Hydraulic Inverse Modeling Using Total-Variation Regularization with Relaxed Variable-Splitting

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Outline

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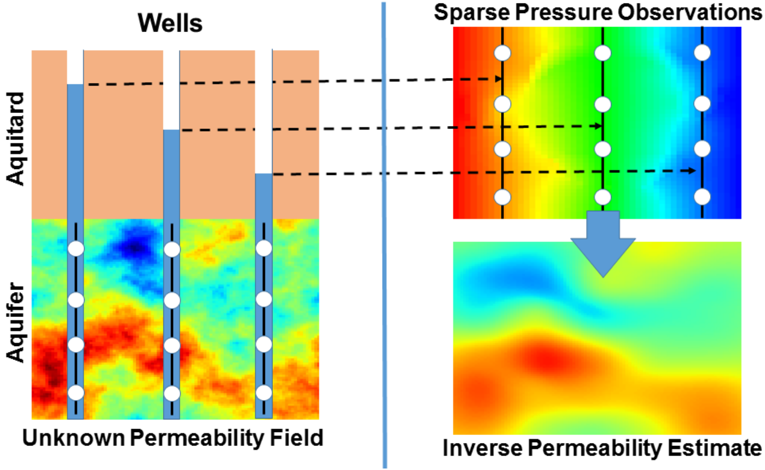
Introduction

- Inverse modeling seeks model parameters given a set of observed-state variables.
- For many practical hydrogeological problems, because the data coverage is limited, the inversion can be ill-posed and unstable.
- To stabilize the inversion, regularization techniques can be employed to eliminate the ill-posedness.
- The most commonly used type of regularization include Tikhonov and Total-Variation (TV).
- However, Tikhonov regularization tends to yield smoothed inversion results, and conventional TV regularization can be computationally unstable and yield unwanted artifacts.
- We have developed a novel hydraulic inverse modeling method using a TV regularization with relaxed variable-splitting scheme to preserve sharp interfaces and improve the accuracy of inversion.

Outline

Hydrogeologic Inverse Modeling - Illustration



- **Input:** Measured values (hydraulic heads) at N observation wells.
- **Output:** Model parameter values (conductivity or transmissivity) at every grid node of the model.

Forward Problem

The forward problem of hydrogeologic inverse modeling is governed by the groundwater flow equation,

Groundwater Flow Equation

$$\nabla \cdot (T \nabla h) = g$$
$$g(x, y) = 0$$
$$\left.\frac{\partial h}{\partial x}\right|_{a,y} = \left.\frac{\partial h}{\partial x}\right|_{b,y} = 0$$
$$h(x, c) = 0, h(x, d) = 1$$

where h is the hydraulic head, T is the transmissivity and g is a source/sink (here, set to zero).

Forward Problem

Using the operator, the forward modeling problem of the hydrogeologic inverse modeling can be simplified as,

Groundwater Flow Equation - Operator Form

$$\mathbf{h} = f(\mathbf{T}),$$

where $f(\cdot)$ is the forward operator mapping from the model parameter space to the measurement space.

Inverse Problem

Correspondingly, the problem of model calibration can be posed as a damped least-squares problem,

Hydrogeologic Inverse Modeling

$$\mathbf{m} = \arg\min_{\mathbf{m}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 \right\},$$

where $\mathbf{d}$ represents a recorded hydraulic head dataset, $\mathbf{m}$ is the calibrated model parameter, $\|\mathbf{d} - f(\mathbf{m})\|_2^2$ measures the data misfit, $||\cdot||_2$ stands for the L_2 norm.

Outline

Regularization Theory

- Inverse modeling with general regularization term can be posed as,

Hydrogeologic Inverse Modeling with Regularization

$$\hat{\mathbf{m}} = \arg\min_{\mathbf{m}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda \mathcal{R}(\mathbf{m}) \right\},$$

where $\mathcal{R}(\mathbf{m})$ is a general regularization term and the parameter λ is a parameter controlling the amount of regularization in the inversion.

Inverse Problem & Regularization Techniques

- General Regularization Methodology

Inverse Modeling with regularization

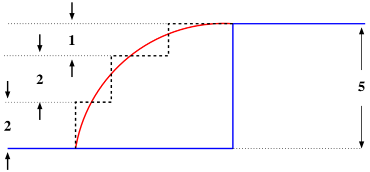
$$\min_{\mathbf{m}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda \mathrm{R}(\mathbf{m}) \right\},$$

where $\|\mathbf{d} - f(\mathbf{m})\|_2^2$ is data fidelity term, $\mathrm{R}(\mathbf{m})$ is the regularization term and λ is the regularization parameter.

- Specific Regularization and Its Characteristics
  - Total-Variation (TV): $\mathrm{R}(\mathbf{m}) = \|\nabla \mathbf{m}\|_1 = \sum_i |(\delta m)_i|$, (1-D)

    Best suited for reconstructing piecewise-constant functions, computationally expensive
  - Tikhonov (TK): $\mathrm{R}(\mathbf{m}) = \|L\mathbf{m}\|_2 = \sum_i (\delta m)_i^2$, (1-D)

    Best suited for reconstructing smooth functions, computationally cheap



- $\mathrm{TV}_{step} = 5$;
  $\mathrm{TV}_{smooth} = 2 + 2 + 1 = 5$.
- $\mathrm{TK}_{step} = 5^2 = 25$;
  $\mathrm{TK}_{smooth} = 2^2 + 2^2 + 1 = \mathbf{9} \leftarrow$.

Outline

Total Variation Regularization with Relaxed Variable-Splitting Scheme

The misfit function of hydraulic inverse modeling using total-variation regularization with relaxed variable-splitting is:

A New Misfit Function of Hydraulic Inverse Modeling

$$E(\mathbf{m}, \mathbf{u}) = \min_{\mathbf{m}, \mathbf{u}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda_1 \|\mathbf{m} - \mathbf{u}\|_2^2 + \lambda_2 \|\nabla \mathbf{u}\|_1 \right\},$$

- $\|\mathbf{d} - f(\mathbf{m})\|_2^2$ is the **data misfit term**;
- $\|\mathbf{m} - \mathbf{u}\|_2^2$ and $\|\nabla \mathbf{u}\|_1$ are the **regularization terms**;
- λ_1 and λ_2 are the **regularization parameters**;

Total-Variation Regularization with Relaxed Variable-Splitting

A New Misfit Function of Hydraulic Inverse Modeling

$$E(\mathbf{m}, \mathbf{u}) = \min_{\mathbf{m},\mathbf{u}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda_1 \|\mathbf{m} - \mathbf{u}\|_2^2 + \lambda_2 \|\mathbf{u}\|_{\mathrm{TV}} \right\},$$

where λ_1 and λ_2 are both positive regularization parameters.

- The regularization terms contain a new variable $\mathbf{u}$ and an additional term $\|\mathbf{m} - \mathbf{u}\|_2^2$ compared to the conventional TV regularization term.

Total-Variation Regularization with Relaxed Variable-Splitting

A New Misfit Function of Hydraulic Inverse Modeling

$$E(\mathbf{m}, \mathbf{u}) = \min_{\mathbf{u}} \left\{ \min_{\mathbf{m}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda_1 \|\mathbf{m} - \mathbf{u}\|_2^2 \right\} + \lambda_2 \|\mathbf{u}\|_{\mathrm{TV}} \right\},$$

where λ_1 and λ_2 are both positive regularization parameters.

- The regularization parameter λ_1 controls the trade-off between the data misfit term and the Tikhonov regularization term, and λ_2 balances the amount of interface-preservation in inverse modeling.

A New Misfit Function of Hydraulic Inverse Modeling (A Closer Look)

A New Misfit Function of Hydraulic Inverse Modeling:

$$E(\mathbf{m},\mathbf{u}) = \min_{\mathbf{u}} \left\{ \min_{\mathbf{m}} \left\{ \|\mathbf{d} - f(\mathbf{m})\|_2^2 + \lambda_1 \|\mathbf{m} - \mathbf{u}\|_2^2 \right\} + \lambda_2 \|\mathbf{u}\|_{TV} \right\},$$

where λ_1 and λ_2 are both positive regularization parameters.

- The inner problem is to solve for **m** using a conventional inverse modeling with the Tikhonov regularization and prior model **u**.
- The outer subproblem is to solve for **u** using a standard L_2-TV minimization method to preserve the sharpness of interfaces in inversion result **m**.
- The interleaving of solving these two subproblems leads to an inversion that not only improves the minimization of the data misfit, but also enhances the sharpness of interfaces.

Outline

Computation Methods

We employ the Alternating Direction Method of Multipliers (ADMM) to solve our new hydraulic inverse modeling

Alternating Direction Method of Multipliers (ADMM)

$$
\begin{aligned}
\mathbf{m}^{(k)} &= \operatorname*{argmin}_{\mathbf{m}} \{E_1(\mathbf{m})\} \\
&= \operatorname*{argmin}_{\mathbf{m}} \left\{ \|d - f(\mathbf{m})\|_2^2 + \lambda_1 \left\|\mathbf{m} - \mathbf{u}^{(k-1)}\right\|_2^2 \right\} \\
\mathbf{u}^{(k)} &= \operatorname*{argmin}_{\mathbf{u}} \{E_2(\mathbf{u})\} \\
&= \operatorname*{argmin}_{\mathbf{u}} \left\{ \left\|\mathbf{m}^{(k)} - \mathbf{u}\right\|_2^2 + \lambda_2 \|\mathbf{u}\|_{\mathrm{TV}} \right\}
\end{aligned}
$$

Selection of the Regularization Parameter: λ_1

- The subproblem of $\mathbf{m}^{(k)}$ is a classical inverse modeling with Tikhonov regularization.
- Various parameter estimation method has been developed: L-Curve, GCV, etc.

Selection of the Regularization Parameter: λ_2

- The subproblem of $\mathbf{u}^{(k)}$ is a classical L_2-TV minimization.
- Surprisingly, not many effective methods in existing references.
- We employ the unbiased predictive risk estimator (UPRE):

Selection of λ_2, (Lin et. al., SP (90) 2010):

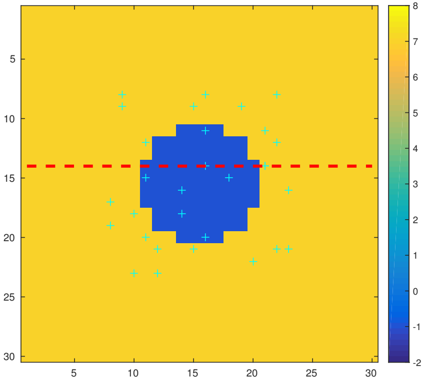
$$\lambda_2 = \underset{\lambda_2}{\operatorname{argmin}}\{\frac{1}{n}\|\mathbf{r}_{\lambda_2}\|_2^2 + \frac{2\sigma^2}{n}\text{trace}(A_{\text{TV},\lambda_2}) - \sigma^2\}.$$

Outline

Problem Setup and Model Discretization

- The reference problem is steady-state groundwater flow on the square domain, $[0, 1] \times [0, 1]$, with fixed hydraulic head at $y = 0$ and $y = 1$, zero flux boundaries at $x = 0$ and $x = 1$, and zero recharge.
- We run the tests on a Linux desktop with 32 cores of 2.0 GHz Intel Xeon E5-2650 CPU, and 16.0 GB memory.
- The groundwater flow equation is solved using the finite difference method on a uniform grid. The parameter grids are composed of horizontal and vertical transmissivity nodes (as are illustrated in figure below).

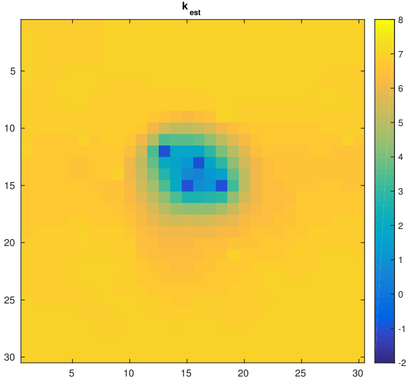
Model Calibration in Hydrology - True Model



True Model

- The plus (“+”) are the hydraulic-head observation points (wells).
- A horizontal profile indicated by the red dotted line will be used to compare the results.

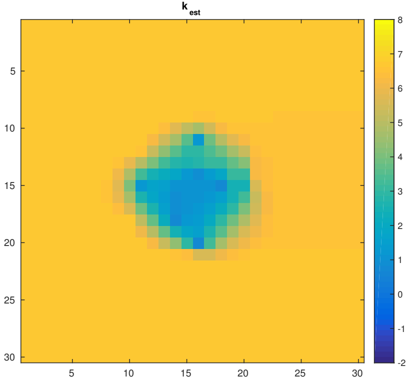
Inverse Modeling Result - 2D Inversion



2D Inversion

- Inversion result using inverse modeling with conventional TV regularization

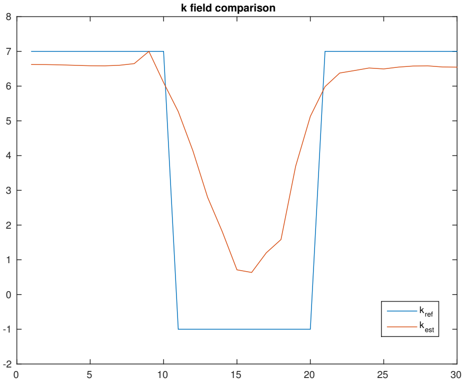
Inverse Modeling Result - 2D Inversion



2D Inversion

- Inversion result using inverse modeling with our new TV regularization

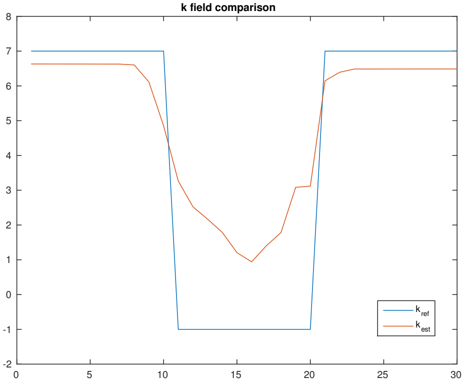
Inverse Modeling Result - 1D Profile



1D Horizontal Profile

- Profile of the inversion (red) v.s. the true value (blue)
- Inverse modeling with conventional TV method

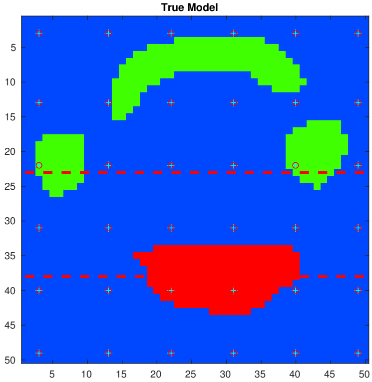
Inverse Modeling Result - 1D Profile



1D Horizontal Profile

- Profile of the inversion (red) v.s. the true value (blue)
- Inverse modeling with our new TV method
- The interface is much better preserved

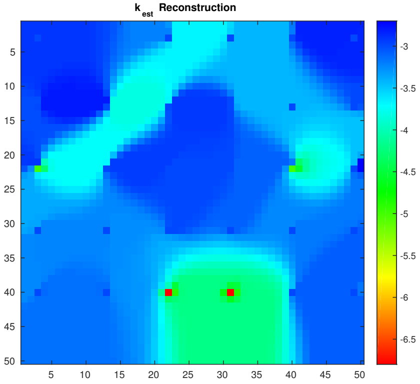
Model Calibration in Hydrology - True Model



True Model

- The dimension of the true model is 50×50.
- Two low-permeable geologic facies are included in the true model representing: sand (green) and clay (red). The background is highly permeable (gravel; blue). The permeability within all the three facies is assumed to be uniform.

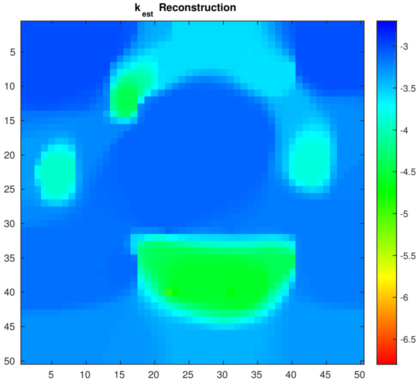
Inverse Modeling Result - 2D Inversion



2D Inversion

- Inversion result using inverse modeling with conventional TV regularization

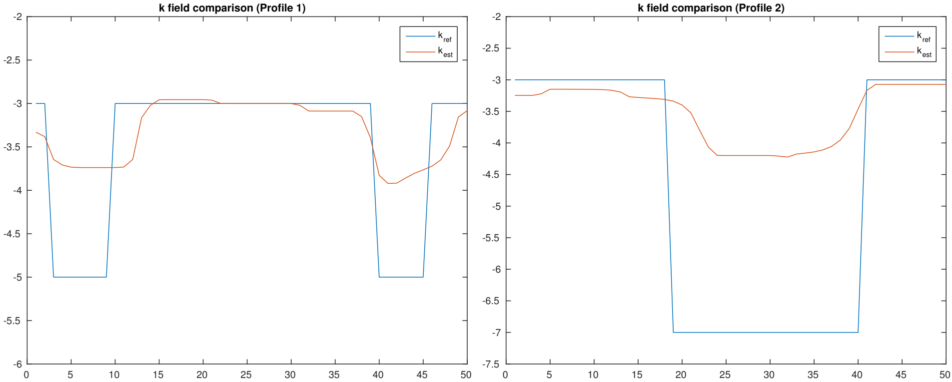
Inverse Modeling Result - 2D Inversion



2D Inversion

- Inversion result using inverse modeling with our new TV regularization

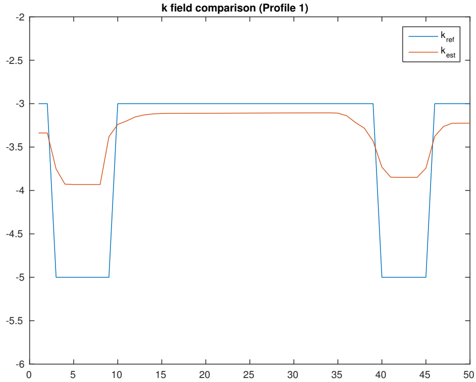
Inverse Modeling Result - 1D Profile

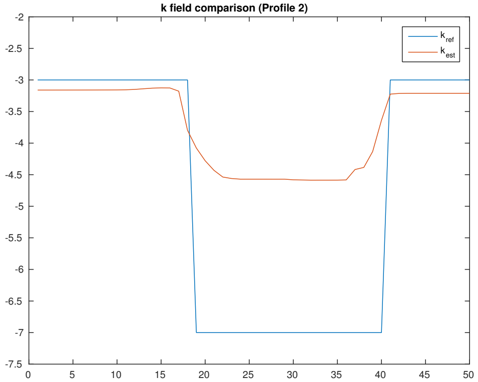


Location 1 Location 2

- Profile of the inversion (red) v.s. the true value (blue)
- Inverse modeling with conventional TV method

Inverse Modeling Result - 1D Profile





Location 1

Location 2

- Profile of the inversion (red) v.s. the true value (blue)
- Inverse modeling with our new TV method
- The interface is much better preserved

Outline

Conclusions

- We have developed a hydraulic inverse modeling using total-variation regularization with relaxed variable-splitting.
- Our numerical examples using synthetic data show that our new methods not only preserve sharp interfaces between facies with contrasting permeabilities, but also significantly improve the accuracy of the inversion. Therefore, our method has great potential in characterizing the subsurface heterogeneity problems.
- We implement our new inverse modeling method using Julia in the MADS computational framework (http://madsjulia.lanl.gov/), which can be downloaded at https://github.com/madsjulia/Mads.jl.

Acknowledgement

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