\text{cal})} \in \mathbb{R}^{N_{(\text{c})}}$ denotes the model parameters, whose values are obtained through calibration, namely, as a solution of a DIP. The number of elements of $\mathbf{p}^{(\text{cal})}$ is $N_{(\text{c})}$. In general, one can write

$$\mathbf{p} = \left(\mathbf{p}^{(\text{fix})}, \mathbf{p}^{(\text{cal})} \right)^t = \left(\mathbf{p}_1^{(\text{fix})}, \dots, \mathbf{p}_{N_{(\text{f})}}^{(\text{fix})}, \mathbf{p}_1^{(\text{cal})}, \dots, \mathbf{p}_{N_{(\text{c})}}^{(\text{cal})} \right)^t, \quad (7)$$

or equivalently in set theory notation

$$\mathbf{p} = \mathbf{p}^{(\text{fix})} \cup \mathbf{p}^{(\text{cal})} = \left\{ \mathbf{p}_1^{(\text{fix})}, \dots, \mathbf{p}_{N_{(\text{f})}}^{(\text{fix})}, \mathbf{p}_1^{(\text{cal})}, \dots, \mathbf{p}_{N_{(\text{c})}}^{(\text{cal})} \right\},$$

where $N_{(\text{f})} + N_{(\text{c})} = N_{(\text{p})}$.

For the paradigmatic example, $N_{(\text{c})} = N$ and $\mathbf{p}^{(\text{cal})} = \{a_{i-1/2}, i = 1, \dots, N\}$.

3.3. Terminology About Results and Forecast of a Mathematical Model

The great variety of goals of mathematical models that were mentioned at the beginning of this section implies that model results are qualified with different words, which are usually considered as synonyms in common language [83–86]: estimate, forecast, guess, outlook, prediction, projection, and prospect. Other synonyms, which would not be used in scientific language, are foretelling, premonition, and prophecy. In the author’s opinion, a “fine-tuned” differentiation in the technical language is important.

Results or outcomes of a forward model should be considered as the state of the system array $\mathbf{s}$ that is the solution to the forward problem, i.e., the solution of (4), when the parameters $\mathbf{p}$ are given. Instead, forecasts of the model could be considered as a set of quantities that are derived from the model results, possibly also with the use of model parameters $\mathbf{p}$ and data $\mathbf{d}$. The terms reanalysis and products are sometimes used to denote similar quantities, especially when data assimilation is performed. In particular, climatic and meteorological reanalysis is often considered in atmospheric physics (e.g., [87,88]). With reference to the paradigmatic example, flow rates could be computed by using the state of the system and the internode conductances. Therefore, the model forecasts are expressed as an array $\mathbf{y}$ that is a function of $\mathbf{s}$, $\mathbf{p}$, and $\mathbf{d}$: $\mathbf{y}(\mathbf{s}, \mathbf{p}, \mathbf{d})$.

The distinction between prediction and projection finds wide consensus in the scientific community. In fact, such a distinction is quite clearly stated in climate science and is well

summarised in the Annex II. Glossary by IPCC [89] in 2007, from which the following sentences are borrowed.

Climate prediction

A climate prediction or climate forecast is the result of an attempt to produce an estimate of the actual evolution of the climate in the future, for example, at seasonal, interannual, or long-term time scales. Since the future evolution of the climate system may be highly sensitive to initial conditions, such predictions are usually probabilistic in nature. See also Climate projection and climate scenario.

Climate projection

A projection of the response of the climate system to emission or concentration scenarios of greenhouse gases and aerosols, or radiative forcing scenarios, often based upon simulations by climate models. Climate projections are distinguished from climate predictions in order to emphasise that climate projections depend upon the emission/concentration/radiative forcing scenario used, which are based on assumptions concerning, for example, future socioeconomic and technological developments that may or may not be realised and are therefore subject to substantial uncertainty.

Instead, the distinction between prediction and forecast is rather subtle and debatable (e.g., [90]). In many websites and blogs, forecast is often claimed to refer to the numerical simulation and prediction of the future behaviour of a system on the basis of past data. Prediction is used in a more general and wide sense. For instance, in statistics, linear regression of a variable against several other variables can be performed by comparing predicted values of the variable under examination with measured or observed values. In some cases, prediction is also considered to be a guess or an estimate of the behaviour of a system without referring to scientific arguments or data but based on assumptions, expert opinions, intuition, or subjective judgement. Therefore, as it is sometimes claimed on websites and blogs, all forecasts are predictions, but some predictions are not forecasts. When mathematical models are used in natural sciences, it seems that “forecast” is the most appropriate term to denote the estimate of quantities derived from the processing of the outcomes of a numerical model for a dynamical system and should be preferred to “prediction”.

4. Discrete Inverse Problems

With the notation and the definitions given in Section 3, the DIP should aim to solve the system

$$\mathbf{y}(\mathbf{s}, \mathbf{p}, \mathbf{d}) = \mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})}), \quad (8)$$

with respect to $\mathbf{p}^{(\text{cal})}$, which is a sub-array of $\mathbf{p}$, as shown by (7). Array $\mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})})$ consists in the calibration target, i.e., the values of the model forecast that are expected to be obtained from model outcomes. The calibration target is obtained from data processing, possibly supported by fixed parameters, i.e., $\mathbf{p}^{(\text{fix})}$; this phase might be tricky, because data and model parameters often refer to different spatial and temporal scales. The calibration target cannot depend on $\mathbf{p}^{(\text{cal})}$.

An exact solution to (8) can rarely be found. The most common approach is to cast the DIP in the framework of optimal control and to look for the set of model parameters that minimises the discrepancy between the two sides of (8). This is performed by introducing an objective function O , given by

$$O(\mathbf{p}^{(\text{cal})}) = d(\mathbf{y}(\mathbf{s}, \mathbf{p}, \mathbf{d}), \mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})})), \quad (9)$$

where d is a discrepancy function such that

- $d : \mathbb{R}^{N(t)} \times \mathbb{R}^{N(t)} \rightarrow [0, +\infty)$,
- $\mathbf{x}' = \mathbf{x}'' \iff d(\mathbf{x}', \mathbf{x}'') = 0$.

The classical choice is the least-squares approach, for which

$$d\left(\mathbf{y}(\mathbf{s}, \mathbf{p}, \mathbf{d}), \mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})})\right) = \sum_{i=1}^{N(\mathbf{t})} \left| y_i(\mathbf{s}, \mathbf{p}, \mathbf{d}) - t_i(\mathbf{d}, \mathbf{p}^{(\text{fix})}) \right|^2. \quad (10)$$

Of course, many other choices are possible for the d function, among which are the sum of absolute differences (ℓ^1 norm) and the maximum absolute difference (ℓ^∞ norm), or any ℓ^p norm of the difference $\mathbf{y}(\mathbf{s}, \mathbf{p}, \mathbf{d}) - \mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})})$. Therefore, the discrete inverse problem can be stated as follows:

Problem 2 (Discrete inverse problem—DIP). Let $\mathbf{s} = \mathbf{g}(\mathbf{p})$ be the solution to the FP from (6). Given $\mathbf{p}^{(\text{fix})}$ and $\mathbf{d}$, given

$$\mathcal{P}^{(\text{cal})} = \left\{ \mathbf{p}^{(\text{cal})} : \left(\mathbf{p}^{(\text{fix})^t}, \mathbf{p}^{(\text{cal})^t} \right)^t \in \mathcal{P} \right\},$$

given the functions $\mathbf{y}$ and $\mathbf{t}$ —in particular, the values of $\mathbf{t}(\mathbf{d}, \mathbf{p}^{(\text{fix})})$, and given the objective function O from (9), the DIP is stated as finding $\mathbf{p}^{(\text{cal})^*} \in \mathcal{P}^{(\text{cal})}$ such that

$$\begin{aligned} O(\mathbf{p}^{(\text{cal})^*}) &\leq O(\mathbf{p}^{(\text{cal})}), \quad \forall \mathbf{p}^{(\text{cal})} \in \mathcal{P}^{(\text{cal})} \\ \text{or equivalently} \\ \mathbf{p}^{(\text{cal})^*} &= \arg \min_{\mathbf{p}^{(\text{cal})} \in \mathcal{P}^{(\text{cal})}} O(\mathbf{p}^{(\text{cal})}). \end{aligned} \quad (11)$$

A graphical scheme of the arrays used to state the FP and the DIP is shown in Figure 2. In that picture, the red arrows is the symbol to show the comparison between model forecast $\mathbf{y}$ and calibration target $\mathbf{t}$.

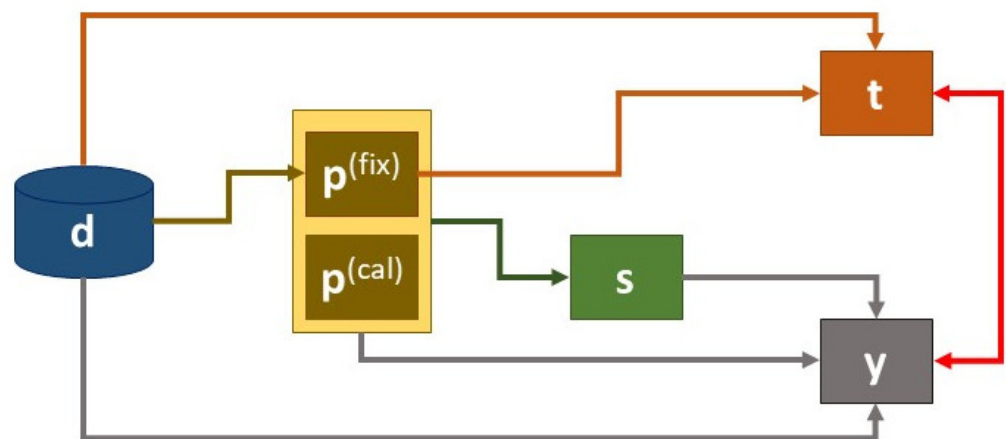


Figure 2. Scheme of the arrays introduced in the text to state the FP, the DIP, and their relationships.

As pointed out by one of the reviewers, the proposed formalism can embrace the approach to inversion through Physics-Informed Machine Learning [91], an approach that has been increasingly applied in geophysics [92] and in hydrology [93] in the last few years. Moreover, the training phase of Artificial Neural Networks can be included in this framework and shares some of the properties and difficulties of physical-based DIPs [94].

4.1. Remarks About the Discrepancy Function

The conditions that have been introduced for the discrepancy function are very similar to those that define a distance or metric among the elements of a given set. However, this function does not necessarily correspond to a distance as two of the properties that define a distance, in a rigorous mathematical sense, are not required here, namely, symmetry and

triangle inequality. As an example, it is important to mention that even some commercial codes use the root mean square relative error given by

$$d(\mathbf{y}, \mathbf{t}) = \left[\frac{1}{N_{(t)}} \sum_{i=1}^{N_{(t)}} \left| \frac{\mathbf{y}_i - \mathbf{t}_i}{\mathbf{t}_i} \right|^2 \right]^{1/2}. \quad (12)$$

The idea behind this choice is to weight the discrepancy between model forecast and calibration target by considering the magnitude of the target. In other words, a small discrepancy could be negligible if the target value is great, whereas it is of great relevance if the target value is small, of the same order of magnitude as the discrepancy. Under this premise, the symmetry condition is not physically significant, i.e., it is physically very different to normalise with respect to $\mathbf{t}$ or to $\mathbf{y}$. This also impacts on the asymmetry of the function.

Nevertheless, even if one disregards this conceptual point, it is easy to check that the function d defined by (12) does not satisfy the triangle inequality. For this, it suffices to consider $N_{(t)} = 1$ so that $d(y, t) = |(y - t) \cdot t^{-1}|$, and the three numbers $\alpha = 4$, $\beta = 1$, and $\gamma = 2$ to see that

$$3 = d(\alpha, \beta) = \left| \frac{\alpha - \beta}{\beta} \right| > \left| \frac{\alpha - \gamma}{\gamma} \right| + \left| \frac{\gamma - \beta}{\beta} \right| = d(\alpha, \gamma) + d(\gamma, \beta) = 2,$$

which violates the triangle inequality.

A generalisation of the relative error has been recently proposed in a COVID-19 spread model [95]. In that example, $\mathbf{y}$ and $\mathbf{t}$ include the cumulative number of infected (I), recovered (R), and deceased (D) persons:

$$\mathbf{y} = \left\{ y_n = (y_n^{(1)}, y_n^{(2)}, y_n^{(3)}) \in \mathbb{R}^3 \mid \begin{aligned} y_n^{(1)} &= I_n, y_n^{(2)} = R_n, y_n^{(3)} = D_n, \\ n &= n_{\min}, \dots, n_{\max} - 1 \end{aligned} \right\}; \quad (13)$$

$$\mathbf{t} = \left\{ t_n = (t_n^{(1)}, t_n^{(2)}, t_n^{(3)}) \in \mathbb{R}^3 \mid \begin{aligned} t_n^{(1)} &= I_n^{(\text{ref})}, t_n^{(2)} = R_n^{(\text{ref})}, t_n^{(3)} = D_n^{(\text{ref})}, \\ n &= n_{\min} \dots, n_{\max} - 1 \end{aligned} \right\}, \quad (14)$$

where $^{(\text{ref})}$ means “obtained from reference data” taken from the Johns Hopkins University Coronavirus Resource Center (CRC), and $n_{\min}$ and $n_{\max}$ are the minimum and maximum time steps for which data are available, whereas $n = 0$ is the moment when the first person is infected. In the referenced work, the misfit between model forecast and calibration target is computed by means of the following objective function:

$$O(\mathbf{p}^{(\text{cal})}) = \sum_{i=1}^3 O^{(i)}(\mathbf{p}^{(\text{cal})}), \quad (15)$$

where

$$O^{(j)}(\mathbf{p}^{(\text{cal})}) = \left\{ \frac{1}{n_{\max} - n_{\min}} \sum_{n=n_{\min}}^{n_{\max}-1} \left[\frac{y_n^{(j)} - t_n^{(j)}}{\max\{\xi, t_n^{(j)}\}} \right]^2 \right\}^{1/2}, \quad (16)$$

for $i = 1, 2, 3$, where $\xi \geq 1$ is a threshold-and-weight parameter. Such a parameter plays a double role:

1. A threshold that keeps positive the denominator of $(y_n^{(j)} - t_n^{(j)}) \times (\max\{\xi, t_n^{(j)}\})^{-1}$, even in the particular case when $t_n^{(j)} = 0$;
2. A weight that controls some characteristics of the objective function:

- If $\xi = 1$ and $t_n^{(j)} \geq 1$, then $O^{(j)}$ reduces to the root-mean-squared relative difference between $t_n^{(j)}$ and $y_n^{(j)}$.
- If ξ assumes large values, it dampens the errors for low values of $t_n^{(j)}$, namely, if $t_n^{(j)} \ll \xi$; therefore, the relative errors corresponding to large values of $t_n^{(j)}$ will be dominant, so that early-time behaviour, when $I_n^{(\text{ref})}$, $R_n^{(\text{ref})}$, and $D_n^{(\text{ref})}$ are small, is less relevant to the model fitting.
- If $\xi > \max\{t_n^{(j)}, n = n_{\min} \dots, n_{\max} - 1\}$, then $O^{(j)}$ reduces to the standard root-mean-squared error.

4.2. Remarks About the DIP for the Paradigmatic Example

The paradigmatic example introduced in section 2 is useful to discuss possible alternative choices for $\mathbf{y}$ and $\mathbf{t}$. Four cases are mentioned here.

The first approach is to use measured data to build $\mathbf{t}$ in a straightforward way by assigning measured values of potential as the elements of $\mathbf{t}$: $\mathbf{t} = (u_1^{(\text{meas})}, \dots, u_{N_m}^{(\text{meas})})^t$, where $u_j^{(\text{meas})}$ is the potential measured at a measurement point $\mathbf{x}_j$. On the other hand, $\mathbf{y}$ is obtained by interpolation of the elements of $\mathbf{s}$, so that the model forecast is the simulated potential at each measurement position: $\mathbf{y} = (u_1^{(\text{int})}, \dots, u_{N_m}^{(\text{int})})^t$, where $u_j^{(\text{int})}$ is the potential interpolated at $\mathbf{x}_j$ from $\mathbf{s} = (u_0, \dots, u_N)^t$.

The second approach is the interpolation of field data at the node positions as a target: $\mathbf{t} = \mathbf{s}^{(\text{int})}(\mathbf{d}, \mathbf{p}^{(\text{fix})})$. This array should be compared with the results of the model, i.e., with the solution to (4): in this case, $\mathbf{y} = \mathbf{s}$.

The third approach assumes that the model results are used to forecast the values of other quantities. For instance, if it is possible to estimate fluxes from field data and they can be included in the $\mathbf{t}$ array, then the $\mathbf{y}$ vector should include the forecast for the same quantities obtained from model results.

The fourth approach consists in substituting the interpolated field $\mathbf{s}^{(\text{int})}(\mathbf{d}, \mathbf{p}^{(\text{fix})})$ in (4), or equivalently in (5) for this paradigmatic example. Then, $\mathbf{y} = \mathbf{A}(\mathbf{p})\mathbf{s}^{(\text{int})}(\mathbf{d}, \mathbf{p}^{(\text{fix})}) - \mathbf{b}(\mathbf{p})$, which is often called equation (or balance) error. For this approach, the target is trivial: $\mathbf{t} = 0$. This approach is known in the literature on groundwater hydrology as the “direct approach” [12]. The conceptual framework used here [71] permits consideration of the whole process from data collection to parameter identification, if $\mathbf{p}^{(\text{fix})}$ includes the parameters that control the interpolation of field data. Then, the direct formulation of the DIP reduces to finding the parameters $\mathbf{p}^{(\text{cal})}$ that satisfy

$$\mathbf{f}(\mathbf{p}, \mathbf{s}^{(\text{int})}(\mathbf{d}, \mathbf{p}^{(\text{fix})})) = 0. \quad (17)$$

4.3. Insights into the DIP Through the Example of the Curve Number Approach

In order to give further insights in the proposed framework, the simple curve number approach [81] could be considered. In its simplest formulation, it computes runoff (Q) as a function of rainfall (P), potential maximum retention after runoff begins (S), and initial abstraction (I_a), i.e., all losses before runoff begins, including interception by vegetation, evaporation, infiltration, and water retention in surface depressions:

$$Q = \frac{(P - I_a)^2}{P - I_a + S}, \quad (18)$$

where all the quantities are expressed as a length, i.e., they are specific per unit surface, possibly integrated over a given monitoring interval (24 h in many applications). Then, a simple linear relationship between I_a and S is proposed, namely, $I_a = c_1 S$; moreover, the curve number CN is used to compute S through the relationship $S = c_2 \cdot CN^{-1} - c_3$.

$c_1 = 0.2$, $c_2 = 1000 \text{ in} = 25,400 \text{ mm}$, and $c_3 = 100 \text{ in} = 2540 \text{ mm}$ are the reference values that were originally proposed [81].

Under the light of the formalism used in this paper, one could collect field measurements for different rainfall events, which are denoted with the index $m = 1, \dots, M$. Rainfall measured at different stations could be included in $\mathbf{d}$, together with discharge measurements at a gauge station. Array $\mathbf{t}$ could be simply obtained by the time integration of instantaneous discharge data over the prescribed time interval, whose duration is included in $\mathbf{p}^{(\text{fix})}$. Some interpolation of the point measurements from the meteorological stations could provide the value of P_m to be inserted in (18), to yield Q_m . In other words, $\mathbf{y} = \mathbf{s} = \{Q_m, m = 1, \dots, M\}$, and $\mathbf{g}$ is built with the application of (18) to each of the M -th rainfall events.

For this simple example, the optimal determination of the values of the parameters c_1 , c_2 , and c_3 , together with CN , could be the goal of model calibration. In this case, one could consider all these parameters as elements of $\mathbf{p}^{(\text{cal})}$. An alternative choice could be to consider CN only as the fitting parameter and to fix the values of c_1 , c_2 , and c_3 to the reference values so that they belong to $\mathbf{p}^{(\text{fix})}$.

5. Further Remarks About the DIP

The definitions given in the previous sections could be used to discuss several concepts relevant for the DIP, like identifiability, regularisation, multi-objective inversion, sensitivity analysis, and the use of the adjoint-state equation to compute sensitivity methods for the minimisation of the objective function. These aspects are discussed elsewhere ([71] and the references therein). Here, the focus is on the ill-posedness or ill-conditioning of the DIP and on different calibration methods that can only partially be embedded in the above-referenced conceptual framework. However, it is worth mentioning some literature references that are related to the importance of multi-objective calibration [96–98] and to the use of different metrics to assess and quantify model performance [7,99–101].

5.1. Some Remarks About Ill-Posedness of DIP

Since the beginning of the XX century, well-posedness (i.e., existence, uniqueness, and stability) is a key concept in mathematical problems [102]. Inverse problems are often ill-posed; because it is difficult to provide reasonable conditions to guarantee the existence of a solution, the latter is often non-unique and can depend in an unstable way on the input data. The framework considered in this paper permits stating the uniqueness and stability of the DIP in a relatively simple way, as follows:

Definition 1 (Uniqueness). Let $\mathbf{p}'$ and $\mathbf{p}''$ be two solutions to Problem 2. The DIP is said to admit a unique solution if $\mathbf{p}' = \mathbf{p}''$.

Definition 2 (Stability). Let $\mathbf{p}'$ and $\mathbf{p}''$ be two solutions to Problem 2, corresponding, respectively, to two data sets $\mathbf{d}'$ and $\mathbf{d}''$. The DIP is said to admit a stable solution if $\|\mathbf{d}' - \mathbf{d}''\| \rightarrow 0$ implies $\|\mathbf{p}' - \mathbf{p}''\| \rightarrow 0$.

From the practical point of view, the DIP could be affected by ill-conditioning—that is, even if a DIP admits a stable solution, a small error on the data could be sufficient to yield big, or even huge, errors in the identified parameters. This concept can be defined in a formal, but still qualitative, way as follows:

Definition 3 (Lipschitz condition). Under the same hypotheses of Definition 2, the solution to the DIP is said to satisfy the Lipschitz condition if there exists a constant $C > 0$ such that $\|\mathbf{p}' - \mathbf{p}''\| \leq C \cdot \|\mathbf{d}' - \mathbf{d}''\| \rightarrow 0$.

Definition 4 (Conditioning). Under the same hypotheses of Definition 2, and if the solution to the DIP satisfies the Lipschitz condition, the DIP is said to be ill- (or, respectively, well-) conditioned if C is big (or, respectively, small).

In practical applications, the problems due to non-uniqueness, instability, and ill-conditioning might appear in a very similar manner. Moreover, the presence of local minima of the objective function is a very relevant and typical problem that arises in the solution of a DIP. It causes the failure of several algorithms, mostly those based on gradient descent: their final outcome depends on the initial guess and is often a local minimum. In addition, those algorithms suffer big problems when the objective function is almost flat around the minimum. However, no matter which minimisation algorithm is applied, the flatness of O implies that a large set of arrays $\mathbf{p}^{(\text{cal})}$ yields values of O , which differ by quantities smaller than the uncertainties due to measurement and modelling errors. This problem is somehow linked with the concept of “resolution” and is strictly related to the sensitivity of the model outcomes and forecast on the model parameters. These issues triggered the introduction of the concept of “equifinality” [56,103–105] and of the study of parameter uncertainty [106–108]. The latter, together with proper management of data and modelling errors, should be cast in the frame of probability theory and stochastic processes (see Section 5.3).

5.2. Solution Methods Based on Comparison Among Model Forecasts

Some methods of solution of the DIP are based on the comparison among different model forecasts; here, the focus is on two of them: the Comparison Model Method ([109–116], CMM), together with its variation named successive flux estimation [117], and the Dual Constraint Method ([118–120], DCM). Both methods are based on the use of the solution to the FP for a tentative set of parameters ($\mathbf{p}^{(0)}$), namely, for a tentative a field for the applications related to the paradigmatic example. The iterative updating of parameters is based on the use of phenomenological laws (Darcy’s law in the case of groundwater hydrology, Fourier’s law in the case of heat flow, etc.). Therefore, these methods have quite a strong physical foundation but are not based on the use of the gradient of O to search the minimum of the objective function.

Starting from a first guess of $\mathbf{p}^{(\text{cal})}$, i.e., $a_{i-1/2}^{(0)}$, $i = 1, \dots, N$ for the paradigmatic example, CMM solves the FP and obtains $\mathbf{s}^{(0)}$, i.e., the values of $u_i^{(0)}$, $i = 1, \dots, N - 1$ for the solution of (5). Then, in its simplest formulation, the method is applied iteratively by means of the following simple formula:

$$a_{i-1/2}^{(\ell+1)} \frac{u_i^{(\text{int})} - u_{i-1}^{(\text{int})}}{\Delta x_{i-1/2}} = a_{i-1/2}^{(\ell)} \frac{u_i^{(\ell)} - u_{i-1}^{(\ell)}}{\Delta x_{i-1/2}}, \quad i = 1, \dots, N. \quad (19)$$

In other words, the fluxes computed at the ℓ -th step of the iterative algorithm are assumed to be equal to the fluxes that are computed from the internode conductivities at the next iteration and the potential interpolated at each node. Roughly speaking, from the physical point of view, at each iteration, the method increases the values of $a_{i-1/2}$, where the modelled discrete potential gradient is greater than the one computed with the interpolated potential and vice versa.

By abstracting from the specific paradigmatic example, the CMM algorithm could be specified as follows: starting from an initial guess of the parameters to be calibrated, compute the parameters at the ℓ -th iteration as the solution to

$$\mathbf{y}(\mathbf{s}^{(\ell-1)}, \mathbf{d}, \mathbf{p}^{(\ell-1)}) = \mathbf{y}(\mathbf{s}^{(\text{int})}, \mathbf{d}, \mathbf{p}^{(\ell)}), \quad (20)$$

where $\ell = 0, 1, \dots$ and $\mathbf{s}^{(\ell-1)} = \mathbf{g}(\mathbf{p}^{(\ell-1)})$.

DCM starts from the idea of Calderón’s problem [121], who worked on the problem of obtaining images of the subsurface through electrical tomography inversion. He stated the inverse problem as the determination of the conductivity field in a region of the subsurface by means of potential and current measured at the border, through the use of the Dirichlet-to-Neumann map. The latter is the mathematical mapping that assigns to a given set of Dirichlet boundary values the correspondent currents at the border. In the case of DCM, two FPs are considered: the first FP uses “Dirichlet BCs”, i.e., it prescribes the values of the potential at some points, possibly corresponding to measurement points (the fixed

parameters used for this FP and the corresponding solution are denoted with apex ^(D); the second FP is solved by using “Neumann BCs”, i.e., it prescribes fluxes at the same measurement points as for the previous FP (the apex ^(N) is used for quantities referred to this FP). For the paradigmatic example, starting from an initial guess $a_{i-1/2}^{(0)}$, $i = 1, \dots, N$, the solution is obtained by iteratively applying the following equation:

$$a_{i-1/2}^{(\ell)} = a_{i-1/2}^{(\ell)} \left| \frac{u_i^{(N)} - u_{i-1}^{(N)}}{u_i^{(D)} - u_{i-1}^{(D)}} \right|, \quad i = 1, \dots, N. \quad (21)$$

In the general case, the method can be stated as follows: starting from an initial guess of $\mathbf{p}^{(\text{cal})}$, and considering two different subsets of fixed model parameters, corresponding, e.g., to different BCs, and denoted with $\mathbf{p}^{(\text{fix,D})}$ and $\mathbf{p}^{(\text{fix,N})}$, compute $\mathbf{p}^{(\text{cal})}$ at the ℓ -th iteration as the solution to

$$\mathbf{y} \left(\mathbf{s}^{(\text{D})}, \mathbf{d}, \left(\mathbf{p}^{(\text{fix,D})^t}, \mathbf{p}^{(\text{cal}),\ell^t} \right)^t \right) = \mathbf{y} \left(\mathbf{s}^{(\text{N})}, \mathbf{d}, \left(\mathbf{p}^{(\text{fix,N})^t}, \mathbf{p}^{(\text{cal}),\ell-1^t} \right)^t \right), \quad (22)$$

where $\ell = 0, 1, \dots$,

$$\mathbf{s}^{(\text{D})} = \mathbf{g} \left(\left(\mathbf{p}^{(\text{fix,D})^t}, \mathbf{p}^{(\text{cal}),\ell-1^t} \right)^t \right),$$

and

$$\mathbf{s}^{(\text{N})} = \mathbf{g} \left(\left(\mathbf{p}^{(\text{fix,N})^t}, \mathbf{p}^{(\text{cal}),\ell-1^t} \right)^t \right).$$

5.3. Bayesian Approach

The role of the measurement, approximation, and modelling errors on the solution of DIP is emphasised in [71]. Since such errors are very complex to predict (this verb is used here in a proper way, in the sense that, in some cases, only educated guesses can be applied on such errors), the Bayesian approach (see, e.g., [122] for an interesting discussion of the approach) could be of particular interest for model calibration. The common strategy invokes Bayes’ theorem, which can be cast as follows:

$$f_{\text{posterior}} \left(\mathbf{p}^{(\text{cal})} | \mathbf{y} - \mathbf{t} \right) = \frac{f_{\text{likelihood}} \left(\mathbf{y} - \mathbf{t} | \mathbf{p}^{(\text{cal})} \right) \cdot f_{\text{prior}} \left(\mathbf{p}^{(\text{cal})} \right)}{f_{\text{marginal}} \left(\mathbf{y} - \mathbf{t} \right)}, \quad (23)$$

where

- $f_{\text{posterior}} \left(\mathbf{p}^{(\text{cal})} | \mathbf{y} - \mathbf{t} \right)$ is the posterior probability density function (pdf);
- $f_{\text{likelihood}} \left(\mathbf{y} - \mathbf{t} | \mathbf{p}^{(\text{cal})} \right)$ is the likelihood [123], i.e., the conditional pdf of the discrepancy between model forecasts and target values conditioned with respect to the $\mathbf{p}^{(\text{cal})}$ array;
- $f_{\text{prior}} \left(\mathbf{p}^{(\text{cal})} \right)$ is the prior pdf of $\mathbf{p}^{(\text{cal})}$, i.e., the pdf of the values of the parameters to be calibrated, without any information from measured data and model outcomes;
- $f_{\text{marginal}} \left(\mathbf{y} - \mathbf{t} \right)$ is the marginal pdf, i.e., the pdf of the discrepancies between $\mathbf{y}$ and $\mathbf{t}$, without any information from measured data and model outcomes.

The application of the Bayesian approach requires some guesses about the pdfs appearing in (23). The most common guess consists in assuming that both the likelihood and the prior pdf can be expressed as multi-Gaussian distributions. Under these hypotheses, the search for the maximum of the posterior pdf reduces to the least-squares approach. More precisely, it reduces to the weighted least-squares, where the differences $\mathbf{y} - \mathbf{t}$ and the discrepancy of $\mathbf{p}^{(\text{cal})}$ from its prior expected-value have zero mean and are weighted by the inverse of the corresponding covariance matrices. Such matrices take a diagonal form if the elements of $\mathbf{y} - \mathbf{t}$ are independent of each other; moreover, if the variances of each element of $\mathbf{y} - \mathbf{t}$ are equal, then the optimal set of parameters obtained from the Bayesian approach reduces to the standard least-squares solution. However, this is not the only possible choice. In fact, if outliers are present—i.e., if some values of $\mathbf{y}$ are very far from the expected target

value $\mathbf{t}$ —an exponential distribution might provide a better approximation of the pdfs, particularly of the likelihood, and it practically leads to the minimisation of ℓ^1 -like norms.

The above remarks are fundamental, because they implicitly show which are the conditions and the physical requirements at the basis of the classical least-squares approach. Those remarks should not be considered as limitations to the relevance of the Bayesian approach, which is not restricted to find a single optimal set of parameter values. Such an approach should be applied to find the posterior pdf of parameter values so that it provides a potentially powerful tool to analyse uncertainties in the model parameters and, therefore, in the model outcomes and forecasts.

At the beginning of this section, it was mentioned that the discrepancy between model forecast and calibration target depends on measurement errors, on the non-optimal choice of parameter values, and also on model errors. An interesting and more thorough discussion about this topic, particularly about the different role of uncertainties in the model and in the model parameters, can be found in [106]. The fact that (23) is slightly different from the standard formulation proposed by other authors, who consider $\mathbf{y} - \mathbf{t} = \mathbf{s} - \mathbf{d}$, can be useful to stress some remarks. In fact, the framework applied in this paper allows the inclusion of different types of model forecasts and calibration targets. Some sort of prior information is contained not only in the prior pdf, which, by the way, implicitly introduces a regularisation. The likelihood and the marginal pdf depend on the prior assumptions and approximations introduced in the model, although this could be somehow masked by the notation. Moreover, few applications of the Bayesian approach consider the marginal pdf, because the latter is often assumed to be independent of $\mathbf{p}^{(\text{cal})}$. However, the definition given here shows in a quite explicit way that this quantity is affected by modelling assumptions. One could discard this problem, if only the optimal set of parameters is sought. But if the ultimate goal is to obtain a posterior pdf to be used for further analysis, e.g., to infer the uncertainty on model forecast from the uncertainty on model parameters, an accurate estimate of the marginal pdf is necessary and cannot be substituted with a trivial, straightforward assumption.

6. Conclusions

The goal of this paper was to propose a discussion of some properties of forward and inverse modelling in hydrology. The work is focused on the paradigmatic example of the transport equation, which is very commonly used in hydrology, and particularly for the simplest case of a purely diffusive, stationary, 1D transport.

A few essential messages can be summarised here.

The conceptual framework proposed by the author of this paper and some of his coworkers [71] can be very useful to cast the FP and the DIP in a proper way.

Some methods of model calibration, e.g., CMM, DCM, and the Bayesian approach, do not perfectly fit that framework. Nevertheless, such a conceptual framework and its formalism can be useful to cast those methods in more general cases. Furthermore, it provides a non-standard approach that can be useful to discuss some problems, like the role of uncertainties on the model structure, as mentioned in the last remarks of Section 5.3.

With regard to the terminology used to describe the results of mathematical models for hydrology, and more generally for natural sciences, this work has the ambition to clarify the distinction between words that are considered as synonyms in common language and that are sometimes used without any specific care in scientific papers and technical reports. In particular, the conceptual framework permits us to differentiate model results or outcomes (i.e., the state of the system obtained from the solution to the FP) from model forecasts (or reanalysis, or products, whose evaluation could involve data and parameters). On the other hand, words like prediction should be carefully used, possibly only in specific contexts like, e.g., statics.

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Abbreviations and Symbols

The following abbreviations are used in this paper:

BCs	boundary conditions;
BICs	boundary and initial conditions;
CMM	comparison Model Method;
DCM	dual constraint Method;
DIP	discrete inverse problem;
FP	forward problem;
pdf	probability density function.

The following mathematical symbols are used in this paper.

For the description of the general framework of the FP and the DIP:

d	array of data;
f	array of functions describing the FP;
g	function of p denoting the solution to the FP;
p	array including model parameters;
p ^(cal)	array of model parameters whose values must be fitted;
p ^(fix)	array of model parameters whose values are fixed;
p ^{(cal)*}	solution to the DIP;
s	array of the state of the system, i.e., the solution to the FP;
t	array of calibration target;
y	array of model forecasts;
P	set of the admissible model parameters;
P ^(cal)	set of potential solutions to the DIP;
S	set of state of the system;
$N_{(c)}$	number of elements of p ^(cal) ;
$N_{(f)}$	number of elements of p ^(fix) ;
$N_{(p)}$	number of model parameters;
$N_{(s)}$	number of elements of s ;
$N_{(t)}$	number of elements of t and y ;
O	objective function;
d	discrepancy function;
x' , x''	elements of $\mathbb{R}^{N_{(t)}}$;
α, β, γ	numbers.

For the paradigmatic example:

a	phenomenological coefficient (e.g., conductivity, diffusivity, and transmissivity);
$a_{i-1/2}$	discrete phenomenological coefficient (e.g., internode or interblock conductance);
b	phenomenological coefficient (capacity);
f	source/sink term;
i	node or cell index;
N	maximum node index;
u	potential (e.g., hydraulic head, solute concentration, and temperature);
u_{i-1}	potential at a node;
φ_i	sum of the source terms in a cell;
$\Delta x_{i-1/2}$	spacing between adjacent nodes;
$\mathbf{A}$	coefficient matrix for the paradigmatic example;
$\mathbf{b}$	known-term, including sink/source terms and BICs;
D_t	Lagrangian derivative;
$\mathbf{x}_j$	measurement points;
$u_j^{(\text{meas})}$	measured value of the potential;
$^{(\text{int})}$	superscript to denote interpolated quantities.

For the discussion of some remarks coming from the application of the DIP to the curve number method:

CN	curve number;
c_1, c_2, c_3	phenomenological coefficients;
I_a	initial abstraction, i.e., losses before runoff begins;
m	index to denote different rainfall events;
M	number of rainfall events considered;
P	rainfall;
Q	runoff;
S	potential maximum retention after runoff begins.

For the discussion of some remarks coming from the application of the DIP to a COVID-19 spread model:

I, R, D	numbers of infected, recovered, and deceased persons;
n	time index;
$n_{\min}, n_{\max}$	minimum and maximum values of n ;
ζ	threshold-and-weight parameter;
$^{(j)}$	apex used in the DIP;
$^{(\text{ref})}$	apex used to denote values obtained from reference data.

For the discussion of the Bayesian approach and of some specific methods of solution to the DIP:

$f_{\text{likelihood}}$	likelihood;
f_{marginal}	marginal pdf;
$f_{\text{posterior}}$	posterior pdf;
f_{prior}	prior pdf;
$^{(D)}$	apex denoting quantities referred to the FP with Dirichlet BCs for DCM;
$^{(N)}$	apex denoting quantities referred to the FP with Neuman BCs for DCM;
ℓ	iteration index for CMM and DCM.

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