IDENTIFICATION OF PARAMETER ZONATION USING LEVEL SET METHODS

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ABSTRACT

We introduce a new inverse approach for efficiently identifying parameter structures (zonation) for the permeability field using the level set method, given spatially distributed observations of the permeability field (both lithology and/or permeability values) and hydraulic head measurements at various times. The permeability field is characterized by a number of zones, each of which represents a different lithology and may have a different permeability value. In this method, the boundaries of zones are represented by a level set function. Starting from an initial choice, these boundaries are implicitly manipulated through the evolution of the level set function, which is sequentially optimized to match the observed data and to satisfy some parameter regularization requirements. No assumption has been made on the shape, size, locations, and the number of these zones, or the correlation structure and the proportion of different lithology. A synthetic example shows that this method can locate those embedded zones efficiently.

1. INTRODUCTION

Accurately identifying geologic conceptual models, which include spatial distributions of stratigraphic units and fault zones and their properties (permeability, porosity, sorption coefficient, etc.), is critical to a wide range of applications, for example, contaminant site cleanup, reservoir simulations for oil/gas recovery, geological carbon sequestration. It is well known that geological systems are intrinsically deterministic but complex. However, these complex geological conceptual models are constrained only at a limited number of locations due to the high costs associated with subsurface measurements. Poor geological constraints leads to uncertainty in determining model structures and their hydrologic properties and thus, to uncertainty in predicting flow and solute transport in the subsurface. Although heterogeneity of hydraulic properties within stratigraphic units or fault zones plays an important role in flow and solute transport (Lu and Zhang, 2002; Lu and Zhang, 2003), it has been recognized recently that the uncertainty in conceptual model structures is the main source of prediction uncertainty (Neuman and Wierenga, 2003). Interfaces between stratigraphic units and fault zones are traditionally determined by geological correlation based on a limited number of boreholes and outcrop, without considering measurements of system state variables (e.g. pressure head, radionuclide concentration).

When observations of such state variables are available at a site, model calibration techniques can be used to improve parameter estimates and characterize uncertainties of these estimates (Neuman and Wierenga, 2003). In this calibration process, subsurface properties (say, permeability) of stratigraphic units and fault zones are iteratively updated such that the residual between the observed and modeled pressure head (or radionuclide concentration) is minimized. It is important to note that all existing model calibration techniques assume that the conceptual model is correct and they are not capable of updating interfaces between stratigraphic units and fault zones. Because these techniques rely on a prescribed geological conceptual model, calibrated parameter estimates are model-dependent. As a consequence, successful identification of parameter values from the model calibration process depends on the correctness of the input geological conceptual model.

Sun and Yeh [1985] were the first to propose a method to identify simultaneously both the parameter zonation and its parameter values for the hydraulic conductivity field. Using some model structure identification criteria, *Carrera and Neuman* [1986] were able to choose the best parameter zonation pattern among a number of given alternatives. *Eppstein and Dougherty* [1996] used a modified version of the extended Kalman filter, a data-driven procedure that dynamically determines and refines zonations. *Tsai et al.* [2003] used Voronoi zonation to parameterize the unknown distributed parameter and solved the inverse problem by a sequential global-local optimization procedure.

In this study, we develop a general methodology for parameter zonation identification based on the level set method and apply the approach to a simple case of one material embedded in another. This method can be used to identify, for example, low-permeability layers in a relatively higher permeability porous media (or vice versa), or highly permeable fault zones in the subsurface.

The level set method is a very powerful tool for solving problems that involve geometry and geometric evolution [*Osher and Sethian*, 1988]. It has also been applied to solving shape optimization problems [*Burger*, 2003]. By a shape we mean a bounded region $D \in R^n$ with a C^1 boundary. Instead of working on D directly, in the level set method a function $\phi(\mathbf{x})$ that corresponds to boundaries is manipulated to adjust D implicitly. The method has been used in several fields, including image segmentation [*Lie et al.*, 2005] and inverse problems [*Santosa*, 1996]. One of the advantages of the level set method is that it is much easier to work with a globally defined function than to keep track of the boundaries of regions of interest, which may split into many regions or merge

2. PROBLEM STATEMENT

We consider transient water flow in saturated porous media governed by the following equation

$$\nabla \cdot [K_s(\mathbf{x}) \nabla h(\mathbf{x}, t)] + g(\mathbf{x}, t) = S_s \frac{\partial h(\mathbf{x}, t)}{\partial t}, \quad \mathbf{x} \in \Omega \tag{1}$$

subject to appropriate initial and boundary conditions

$$h(\mathbf{x}, 0) = H_0(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \tag{2}$$

$$h(\mathbf{x}, t) = H(\mathbf{x}, t), \qquad \mathbf{x} \in \Gamma_D \tag{3}$$

$$-K_s(\mathbf{x}) \nabla h(\mathbf{x}, t) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}, t), \qquad \mathbf{x} \in \Gamma_N, \tag{4}$$

where $h(\mathbf{x},t)$ is hydraulic head, $H_0(\mathbf{x})$ is the initial head in domain Ω, $H(\mathbf{x},t)$ is the prescribed head on Dirichlet boundary segments Γ_D, $K_s(\mathbf{x})$ is hydraulic conductivity, $g(\mathbf{x},t)$ is source/sink term, $Q(\mathbf{x},t)$ is the prescribed flux across Neumann boundary segments Γ_N, $\mathbf{n}(\mathbf{x}) = (n_1, \cdots, n_d)^T$ is an outward unit vector normal to the boundary $\Gamma = \Gamma_D \cup \Gamma_N$, n_d is the dimensionality of domain Ω, and S_s is the specific storage. For simplicity, in this study, we assume that S_s is a constant because its variation is relatively small compared to that of the hydraulic conductivity.

It is also assumed that the saturated hydraulic conditivity is a piecewise constant function, which is defined on Ω that is partitioned into a number of unknown subdomains (zones). We do not know the hydraulic conductivity values for these zones and do not have enough direct information to infer the exact size, shape, and locations of these zones. Given the following measurements:

Log hydraulic conductivity: $\widehat{Y}_0 = (\widehat{Y}_i)$ at locations $\mathbf{x}_i, i = \overline{1, n_Y}$,
Type of stratigraphic units: $\widehat{\phi}_0 = (\widehat{\phi}_i)$ at locations $\mathbf{y}_i, i = \overline{1, n_\phi}$, and
head: $\widehat{h}_0 = (\widehat{h}_{ij})$ at locations $\boldsymbol{\chi}_i$ and times t_j, $i = \overline{1, n_h}$ $j = \overline{1, n_t}$,

our aim is to find the spatial distribution of these zones in the domain and the saturated hydraulic conductivity values for all these zones.

3. MATHEMATICAL FORMULATION

Suppose that there are a number of different stratigraphic units in an area of interest, we want to find a piecewise constant function such that

$$\phi(\mathbf{x}) = m, \qquad \mathbf{x} \in \Omega_m \subset \Omega, \tag{5}$$

where Ω_m, $m = \overline{1, M}$ is a unknown partition of Ω, i.e., $\cup_m \Omega_m = \Omega$, and M is the number of possible stratigraphic units. Here some of these Ω_m, $m = \overline{1, M}$, could be empty. In practice, one should choose M such that it is slightly larger than the number of possible stratigraphic units in the area of interest.

By defining basis functions associated with ϕ:

$$\psi_m(\mathbf{x}) = \frac{1}{\alpha_m} \prod_{j \neq m}^{M} (\phi(\mathbf{x}) - j), \quad \alpha_m = \prod_{j \neq m}^{M} (m - j), \tag{6}$$

it is easy to verify that $\psi_m(\mathbf{x}) = 1$ for $\mathbf{x} \in \Omega_m$ and $\psi_m(\mathbf{x}) = 0$ otherwise, and thus the log hydraulic conductivity can be expressed as a piecewise constant function

$$Y(\mathbf{x}) = \sum_{m=1}^{M} Y_m \psi_m(\mathbf{x}) \tag{7}$$

where Y_m is the log hydraulic conductivity of subdomain Ω_m. It is clear that $Y(\mathbf{x}) = Y_m$ for $\mathbf{x} \in \Omega_m$, as expected. Note that both Y and ψ_m are polynomials of order $M-1$ in terms of ϕ,

The basis functions ψ_m can be used to measure the length of boundary $\partial\Omega_m$ and the area of subdomain Ω_m

$$|\partial\Omega_m| = \int_\Omega |\nabla \psi_m| d\mathbf{x}; \qquad |\Omega_m| = \int_\Omega \psi_m d\mathbf{x}. \tag{8}$$

If we further define

$$W(\phi(\mathbf{x})) = \prod_{m=1}^{M} (\phi(\mathbf{x}) - m) \tag{9}$$

then by enforcing $W(\phi) = 0$, we ensure that a partition of Ω defined by $\Omega_m = \{\mathbf{x}|\phi(\mathbf{x}) = m\}$ is unique and there is no vacuum or overlapped areas among Ω_m, $m = \overline{1, M}$.

The inverse problem can be formulated as a minimization of the following functional

$$\begin{aligned} F(\phi, Y_0) &= \frac{1}{2}\sum_{i=1}^{n_Y} w_i^{(Y)} (Y(\mathbf{x}_i) - \widehat{Y}_i)^2 + \frac{1}{2}\sum_{i=1}^{n_\phi} w_i^{(i)} (\phi(\mathbf{y}_i) - \widehat{\phi}_i)^2 \\ &+ \frac{1}{2}\sum_{i=1}^{n_h}\sum_{j=1}^{n_t} w_{ij}^{(h)} (h(\boldsymbol{\chi}_i, t_j) - \widehat{h}_{ij})^2 + \beta \sum_{m=1}^{M} \int_\Omega |\nabla \psi_m(\mathbf{x})| d\mathbf{x}, \end{aligned} \tag{10}$$

where the first term measures the closeness of the estimated log hydraulic conductivity to the observed values at all observations points $\mathbf{x}_i$, $i = \overline{1, n_Y}$. The second term represents the difference between the observed and estimated types of stratigraphic units. The third term in (10) measures the difference between the observed head and the modeled hydraulic head using the estimated hydraulic conductivity field. The last term in (10) is the length of all boundaries $\partial\Omega_m$. Including this term in the objective function basically means that we prefer to take a partition with a relatively smaller boundary length. The importance of this term can be adjusted by tuning the coefficient β.

The inverse problem becomes a constrained minimization problem:

$$\min_{\phi, Y_0} F(\phi, Y_0), \quad \text{subject to } W(\phi) = 0 \tag{11}$$

where $Y_0 = (Y_1, Y_2, \cdots, Y_M)^T$ is a vector of permeability values for all units. The minimization in (11) can be solved by finding a saddle-point of the augmented Lagrangian functional [Lie et al., 2005]

$$L(\phi, Y_0, \lambda) = F(\phi, Y_0) + \int_\Omega \lambda(\mathbf{x}) W(\phi) d\mathbf{x} + \frac{r}{2}\int_\Omega |W(\phi)|^2 d\mathbf{x} \tag{12}$$

where $r > 0$ is a penalty parameter, and $\lambda(\mathbf{x})$ is the Lagrange multipler, which is a function defined on Ω. At the saddle point we have

$$\frac{\partial L}{\partial \phi} = 0; \quad \frac{\partial L}{\partial Y_m} = 0, \;\; m = \overline{1, M}; \quad \frac{\partial L}{\partial \lambda} = 0. \tag{13}$$

3.1. $\partial L/\partial\phi$. Taking the derivative of (12) with respect to ϕ yields

$$\begin{aligned} \frac{\partial L}{\partial \phi} &= \sum_{i=1}^{n_Y} (Y(\mathbf{x}_i) - \widehat{Y}_i) \frac{\partial Y(\mathbf{x}_i)}{\partial \phi} + \sum_{i=1}^{n_h}\sum_{j=1}^{n_t} (h(\boldsymbol{\chi}_i, t_j) - \widehat{h}_{ij}) \frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial \phi} \\ &- \beta \sum_{m=1}^{M} \nabla \cdot \left(\frac{\nabla \psi_m}{|\nabla \psi_m|} \right) \frac{\partial \psi_m}{\partial \phi} + \lambda \frac{\partial W}{\partial \phi} + r W(\phi) \frac{\partial W}{\partial \phi}, \end{aligned} \tag{14}$$

which involves computation of $\partial Y/\partial\phi$, $\partial h/\partial\phi$, $\partial\psi/\partial\phi$, and $\partial W/\partial\phi$. They can be derived from (6), (7), and (9):

$$\frac{\partial\psi_m}{\partial\phi} = \frac{1}{\alpha_m}\sum_{k\neq m}^{M}\prod_{j\neq m,k}^{M}(\phi - j), \tag{15}$$

$$\frac{\partial Y(\mathbf{x}_i)}{\partial\phi} = \sum_{m=1}^{M} Y_m \frac{\partial\psi_m(\mathbf{x}_i)}{\partial\phi}, \tag{16}$$

$$\frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial\phi} = \int_\Omega \frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial Y(\mathbf{x})}\frac{\partial Y(\mathbf{x})}{\partial\phi} d\mathbf{x}, \tag{17}$$

and

$$\frac{\partial W(\phi)}{\partial\phi} = \sum_{k=1}^{M}\prod_{j\neq k}^{M}(\phi(\mathbf{x}) - j). \tag{18}$$

3.2. $\partial L/\partial Y_m$**.** Taking the derivative of (12) with respect to Y_m yields

$$\frac{\partial L}{\partial Y_m} = \sum_{i=1}^{n_Y}(Y(\mathbf{x}_i) - \widehat{Y}_i)\frac{\partial Y(\mathbf{x}_i)}{\partial Y_m} + \sum_{i=1}^{n_h}\sum_{j=1}^{n_t}(h(\boldsymbol{\chi}_i, t_j) - \widehat{h}_{ij})\frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial Y_m} \tag{19}$$

Using the properties of the basis functions, (**??**) can be reduced to

$$\frac{\partial L}{\partial Y_m} = \sum_{\{k:\, \mathbf{x}_k \in \Omega_m\}}(Y_m - \widehat{Y}_k) + \sum_{i=1}^{n_h}\sum_{j=1}^{n_t}(h(\boldsymbol{\chi}_i, t_j) - \widehat{h}_{ij})\int_{\Omega_m}\frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial Y(\mathbf{x})}d\mathbf{x} \tag{20}$$

In the minimization process, we let $\partial L/\partial Y_m = 0$, which is equivalent to

$$Y_m = \frac{1}{N_m}\sum_{\{k:\, \mathbf{x}_k \in \Omega_m\}}\widehat{Y}_k - \frac{1}{N_m}\sum_{i=1}^{n_h}\sum_{j=1}^{n_t}(h(\boldsymbol{\chi}_i, t_j) - \widehat{h}_{ij})\int_{\Omega_m}\frac{\partial h(\boldsymbol{\chi}_i, t_j)}{\partial Y(\mathbf{x})}d\mathbf{x} \tag{21}$$

where N_m is the number of direct measurements in Ω_m. The first term in the above equation represents the arithmetic mean of all Y measurements in subdomain Ω_m, and the second term is the correction due to unfit between the modeled and measured head.

4. Illustrative Example

In this section, we illustrate the level set method with a two-dimensional synthetic binary field. The test system consists of steady-state, saturated water flow in a rectangular domain of 100 $m \times$ 100 m, discretized into elements of a size 1 $m \times$ 1 m. The true (synthetic) permeability field is shown in Figure 1(a), in which a lower-permeable layer ($k = 10^{-13}$ m^2) is embedded in the background material ($k = 10^{-10}$ m^2), offset by a fault, and observed at two boreholes. Lacking other constraining information, the geometry of the lower-permeable unit based on the traditional geological correlation will be incorrectly interpreted as a laterally connecting bed in the region between the two dashed lines. No matter how many observed head or concentration data are available, the parameter estimates from model calibration using this incorrect geological model certainly will yield erroneous results, and thus the prediction of flow and solute transport based on these parameter estimates will also be incorrect. The boundary conditions are prescribed as constant head at left (H_1 = 10.5 m) and right (H_2 = 10.0 m) boundaries and no flow at the two lateral boundaries. The steady-state flow equation is solved for the synthetic permeability field, and 36 steady-state head measurements at various locations (see Fig. 1a) are assumed to be available.

Since the lower-permeable unit has been observed at two wells, we initialize the iterative procedure by choosing an initial setting of lower-permeable zones as depicted in Fig. 3(b). The new boundary of low-permeability zones is determined iteratively. This process is repeated until either the prescribed number of updates has been reached or the difference between the modeled head and the observed head is smaller than a prescribed value. The evolution of the boundary ∂D is depicted in Figure 1c-1f, where the artificial time τ represents the number of updates. The final inversion results (Fig. 1f) are very similar to the true structures and head distribution, indicating that the level set method can be used to efficiently identify parameter zonation.

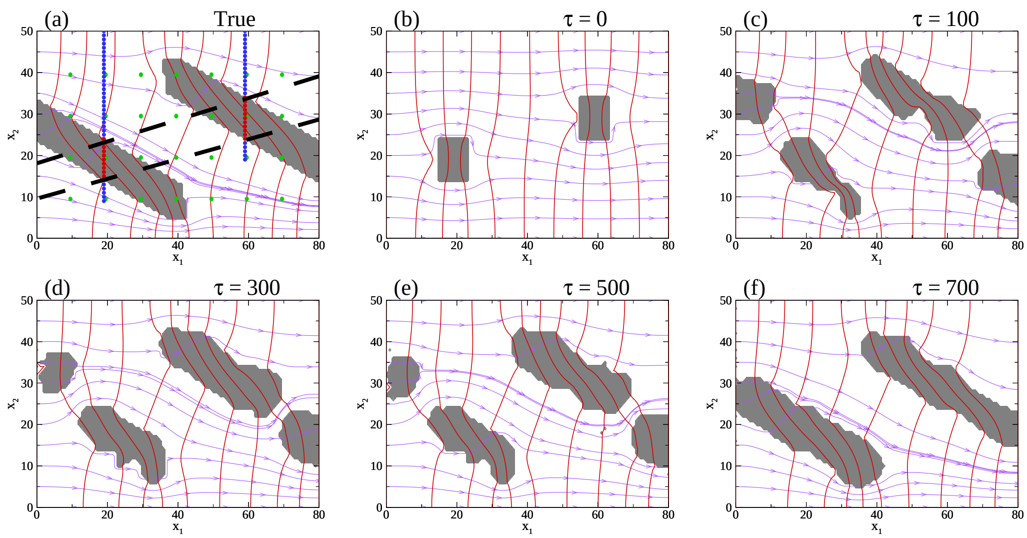

FIGURE 1. An illustrative example. (a) The problem configuration where the lower-permeable layer is offset by a fault and observed in two boreholes. The region between two dashed-lines is the possible lower-permeable zone identified by the traditional geological correlation. (b) Initial lower permeable zones in the proposed approach, based on borehole observation. (c-f) Identified lower-permeable units at several iteration steps.

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