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Control Function Measures for Hydrodynamic Problems[1]

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This short paper shows that different choices made for control functions of information in hydrodynamic flow problems can have significant implications for interpretations of the system. Using as a simple illustration the case of a steady-state, one-dimensional flow model with no internal sources or sinks and with the hydraulic conductivity depending on a single parameter and the distance from the origin, it is shown that, even when a continuous, error-free head data set is provided, statements about the uniqueness or not of the inverse solution are conditioned on the choice of the control function. Care has to be exercised in obtaining physically meaningful results and, depending on the model assumptions and the data available, there may not be acceptable models. It is also shown that there may be more than one model behavior that is acceptable. The results have implications for the hydrodynamic upscaling problem for flow in permeable media, for ensemble averaging methods, and for parameter determination for deterministic models of permeable flow.

KEY WORDS: inverse problem, control functions, uniqueness.

INTRODUCTION

The problem of estimating aquifer characteristics from water level data, referred to as "parameter estimation or identification" or "inverse problem," has been studied extensively over the last 40 years (Carrera, 1987; de Marsily and others, 2000; Kitanidis and Vomvoris, 1983; Yeh, 1986). The issue of the uniqueness or not of the solution of the hydraulic conductivity field obtained from such an approach has been dealt with, among others, by Chavent (1974), Neuman (1973), and Neuman and Yakowitz (1979). Chavent (1974) studied the uniqueness problem for the cases of constant and spatially distributed parameters, respectively, and found that in the case of constant parameters the inverse problem returns a unique solution because in general there are more measurements than unknowns, whereas in the case of distributed parameters, and for a limited number of point measurements, the solution is always nonunique. Neuman (1973) and Neuman and Yakowitz (1979)

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have pointed out that the uniqueness of the solution to the inverse problem is affected by noise in water level data and “insufficient information about lateral flow rates or by the lack of sufficiently large hydraulic gradients in some parts of the aquifer.” The problem of uniqueness is related to the notion of identifiability, whether it is possible to obtain unique solutions of the inverse problem from data collected in the spatial and temporal domains. According to Kitamura and Nakagiri (1977) an unknown parameter was defined as identifiable “if it can be determined uniquely in all points of its domain by using the input-output relation of the system and the input-output data.” Chavent (1987) summarized and compared five definitions of identifiability of distributed parameter systems using the output least squares error criterion. Kitanidis and Vomvoris (1983) and Samper and Neuman (1989) cast the identifiability problem in a geostatistical context for estimating spatial covariance structures, and Sun and Yeh (1990) extended the concept of identifiability with three new definitions that were related to the reliability of experimental design.

Additionally, in many problems concerning hydrodynamic flow in permeable media, some form of averaging is usually performed on modeled processes, often using Darcy’s flow equation as a basic starting point for system description. Three fundamental types of averaging are customarily in place: averaging over “small” domains in order to describe the hydrodynamic flow on coarser scales (often referred to as the upscaling problem; Desbarats, 1992; Rubin and Gomez-Hernandez, 1990); averaging to describe an ensemble of possible situations because of uncertainty or variation in system parameters and/or boundary conditions and/or measurement uncertainty (Gomez-Hernandez and Gorelick, 1989); and averaging to describe how well a particular model matches a set of data, often with model parameter determination obtained by minimizing specific functionals describing the global mismatch of data and model behaviors (Carrera and Neumann, 1986a,b; Clifton and Neuman, 1982; Desbarats and Dimitrakopoulos, 1990).

The purpose of this short paper is to illustrate, by specific example, that the choice of the measure of mismatch, the objective function that is used to define uniqueness or not of the solution to the inverse problem, can have profound implications for inferences pertinent to a hydrodynamic system.

SPECIFIC HYDRODYNAMIC FLOW MODEL

Consider one-dimensional, steady-state flow with no internal sources or sinks in which the head is h_0 on $x = 0$, and h_L on $x = L$. This description may represent physically the case of a confined aquifer between two long, parallel, straight rivers with the distance between the rivers being L and the heads in the rivers given by h_0 and h_L, respectively. Alternatively, one may consider that the description represents vertical, steady-state flow across a perfectly stratified aquitard of thickness L

bounded by two constant-head planes. In either case the x-axis is defined normal to the constant head boundaries. Take the hydraulic conductivity $K(x)$ to vary with x in the form

$$K(x) = K_0 \left(1 + \frac{2\eta x}{L}\right)^{-1} \tag{1}$$

where η is a dimensionless scaling constant and K_0 is also constant. This particular form of hydraulic conductivity represents the case of a porous medium composed of material that becomes progressively finer with distance from the origin and hence of decreasing hydraulic conductivity with distance x.

For one-dimensional, steady-state flow Darcy's law describes the relation between flow q and head $h(x)$ in the form

$$q = -K(x)\, dh/dx. \tag{2}$$

Note that Eq. (2) and the continuity equation $dq/dx = 0$ require that the head $h(x)$ is either monotonically increasing or decreasing with increasing x. Using Eq. (1) for the hydraulic conductivity, the solution to Eq. (2) is

$$h(x) = h_0 - \frac{q}{K_0} x \left(1 + \frac{\eta x}{L}\right), \tag{3}$$

which automatically satisfies the boundary condition $h(x) = h_0$ on $x = 0$. On $x = L$, the boundary condition $h(x) = h_L$ requires

$$\frac{Lq(1+\eta)}{K_0} = -(h_L - h_0), \tag{4}$$

so that expression (3) can be written in the more transparent form

$$h(x) = h_0 + (h_L - h_0)\frac{x}{L}\frac{\left(1 + \frac{\eta x}{L}\right)}{(1+\eta)}. \tag{5}$$

Now suppose that this model of head variation is used in an attempt to satisfy a set of continuous, statistically sharp (no measurement error or noise), data on head $H(x)$ in $0 < x < L$, and where the data are taken in the form

$$H(x) = h_0 + (h_L - h_0)\ f(x/L), \tag{6}$$

where $f(x/L)$ is dimensionless with the values $f(0) = 0$ and $f(1) = 1$. Note that the head data $H(x)$ are measured with depth x across the aquitard. The data do *not* have to conform to the assumed one-dimensional model behavior. The aim is to determine how well such models, under their basic assumptions, satisfy the head data.

In particular, one is interested in the value of the parameter η, which provides the "best" fit of the model $h(x)$ to the data field $H(x)$. Customarily, such problems are handled by some form of global measure of mismatch (an objective function) between $h(x)$ and $H(x)$, which is then extremized to obtain the "best" value of η; i.e. the value which minimizes the measure chosen. For instance, one quadratic measure is

$$\Psi_0^2 = \frac{1}{(h_L - h_0)^2} \int_0^L (H(x) - h(x))^2 \, dx = \int_0^L \left\{ f(x/L) - \left(\frac{x}{L}\right) \frac{1 + \frac{\eta x}{L}}{1 + \eta} \right\}^2 dx. \tag{7}$$

But an alternative acceptable objective function is a weighted quadratic measure

$$\begin{aligned} \Psi_1^2 &= \frac{1}{(h_L - h_0)^2} \int_0^L [(1 + \eta)(H(x) - h(x))]^2 \, dx \\ &= \int_0^L \left\{(1 + \eta) f(x/L) - \left(\frac{x}{L}\right) \left(1 + \frac{\eta x}{L}\right)\right\}^2 dx. \end{aligned} \tag{8}$$

And, when minimized with respect to η, Ψ_0^2 and Ψ_1^2 return *different* values for η. This can be seen from the fact that minimization of Eq. (7) entails solving

$$\frac{d\Psi_0^2}{d\eta} = 0, \tag{9}$$

whereas the minima of Eq. (8) are obtained through the algebraic expression

$$\frac{d\Psi_1^2}{d\eta} = \left(\frac{1 + \eta}{2}\right) \frac{d\Psi_0^2}{d\eta} + \Psi_0^2 = 0. \tag{10}$$

Indeed if the optimum solution $\eta = \eta^*$ obtained from Eq. (9) also satisfies expression (10) then one needs to have $\Psi_0^2 = 0$, a condition that is only satisfied when the modeled head captures perfectly the variations of the measured head.

In fact, the generalization

$$\begin{aligned} \Psi_{p+1}^2 &= \frac{1}{(h_L - h_0)^2} \int_0^L [(1 + \eta)^{p+1}(H(x) - h(x))]^2 \, dx \\ &= \int_0^L \left\{(1 + \eta)^{p+1} f(x/L) - (1 + \eta)^p \left(\frac{x}{L}\right) \left(1 + \frac{\eta x}{L}\right)\right\}^2 dx \end{aligned} \tag{11}$$

when minimized with respect to η, returns the relation between the power p and the best value of $\eta(p)$ in the form (for $\eta \neq -1$)

$$\frac{d\Psi_{p+1}^2}{d\eta} = \left(\frac{1+\eta}{2}\right) \frac{d\Psi_0^2}{d\eta} + (p+1)\Psi_0^2 = 0, \tag{12}$$

which for $p = -1$ and $p = 0$ returns Eq. (9) and (10), respectively.

Equation (12), using the transformations $\alpha(u) = x/L \equiv u$, $\beta(u) = (x/L)^2 \equiv u^2$, and the definition of the integral

$$I_{gq} = \int_0^1 [f(u) - g(u)][f(u) - q(u)]\, du, \tag{13}$$

yields the optimum value of $\eta(p)$ in the implicit form of

$$p[I_{\alpha\alpha} + 2\eta I_{\alpha\beta} + \eta^2 I_{\beta\beta}] = -(1+\eta)[I_{\alpha\beta} + \eta I_{\beta\beta}]. \tag{14}$$

Note that if p is chosen to be zero (corresponding to Ψ_1^2) then the solutions to Eq. (14) are

$$\eta = -1 \tag{15}$$

or

$$\eta_1 = -I_{\alpha\beta}/I_{\beta\beta}, \tag{16}$$

whereas if $p = -1$ (corresponding to Ψ_0^2) then Eq. (14) yields

$$\eta_0 = (I_{\alpha\beta} - I_{\alpha\alpha})/(I_{\alpha\beta} - I_{\beta\beta}). \tag{17}$$

Also note that on $\eta = 0$, Eq. (14) returns

$$p_0 = -I_{\alpha\beta}/I_{\alpha\alpha}. \tag{18}$$

For values of p other than $p = 0$ and $p = -1$, Eq. (14) provides two values of η. A sketch of the curve p versus η is given in Figure 1. Thus by choosing different measures of global mismatch (represented here by the power p for the simple purposes of illustration) one obtains different "best" values for η.

There is a physical requirement, however. The value of η may *not* be smaller than -1, because then the model head $h(x)$ would reverse direction at the point $x* = L/|\eta|$, which would lie in the domain $0 < x < L$. On physical grounds such a

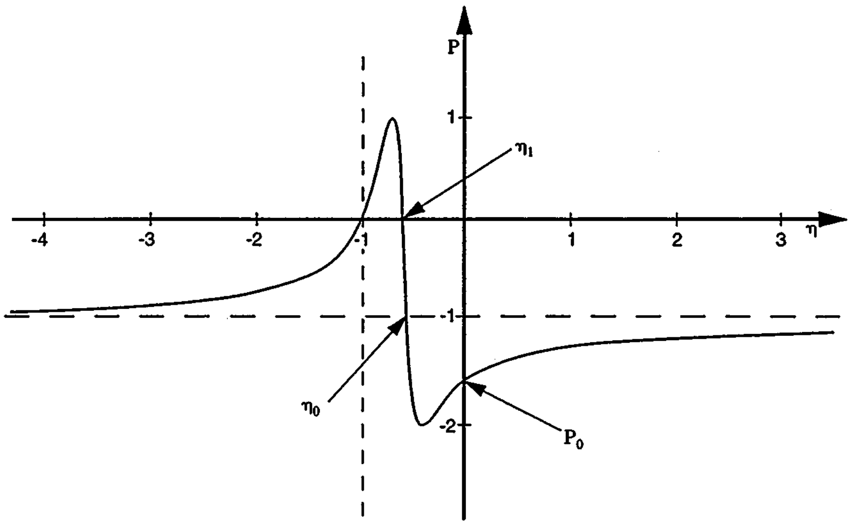

Figure 1. Sketch of the general shape of the p versus η curve represented by Eq. (14). The critical value of $\eta = -1$ is marked by a vertical dashed line. The two values ($p = 0$ and $p = -1$) at which Eq. (14) provides linear equations for η (with $\eta > -1$) are marked as η_1 (for $p = 0$) and η_0 (for $p = -1$), respectively. The value marked p_0 corresponds to $\eta = 0$.

reversal is forbidden because a steady one-dimensional flow model with no internal sources or sinks requires that $h(x)$ be monotonically increasing or decreasing in the range $0 < x < L$. This unphysical region ($\eta \leq -1$) is marked by the vertical dashed line at $\eta = -1$ on Figure 1.

In fact, a second, and much stronger, requirement exists. The value of η *must* exceed $-1/2$. This requirement follows because the model hydraulic conductivity is taken as proportional to $(1 + 2\eta x/L)^{-1}$. If η were to be smaller than $-1/2$, then the model conductivity could not be positive definite everywhere in $0 < x < L$, which it must be physically. Figure 2 provides a sketch of the behaviors allowed depending on whether η_0 and/or η_1 are themselves greater or less than $-1/2$. In Figure 2(a), neither η_1 nor η_0 can represent physically acceptable minima; in Figure 2(b), η_1 is not acceptable but η_0 is; while in Figure 2(c) both η_1 and η_0 are physically acceptable.

The first point to make is that, depending on the global measure of mismatch used, there can be many "best" solutions. The second point is that the "best" solution classes have to be constrained by the requirements of the problem. In the example given, the requirement of a monotone increasing (or decreasing) model head with increasing x demands $\eta > -1$, while the requirement of a positive model hydraulic conductivity everywhere demands enforcement of the stronger constraint $\eta > -1/2$.

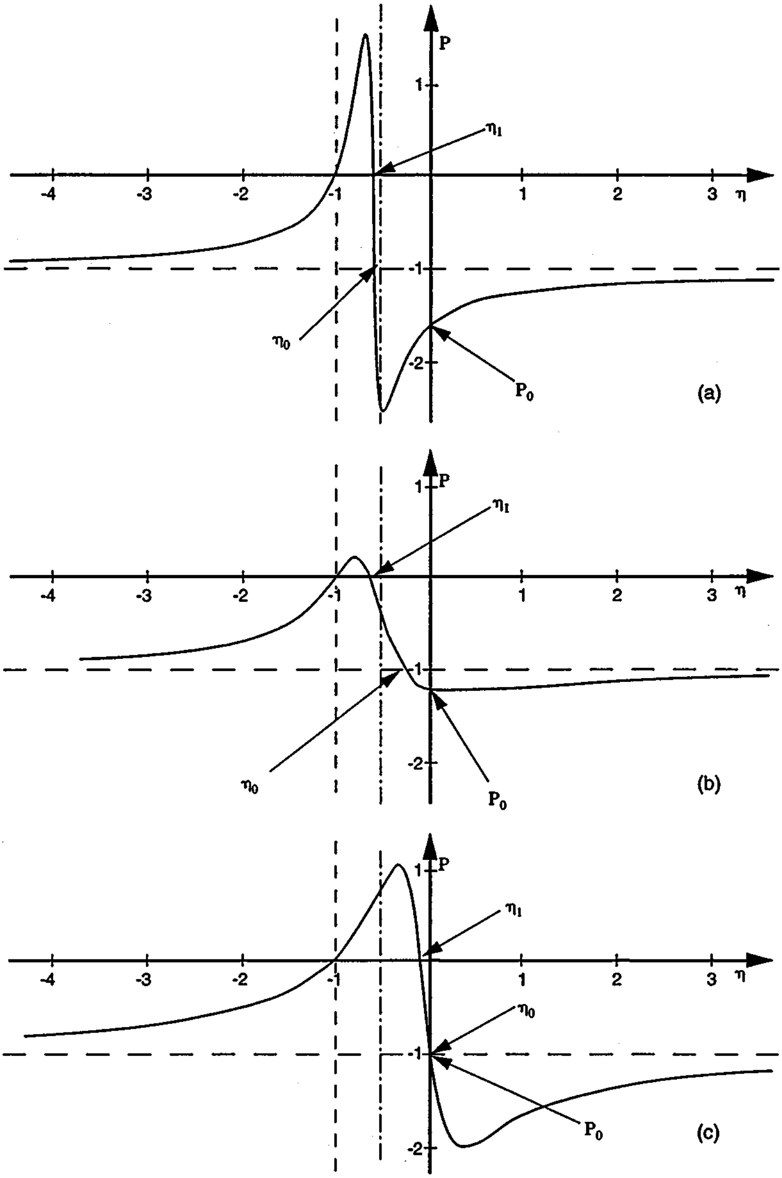

Figure 2. Sketch of the three behaviors for physical solutions of Eq. (14) when the extra constraint $\eta > -1/2$ is added (represented by the vertical dot–dash line at $\eta = -1/2$), as a consequence of requiring that the model hydraulic conductivity be positive everywhere in $0 < x < L$.

But, once these constraints are satisfied, there is still an infinite number of solutions possible for the parameter η, each depending on the value used for the parameter p. Indeed, inspection of Figure 1 or Figure 2 shows that there are always two solutions possible for η for each choice of p.

While it could be argued that the choice of the weighting factor $(1+\eta)^{1+p}$ of the mismatch between observed and modeled head is contrived, and while it could be argued that a different model dependence of hydraulic conductivity could be chosen, those points are not relevant to the argument. The point is that the model choices are not fundamentally forbidden. Thus, for instance, if the spatial dependence of the measured head data, $f(x/L)$, is such that η_0 and η_1 are both smaller than $-1/2$, then one cannot use measures of global mismatch which are of the form of Eq. (7) or (8), for both will yield unphysical values for η. Instead, with a weighting factor $(1+\eta)^{p+1}$, one must then arrange to have a value of p such that the curve of p versus η from Eq. (14) can never intersect the point $p = p^*$ at $\eta = -1/2$, where

$$p^* = -\{2I_{\alpha\beta} - I_{\beta\beta}\}/\{4I_{\alpha\alpha} - 4I_{\alpha\beta} + I_{\beta\beta}\}, \tag{19}$$

or else one cannot obtain physically meaningful results. And there will always be two “best” values of the parameter η for each chosen p value.

Other choices of weighting factors with, similarly, free parameters such as p, would also have to ensure that the corresponding η values exceed $-1/2$.

DISCUSSION

What can be learnt from the simple illustration reported here has implications for general hydrodynamic flow problems.

First, note that it is not sufficient, in general, just to choose arbitrary measures of mismatch for modeled head versus observations. The simple example given shows that any such measure must be constrained in order that parameters determined make physical sense. In more complex, three-dimensional, heterogeneous, partially saturated, time-dependent, anisotropic hydrodynamic problems, it may not be as clear as it is in the simple example considered here to ascertain that all physical conditions have been satisfied. Indeed, it may not even be possible to identify all such conditions.

Second, the weighting one attaches to a global measure of mismatch is, apparently, not only nonunique but also, for a given choice with free parameters, constrained by conditions not incorporated directly in the measure of mismatch, and may also lead to multiple solutions for physical parameter values. There does not seem to be any specific requirement available on what choice of weighting is most appropriate nor, indeed, any objective way of deciding the issue. This particular point is most vexing because the implication is that different authors will (and do) choose different weightings, so that intercomparison of results from different works is often difficult, if not impossible.

In addition, the question of how and what one averages in an upscaling hydrodynamic flow, as correctly representing the finer-scaled averaged information, are major concerns. Also note that the simple illustration dealt only with a spatially independent weighting factor. The complications that can ensue when a spatially dependent weighting factor is used, which may also depend on the physical parameters being sought, and which may also contain its own free parameters akin to the power p, are clearly problems of considerable concern in their own right.

Third, measures of global mismatch for, say, hydrodynamic head, do not contain all the salient information of the system being modeled—else there would be no need to impose extraneously the two requirements $\eta > -1$ (modeled head monotonic) and $\eta > -1/2$ (hydraulic conductivity positive) in the simple illustration. So another question of serious concern in general hydrodynamic flow problems is: When can one be sure that minimization measures used do contain all the information of the system, so that any results are guaranteed to make physical sense?

Fourth, for a minimization measure that returns a best parameter not within a physically acceptable range, one inference is that the model chosen is a poor approximation to the observations and one is advised to seek more relevant model behaviors—or, of course, a more appropriate measure of mismatch, or both.

Finally, while the example presented is extremely simple, it is its very simplicity that sharply illuminates the problems. The complications that arise when complex deterministic (and even more complex stochastic) models of flow are under consideration are, quite frankly, uninviting in this regard. The complexities would merely cloud the salient points, which are better brought out by the simple example used here.

It would, however, seem that the points raised need to be considered in virtually all hydrodynamic flow problems in a manner more detailed than appears to have been the case so far.

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