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Hyper-Differential Sensitivity Analysis to Support Geophysical Inverse Problems

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Motivation

Many geological processes may be modeled using **partial differential equations** (PDEs). Such models have tremendous potential to advance research in geosciences; however, their use is frequently limited by:

- uncertainties in physical parameters in the PDE,
- limitations on data needed for calibration and validation,
- and computational complexity associated with solving the PDEs over large spatial regions with fine resolution.

Inverse problems seek to utilize the available data to estimate uncertain parameters in the PDEs. However, the data available in practice is typically not adequate to estimate all parameters, and in some cases the data itself is uncertain.

Hyper-differential sensitivity analysis is a mathematical tool, suited for large scale applications, which augments the inverse problem to assess the sensitivity of parameter estimates to remaining uncertainties.

Formulation

We consider deterministic inverse problems constrained by PDEs of the form

$$\min_{u,z} J(u,z,\theta) \qquad (1)$$
$$s.t.\ c(u,z,\theta)=0$$

where
- J is an objective function
- c is a system of PDEs
- u are state variables (a solution of the PDEs)
- z is a uncertain parameter being estimated
- θ are parameters and/or data which are fixed in (1)

Goal: Analyze the sensitivity of the solution of (1), the optimal z, to perturbations in θ, the additional uncertain parameters and/or data.

Example: Contaminant Inversion

- Given sparse measurements, solve an inverse problem to determine the contaminant source.
- Modeled by coupling equations for fluid flow in porous media and contaminant transport, which contain uncertainty parameters related to:
  - material properties such as, but not limited too, permeability and porosity,
  - boundary conditions and constitutive laws for the porous media flow PDE(s),
  - fluid properties of the contaminant.
- HDSA is a quantitive assessment of how the contaminant source inversion depends upon these uncertainties.
- HDSA guides model development, data acquisition, and uncertainty quantification

Mathematical Framework

Differentiating Through the Optimality System

Given the local minima

$$x^\star(\theta)=(u^\star(\theta),z^\star(\theta),\lambda^\star(\theta))$$

of (1), with adjoint state $\lambda^\star$, for a user specified θ, the derivative of $x^\star(\theta)$, with respect to θ, is given by

$$\mathcal{D}x^\star(\theta)=-\mathcal{K}^{-1}\mathcal{B} \qquad (2)$$

where

- $\mathcal{K}$ denotes the Karush-Kuhn Tucker (KKT) operator, i.e. hessian of the Lagrangian, $\mathcal{L}$, with respect to (u,z,λ)
- $\mathcal{B}$ denotes the mixed second derivative of $\mathcal{L}$ with respect to (u,z,λ) and θ
- (2) is similar to a Newton step for (1), it may be interpreted as the Newton step taken after perturbing θ

Defining Sensitivity Indices

- define $\Pi(u,z,\lambda)=\mathcal{P}z$ for a projector $\mathcal{P}$
- $\mathcal{P}$ may be the identity, or a projection onto a linear subspace informed by the data
- define a basis $\{\theta_1,\theta_2,\dots,\theta_n\}$ for the fixed parameters

The sensitivity indices

$$S_i=\frac{||\Pi\mathcal{D}x^\star(\overline{\theta})\theta_i||}{||\theta_i||} \qquad i=1,2,\dots,n,$$

may be interpreted as the change in the optimal estimate $z^\star$ when the fixed parameter $\overline{\theta}$ is perturbed in the θ_i direction.

Computational Complexity

- computing all n sensitivity indices directly is computationally intensive for large n (the typical case)
- computing the action of $\mathcal{D}x^\star(\overline{\theta})$ on a perturbations $\delta\theta$ requires solving a large linear system (applying $\mathcal{K}^{-1}$)
- each matrix vector product (applying $\mathcal{K}$) requires two linear PDE solves
- need many PDE solves to explore high dimensional parameter spaces

Algorithmic Overview

- exploit low rank structure, when present, via a truncated Generalized Singular Value Decomposition (GSVD)
- leverage randomized algorithms to parallelize the GSVD computation
- leverage underlying Trilinos linear algebra constructs to parallelize PDE solves
- HDSA only requires linear PDE solves even when the PDE model c is nonlinear

Permeability Inversion

Tracer Injection to Estimate Permeability

$$\min_{p,c,z} M(p,c;d;\theta)+R(z) \qquad \text{misfit plus regularization}$$
$$s.t.$$
$$\nabla\cdot(-\kappa(z)\nabla p)=0 \qquad \text{Darcy's Law}$$
$$\frac{\partial c}{\partial t}+\nabla\cdot(-\epsilon(\theta)\nabla c)+(-\kappa(z)\nabla p)\cdot\nabla c=S(\theta) \qquad \text{Transport}$$
$$p=\psi(\theta) \qquad \text{Pressure Dirichlet BC}$$
$$-\kappa(z)\nabla p\cdot n=0 \qquad \text{Pressure Neuman BC}$$
$$\nabla c\cdot n=0 \qquad \text{Tracer Neuman BC}$$

- Compute sensitivity of the estimated permeability with respect to observed data, tracer uncertainty, and BCs.

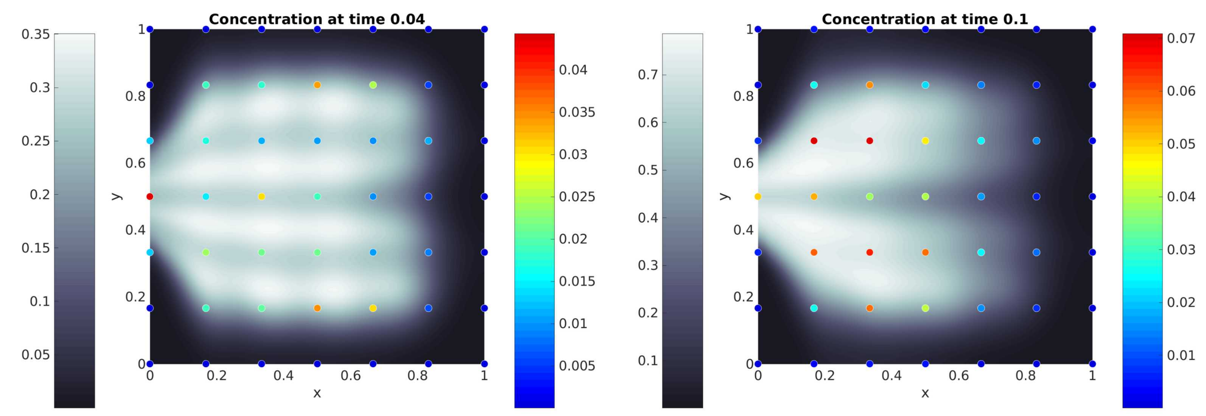

Figure 1: Time snapshots of tracer concentration (in greyscale) with the data sensitivities overlaid.

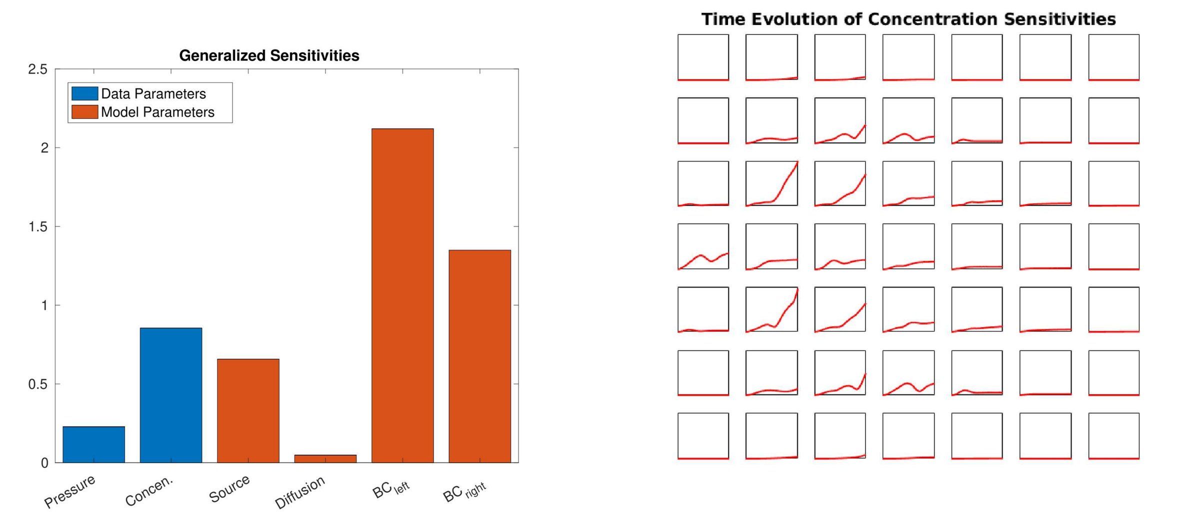

Figure 2: Generalized sensitivities (left) and time evolution of tracer data sensitivities (right).

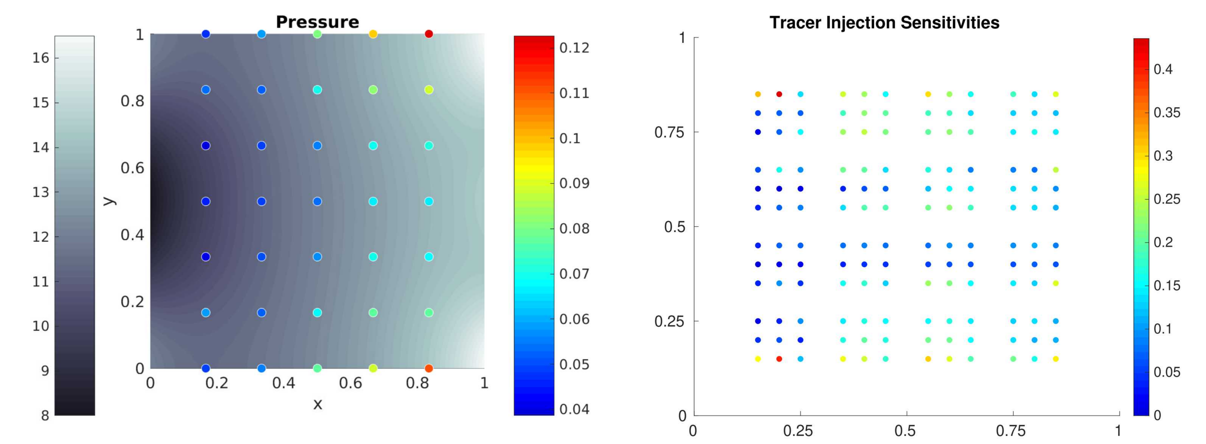

Figure 3: Pressure (in greyscale) with data sensitivities overlaid (left) and tracer injection sensitivities (right).

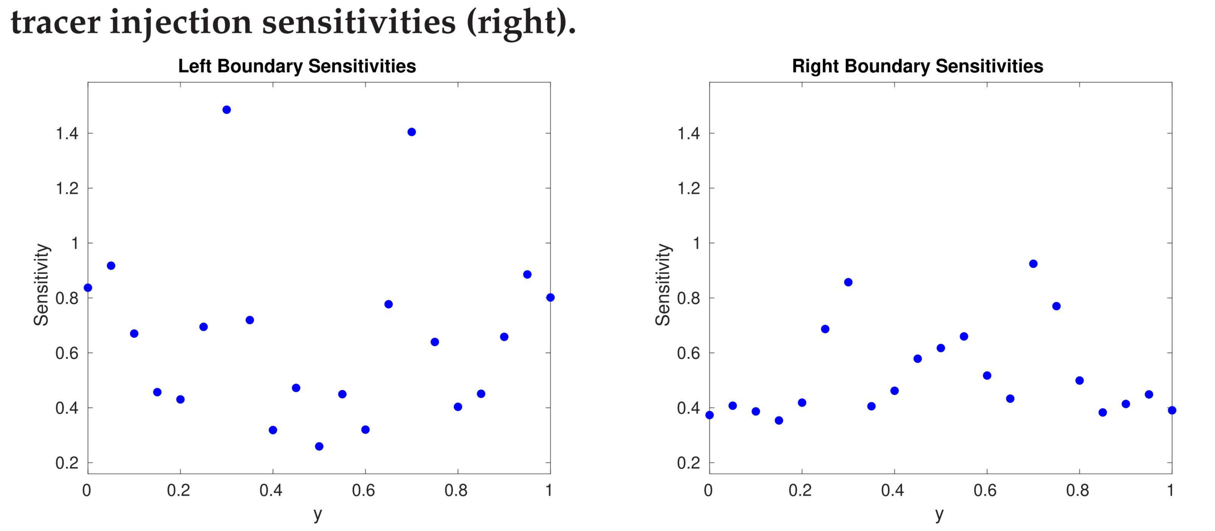

Figure 4: Pressure dirichlet BC sensitivities.

Source Inversion

Contaminant Source Identification

$$\min_{p,c,z} M(c;d)+R(z) \qquad \text{misfit plus regularization}$$
$$s.t.$$
$$\nabla\cdot(-\kappa(\theta)\nabla p)=0 \qquad \text{Darcy's Law}$$
$$\frac{\partial c}{\partial t}+\nabla\cdot(-\epsilon(\theta)\nabla c)+(-\kappa(\theta)\nabla p)\cdot\nabla c=S(z) \qquad \text{Transport}$$
$$p=\psi(\theta) \qquad \text{Pressure Dirichlet BC}$$
$$-\kappa(\theta)\nabla p\cdot n=0 \qquad \text{Pressure Neuman BC}$$
$$\nabla c\cdot n=0 \qquad \text{Contaminant Neuman BC}$$

- Compute sensitivity of the estimated source with respect to permeability, contaminant diffusivity, and BCs.

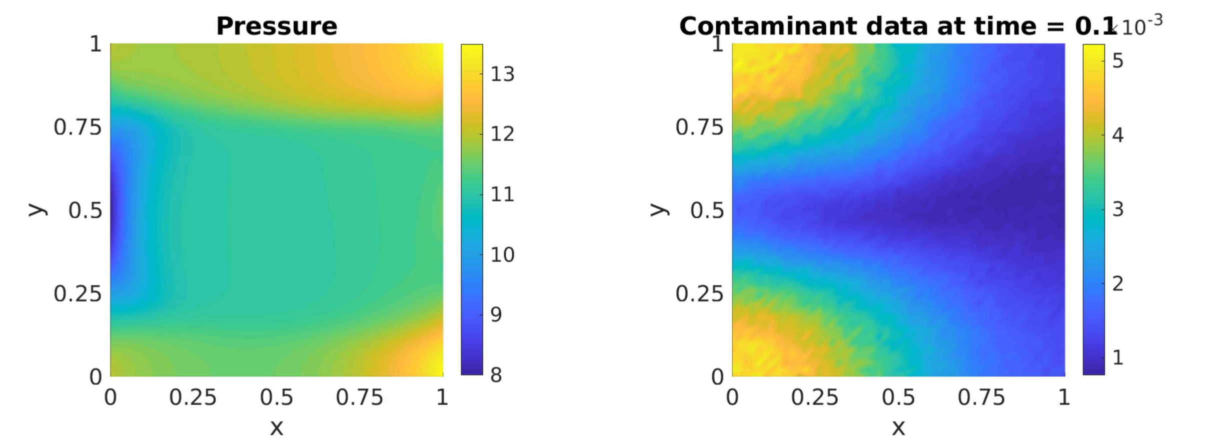

Figure 5: Pressure (left) and contaminant time snapshot (right).

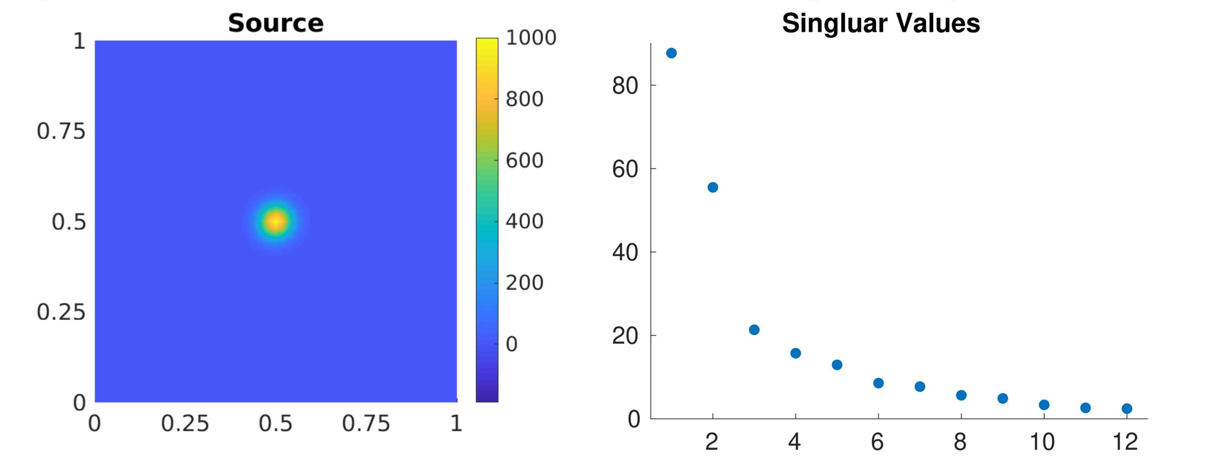

Figure 6: Contaminant source (left) and singular values of $\Pi\mathcal{D}x^\star(\overline{\theta})$ (right).

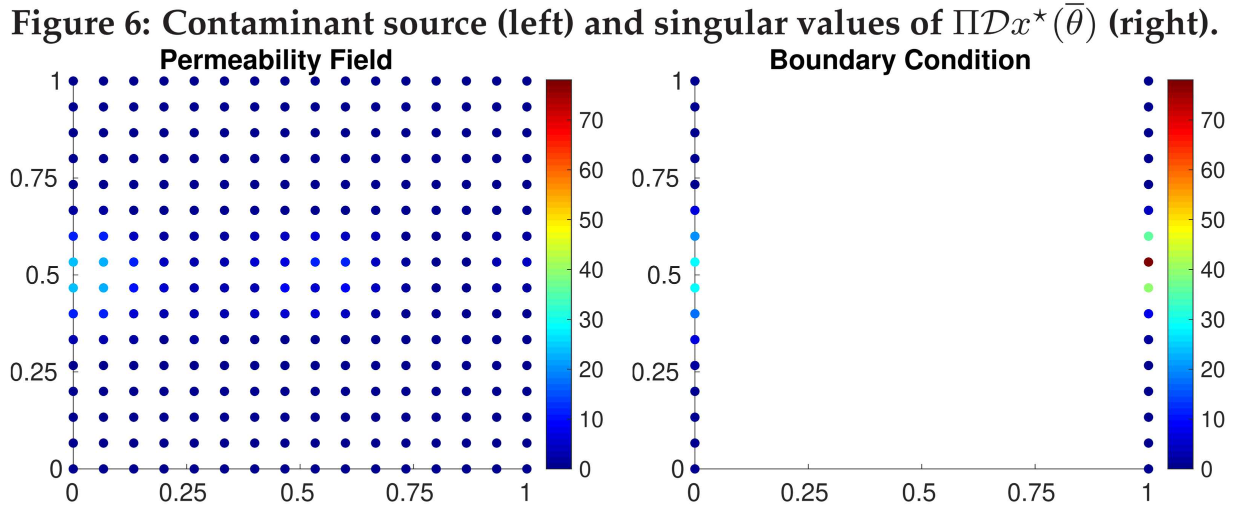

Figure 7: Permeability field (left) and dirichlet BC sensitivities (right).

Conclusions & Acknowledgments

- HDSA provides unique insights which are not given by other sensitivity analysis approaches
- HDSA may be used to assess the relative importance of data sources and model parameters in order to direct experimental design and model development
- HDSA may be used in a real time to provide an estimate of uncertainty in the solution of the inverse problem

- J. Hart, B. van Bloemen Waanders, and R. Herzog. Hyper-differential sensitivity analysis of uncertain parameters in PDE-constrained optimization. Submitted. arXiv: https://arxiv.org/abs/1909.07336
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