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Hyper-differential sensitivity analysis for PDE-constrained optimization: Methods and software

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1 Sensitivity Analysis Framework

- Classical Framework
- Hyper-Differential Sensitivity Analysis (HDSA) Framework

2 Method and Computation

- Overview of the Method
- Computational Considerations

3 Software Design

4 Applications

- Parametric Sensitivity for Optimal Control
- Parametric Sensitivity for Inverse Problems
- Data Source Sensitivity for Inverse Problems
- Distributional Sensitivity for Stochastic Optimization

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Classical Framework

- model mapping uncertain parameters θ to a model output $\mathcal{M}(\theta)$

$$\mathcal{M} : \Theta \rightarrow \mathcal{Y}$$

- Θ and \mathcal{Y} may be \mathbb{R}^n or infinite dimensional function spaces
- common approaches to sensitivity analysis seek to perturb or vary θ and analyze the model output $\mathcal{M}(\theta)$
- a simple example is when θ corresponds to physical parameters (such as material properties) in a partial differential equation (PDE) and $\mathcal{M}(\theta)$ is a functional of the solution of the PDE
- some possible sensitivity analysis approaches are to
 - compute the derivative of $\mathcal{M}(\theta)$ with respect to θ
 - generate samples $\{\theta_i\}_{i=1}^N$ in Θ , evaluate $\mathcal{M}(\theta_i)$, $i = 1, 2, \dots, N$, and estimate statistical properties of the model output

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Consider the PDE-constrained optimization problem

$$\begin{aligned} \min_{u,z} J(u, z, \theta) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

where

- J is an objective function
- u is a (infinite dimensional) state variable
- z is a (possibly infinite dimensional) optimization variable
- c is a PDE
- θ corresponding to (possibly infinite dimensional) physical parameters, data, and/or probability distributions

Goal: Determine the sensitivity of the **solution** of (1) to changes in θ .

Comparison with the Classical Framework

$$\begin{aligned} \min_{u,z} J(u, z, \theta) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

where

- the model $\mathcal{M}(\theta)$ in the classical framework corresponds to the solution of $c(u, z, \theta) = 0$ (given a particular z)
- in many applications our ultimate goal is the optimal solution of (1) or the PDE state evaluated at the optimal solution
- HDSA is a goal-oriented sensitivity analysis
- HDSA has various interpretations and uses depending upon:
 - if (1) is a control, design, or inverse problem
 - if (1) is a deterministic or stochastic optimization problem
 - if θ corresponds to physical parameters, data, or probability distributions

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Optimization Problem

$$\begin{aligned} \min_{u, z} J(u, z, \theta) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

- denote the Lagrangian for (1) by

$$\mathcal{L}(u, z, \lambda, \theta) = J(u, z, \theta) + \langle c(u, z, \theta), \lambda \rangle$$

- assume that (u^*, z^*, λ^*) is a local minimum of (1) with $\theta = \theta_0$

Under mild assumptions ², there exists a function

$$\mathcal{F} : \mathcal{N}(\theta_0) \rightarrow \mathcal{N}(u^*, z^*, \lambda^*)$$

such that

$$\nabla \mathcal{L}(\mathcal{F}(\theta), \theta) = 0$$

for any θ in a neighborhood of θ_0 .

²K. Brandes and R. Griesse, Quantitative stability analysis of optimal solutions in PDE-constrained optimization.

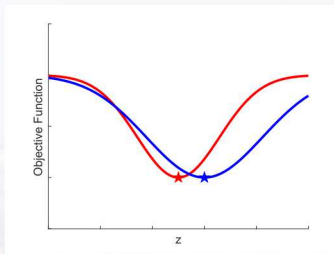
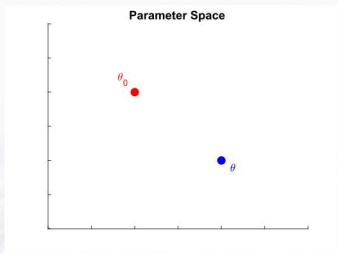
Parameter to Optimal Solution Mapping

$$\mathcal{F} : \mathcal{N}(\theta_0) \rightarrow \mathcal{N}(u^*, z^*, \lambda^*)$$

such that

$$\nabla \mathcal{L}(\mathcal{F}(\theta), \theta) = 0$$

$$\theta \quad \mapsto \quad \mathcal{F}(\theta)$$



Parameters



Optimal Solution

Differentiating through the Optimization Problem

$$\begin{aligned} \min_{u,z} J(u, z) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

$$\mathcal{F} : \mathcal{N}(\theta_0) \rightarrow \mathcal{N}(u^*, z^*, \lambda^*)$$

- $\mathcal{F}(\theta)$ is the solution of (1) with parameters θ
 - it depends on the particular local minimum (u^*, z^*, λ^*)
 - evaluating $\mathcal{F}(\theta)$ requires the solving (1) (expensive)
- the Fréchet derivative of \mathcal{F} with respect to θ is given by ³

$$D\mathcal{F}(\theta) = -\mathcal{K}^{-1}\mathcal{B}$$

where \mathcal{K} is the hessian of \mathcal{L} and \mathcal{B} is the Fréchet derivative of $\nabla\mathcal{L}$ with respect to θ (both evaluated at (u^*, z^*, λ^*))

³K. Brandes and R. Griesse, Quantitative stability analysis of optimal solutions in PDE-constrained optimization.

An Illustrative Example

$$\min_{u,z} J(u, z) = (u - 2)^2 + .0005z^2 \quad (2)$$

$$\text{s.t.} \quad u = \frac{1}{1 + e^{-\theta_1 z}} + \theta_2$$

- $u_{opt}(\theta), z_{opt}(\theta)$ be the optimal solution of (2) (as a function of θ), then

$$\frac{\partial z_{opt}}{\partial \theta_1}(0.5, 0.5) = 9.99 \quad \text{and} \quad \frac{\partial z_{opt}}{\partial \theta_2}(0.5, 0.5) = 3.12.$$

- If instead, (2) is solved with $\theta = (0.5, 0.5)$ and the derivative of

$$g(\theta_1, \theta_2) = \left(\frac{1}{1 + e^{-\theta_1 z_{opt}(0.5, 0.5)}} + \theta_2 - 2 \right)^2 + .0005 z_{opt}(0.5, 0.5)^2$$

is computed with respect to (θ_1, θ_2) we get

$$\frac{\partial g}{\partial \theta_1}(0.5, 0.5) = 0.135 \quad \text{and} \quad \frac{\partial g}{\partial \theta_2}(0.5, 0.5) = 1.03.$$

An Illustrative Example

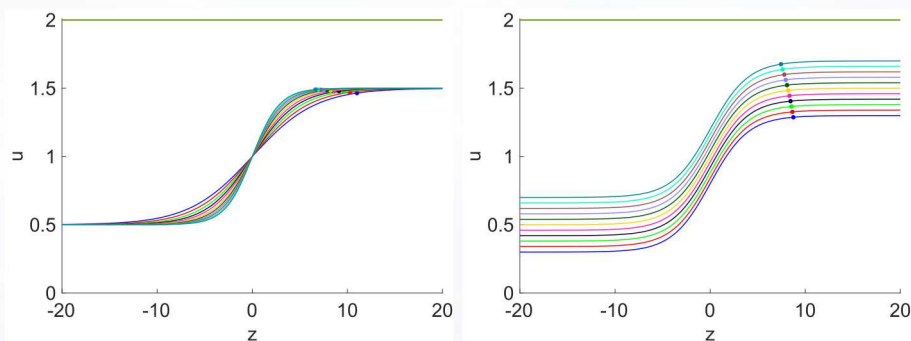


Figure: Plots of $u = \frac{1}{1+e^{-\theta_1 z}} + \theta_2$ and the optimal control strategies for different values of $\theta = (\theta_1, \theta_2)$. Left: varying θ_1 from 0.3 to 0.7 with $\theta_2 = 0.5$ fixed; right varying θ_2 from 0.3 to 0.7 with $\theta_1 = 0.5$ fixed.

Local Sensitivity Indices

$$\begin{aligned} \min_{u,z} J(u, z) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

$$\mathcal{DF} : \mathcal{N}(\theta_0) \rightarrow \mathcal{N}(u^*, z^*, \lambda^*)$$

- define $\Pi(u, z, \lambda) = z$ (or $\Pi(u, z, \lambda) = u$)
- define the local sensitivity function $\mathcal{S} : \Theta \rightarrow \mathbb{R}$ by

$$\mathcal{S}(\theta) = \frac{\|\Pi \mathcal{K}^{-1} \mathcal{B} \theta\|}{\|\theta\|} \quad \theta \in \Theta$$

- $\mathcal{S}(\theta)$ measures the sensitivity of the solution of (1) to parameter perturbations in the direction θ
- if $\{\theta_1, \theta_2, \dots, \theta_n\}$ is a finite dimensional basis for θ , define the local sensitivity indices

$$S_i = \mathcal{S}(\theta_i), \quad i = 1, 2, \dots, n$$

Global Sensitivity Indices

$$S_i = \frac{\|\Pi \mathcal{K}^{-1} \mathcal{B} \theta_i\|}{\|\theta_i\|} \quad i = 1, 2, \dots, n$$

- $\{S_i\}_{i=1}^n$ are local because the derivative $\mathcal{D}\mathcal{F}$ is evaluated at an optimal solution (u^*, z^*, λ^*) corresponding to a nominal parameter θ_0
- we can define global sensitivity indices by sampling different nominal parameters
 - care must be taken to account for multiple local minima, we handle this by associating the local minima with the initial iterate of the optimization routine
 - extensive sampling of local sensitivities is intractable in most applications, but useful insight may be gained from sparse sampling

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Local Sensitivity: Computation

$$S_i = \frac{\|\Pi\mathcal{K}^{-1}\mathcal{B}\theta_i\|}{\|\theta_i\|} \quad i = 1, 2, \dots, n$$

- requires solving the PDE-constrained optimization problem once, followed by n linear system solves with coefficient matrix \mathcal{K}
- n is large when, for instance, $\{\theta_1, \theta_2, \dots, \theta_n\}$ is a discretization of an infinite dimensional parameter field
- in many applications \mathcal{B} possesses a low rank structure, leveraging the singular value decomposition (SVD) yields

$$\|\Pi\mathcal{K}^{-1}\mathcal{B}\theta_i\| = \left\| \sum_{k=1}^{\infty} \sigma_k(v_k, \theta_i) u_k \right\| \approx \sqrt{\sum_{k=1}^m \sigma_k^2(v_k, \theta_i)^2}$$

where (σ_k, u_k, v_k) , $k = 1, 2, \dots$ are the singular triplets of $\Pi\mathcal{K}^{-1}\mathcal{B}$

- estimating the truncated SVD of $\Pi\mathcal{K}^{-1}\mathcal{B}$ allows efficient estimation of S_i , $i = 1, 2, \dots, n$

Singular Value Decomposition (SVD)

- the computational challenge is computing the truncated SVD (with appropriate inner products) of

$$\Pi \mathcal{K}^{-1} \mathcal{B} \quad (3)$$

- let M_θ and M_z denote the mass matrices (defining discretized functional space inner products using coordinate representations)
- the SVD of the discretized operator (3) may be extracted from the generalized eigenvalue problem

$$Ax = \lambda Mx$$

where

$$A = \begin{pmatrix} 0 & M_z \Pi \mathcal{K}^{-1} \mathcal{B} \\ \mathcal{B}^T \mathcal{K}^{-1} \Pi M_z & 0 \end{pmatrix}$$

and

$$M = \begin{pmatrix} M_z & 0 \\ 0 & M_\theta \end{pmatrix}$$

Generalized Eigenvalue Problem

$$\begin{pmatrix} 0 & M_z \Pi \mathcal{K}^{-1} \mathcal{B} \\ \mathcal{B}^T \mathcal{K}^{-1} \Pi M_z & 0 \end{pmatrix} \begin{pmatrix} \tilde{z} \\ \tilde{\theta} \end{pmatrix} = \lambda \begin{pmatrix} M_z & 0 \\ 0 & M_\theta \end{pmatrix} \begin{pmatrix} \tilde{z} \\ \tilde{\theta} \end{pmatrix}$$

- computational cost dominated by applying \mathcal{K}^{-1} (a large linear system solve)
- use conjugate gradient since \mathcal{K} is symmetric positive definite
- use randomized generalized eigenvalue solver from ⁴ to execute linear system solves in parallel on MPI subcommunicators
- postprocess dominant eigenvalues/vectors to estimate the truncated SVD (and hence local sensitivities)

⁴A.K. Saibaba, J. Lee, and P.K. Kitanidis, Randomized algorithms for generalized Hermitian eigenvalue problems with application to computing Karhunen-Loève expansion

Computational Cost Outline

$$\begin{aligned} \min_{u,z} J(u, z, \theta) \\ \text{s.t. } c(u, z, \theta) = 0 \end{aligned} \quad (1)$$

Cost to compute one local sensitivity (assuming all eigenvalue solver matrix vector products are parallelized)

- 1 solve (1) once
- 2 solve 4 large linear systems (whose coefficient matrix is the hessian of the Lagrangian of (1) evaluated at local minimum) for each matrix vector product required by the eigenvalue solver
- 3 many other inexpensive matrix vector products


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- our codes are developed within the Rapid Optimization Library (ROL) in Trilinos⁵
- C++ implementation with
 - parallel linear algebra constructs
 - abstract interfaces
- abstract interfaces enable applications of HDSA in many different problem contexts
- multi-level parallelism facilitates using HDSA on large scale applications

⁵Heroux, M., Bartlett, R., Hoekstra, V.H.R., Hu, J., Kolda, T., Lehoucq, R., Long, K., Pawlowski, R., Phipps, E., Salinger, A., Thornquist, H., Tuminaro, R., Willenbring, J., and Williams, A. An overview of Trilinos, Tech. Rep. SAND2003- 2927, 2003.

Rapid Optimization Library (ROL) ⁶

- contains state-of-the-art matrix free derivative-based optimization algorithms
- enables large scale PDE-constrained optimization for control, design, and inverse problems
- full space and reduced space approaches
- deterministic and stochastic optimization algorithms

⁶Kouri, D.P., von Winckel, G., and Ridzal, D. ROL: Rapid Optimization Library 

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Chemical Vapor Deposition Reactor

$$\min_{u,z} \frac{1}{2} \int_{\Omega} (\nabla \times v)^2 dx + \frac{\gamma}{2} \int_{\Gamma_c} z^2 dx$$

s. t.

$$u = (v_1, v_2, p, T)$$

$$-\epsilon(\theta) \nabla^2 v + (v \cdot \nabla) v + \nabla p + \eta(\theta) T g = 0 \quad \text{in } \Omega$$

$$\nabla \cdot v = 0 \quad \text{in } \Omega$$

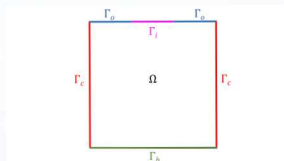
$$-\kappa(\theta) \Delta T + v \cdot \nabla T = 0 \quad \text{in } \Omega$$

$$T = 0 \quad \text{and} \quad v = v_i \quad \text{on } \Gamma_i$$

$$\kappa(\theta) \frac{\partial T}{\partial n} = 0 \quad \text{and} \quad v = v_o \quad \text{on } \Gamma_o$$

$$T = T_b(\theta) \quad \text{and} \quad v = 0 \quad \text{on } \Gamma_b$$

$$\kappa(\theta) \frac{\partial T}{\partial n} + \nu(\theta)(z - T) = 0 \quad \text{and} \quad v = 0 \quad \text{on } \Gamma_c$$



Chemical Vapor Deposition Reactor

$$\min_{u,z} \frac{1}{2} \int_{\Omega} (\nabla \times v)^2 dx + \frac{\gamma}{2} \int_{\Gamma_c} z^2 dx$$

s.t.

$$u = (v_1, v_2, p, T)$$

$$-\epsilon(\theta) \nabla^2 v + (v \cdot \nabla) v + \nabla p + \eta(\theta) T g = 0 \quad \text{in } \Omega$$

$$\nabla \cdot v = 0 \quad \text{in } \Omega$$

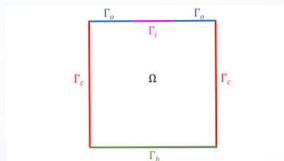
$$-\kappa(\theta) \Delta T + v \cdot \nabla T = 0 \quad \text{in } \Omega$$

$$T = 0 \quad \text{and} \quad v = v_i \quad \text{on } \Gamma_i$$

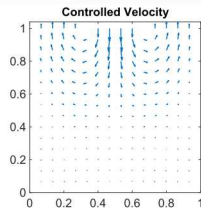
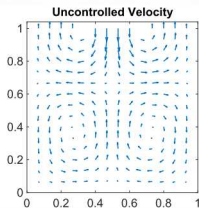
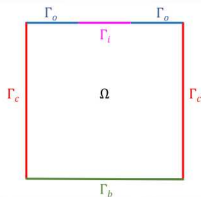
$$\kappa(\theta) \frac{\partial T}{\partial n} = 0 \quad \text{and} \quad v = v_o \quad \text{on } \Gamma_o$$

$$T = T_b(\theta) \quad \text{and} \quad v = 0 \quad \text{on } \Gamma_b$$

$$\kappa(\theta) \frac{\partial T}{\partial n} + \nu(\theta)(z - T) = 0 \quad \text{and} \quad v = 0 \quad \text{on } \Gamma_c$$



Chemical Vapor Deposition Reactor



- particles are injected into the top of a container
- the temperature on side walls is controlled to minimize vorticities in the fluid
- uncertainties enter through properties of the fluid and spatially distributed thermal boundary conditions

Control Solutions

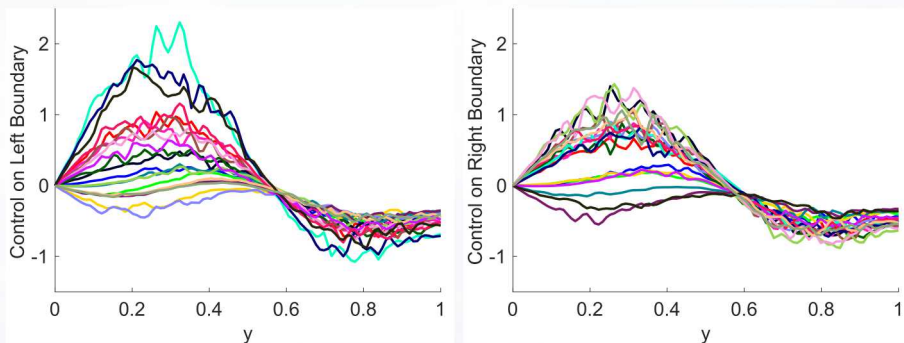


Figure: Control solutions corresponding to 20 different parameter samples. The left and right panels are the controllers on the left and right boundaries, respectively. Each curve is a control solution for a given parameter sample.

Singular Values

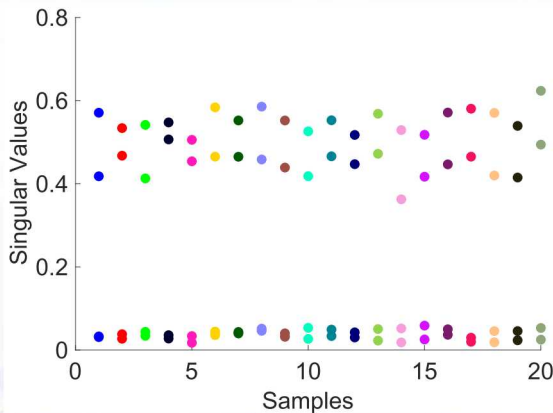


Figure: Leading 4 singular values at 20 different parameter samples. Each vertical slice corresponds to the leading 4 singular values for a fixed sample.

Local Sensitivities

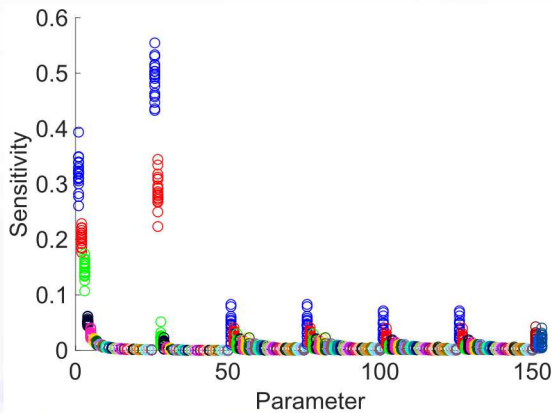


Figure: Local sensitivities for the 153 uncertain parameters. The 20 circles in each vertical slice indicates the sensitivity index for a fixed parameter as it varies over the 20 parameter samples.

Controller Singular Vectors

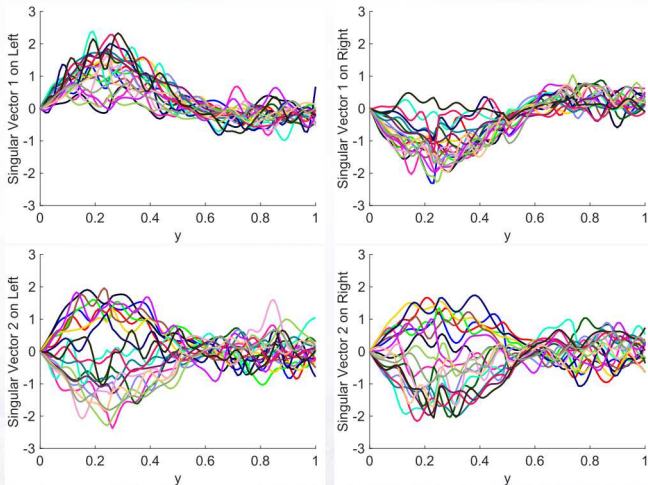


Figure: The top (bottom) row shows the first (second) singular vector on the left and right boundaries, respectively. Each curve corresponds to a different parameter sample.

Observations and Applications

Observations:

- local sensitivity analysis yields similar results for each parameter sample
- only around 10% of the uncertain parameters exhibit significant influence on the control strategy
- the bottom boundary condition, T_b , has the greatest influence on the control strategy

Applications:

- experimental efforts and/or modeling efforts should be invested toward characterizing the bottom thermal boundary condition

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Subsurface Contaminant Source Inversion

$$\min_{u,z} \frac{1}{2} \sum_{i=1}^T \sum_{j=1}^M (\mathcal{P}_{i,j}y - d_{i,j})^2 + \frac{\alpha}{2} \int_{\Omega} z(x,y)^2 dx dy$$

s.t.

$$u = (p, y)$$

$$\nabla \cdot (-\kappa(\theta)\nabla p) = 0$$

$$\frac{\partial y}{\partial t} + \nabla \cdot (-\epsilon(\theta)\nabla y) + (-\kappa(\theta)\nabla p) \cdot \nabla y = \chi_{[.01,.02]}(t)z$$

$$p = \psi(\theta)$$

$$-\kappa(\theta)\nabla p \cdot n = 0$$

$$\nabla u \cdot n = 0$$

$$u = 0$$

in Ω for

on Γ_L

on Γ_B

on $\Gamma_L \cup \Gamma_R \cup \Gamma_B \cup \Gamma_T$ for

in Ω for

Subsurface Contaminant Source Inversion

$$\min_{u,z} \frac{1}{2} \sum_{i=1}^T \sum_{j=1}^M (\mathcal{P}_{i,j}y - d_{i,j})^2 + \frac{\alpha}{2} \int_{\Omega} z(x,y)^2 dx dy$$

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$$\frac{\partial y}{\partial t} + \nabla \cdot (-\epsilon(\theta)\nabla y) + (-\kappa(\theta)\nabla p) \cdot \nabla y = \chi_{[.01,.02]}(t)z \quad \text{in } \Omega \text{ for}$$

$$p = \psi(\theta) \quad \text{on } \Gamma_L$$

$$-\kappa(\theta)\nabla p \cdot n = 0 \quad \text{on } \Gamma_B$$

$$\nabla u \cdot n = 0 \quad \text{on } \Gamma_L \cup \Gamma_R \cup \Gamma_B \cup \Gamma_T \text{ for}$$

$$u = 0 \quad \text{in } \Omega \text{ for}$$

Pressure Equation

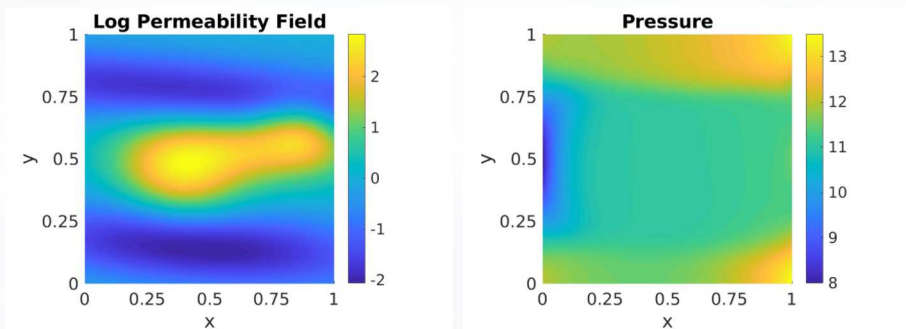


Figure: Left: the log (base 10) of the nominal permeability field; right: the solution of the pressure equation with nominal permeability field and boundary conditions.

- pressure field produces a right to left flow with high velocity around $y = 0.5$
- contaminant enters in the center of the domain and is advected to the left

Transport Equation

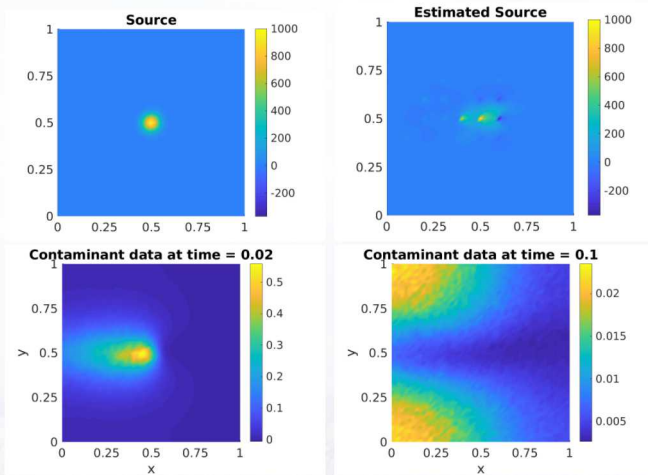


Figure: Top: the “true” source (left) used to generate synthetic data and the estimated source (right). Bottom: the noisy contaminant data at just after the contaminant injection (left) and after several time steps (right).

Singular Values

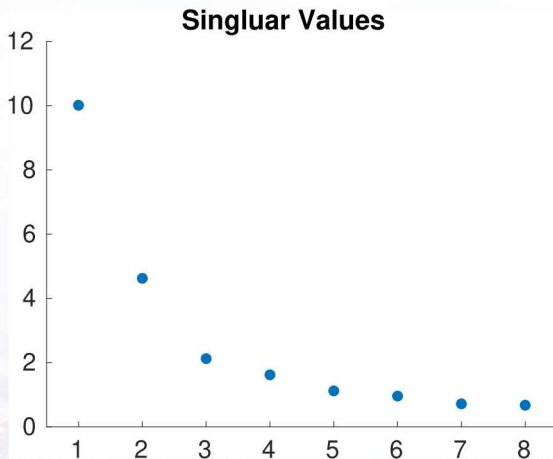


Figure: Singular values for local sensitivities computed at the nominal parameters.

Sensitivity Indices

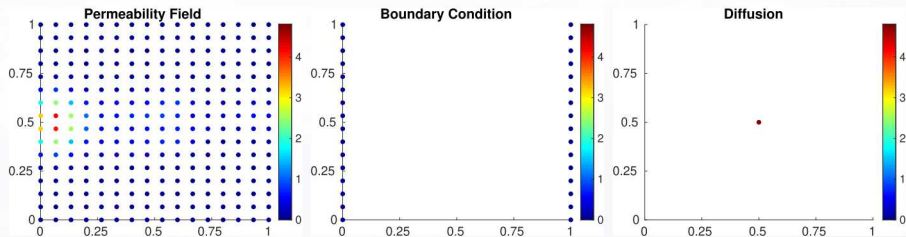


Figure: Sensitivity indices for the permeability field (left), pressure equation Dirichlet boundary conditions (center), and diffusion coefficient (right).

Observations and Applications

Observations:

- the estimated source is most sensitive to the diffusion coefficient
- the permeability field is most important in the region near $x = 0.10$ and $y = 0.50$
- the pressure boundary condition ψ is less influential

Applications:

- the magnitude of the sensitivities relative to the magnitude of the source provides a level of confidence in our estimation
- the localized region of high permeability sensitivity indicates that we may focus data acquisition efforts in a small region
- the high sensitivity of the diffusion coefficient indicates that properties of the contaminant are more important (locally around the nominal estimates) than the subsurface properties (permeability and boundary conditions)

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Tracer Test Permeability Inversion

$$\min_{u,z} \frac{1}{2} \sum_{j=1}^M \left(w_p (\mathcal{P}_j^p p - d_j^p)^2 + \sum_{i=1}^T w_y (\mathcal{P}_{i,j}^y y - d_{i,j}^y)^2 \right) + \frac{\alpha}{2} \int_{\Omega} \|\nabla z\|^2 dx dy$$

s.t.

$$u = (p, y)$$

$$\nabla \cdot (-e^z \nabla p) = 0 \quad \text{in } \Omega$$

$$\frac{\partial y}{\partial t} + \nabla \cdot (-\epsilon \nabla y) + (-e^z \nabla p) \cdot \nabla y = f \quad \text{in } \Omega \text{ for } t > 0$$

$$p = \psi \quad \text{on } \Gamma_L \cup \Gamma_R$$

$$-\kappa \nabla p \cdot n = 0 \quad \text{on } \Gamma_B \cup \Gamma_T$$

$$\nabla u \cdot n = 0 \quad \text{on } \Gamma_L \cup \Gamma_R \cup \Gamma_B \cup \Gamma_T \text{ for } t > 0$$

$$u = 0 \quad \text{in } \Omega \text{ for } t = 0$$

Tracer Test Permeability Inversion

$$\min_{u,z} \frac{1}{2} \sum_{j=1}^M \left(w_p (\mathcal{P}_j^p p - d_j^p - \theta_j^p)^2 + \sum_{i=1}^T w_y (\mathcal{P}_{i,j}^y y - d_{i,j}^y - \theta_{i,j}^y)^2 \right) + \frac{\alpha}{2} \int_{\Omega} \|\nabla z\|^2 dx dy$$

s.t.

$$u = (p, y)$$

$$\nabla \cdot (-e^z \nabla p) = 0 \quad \text{in } \Omega$$

$$\frac{\partial y}{\partial t} + \nabla \cdot (-\epsilon \nabla y) + (-e^z \nabla p) \cdot \nabla y = f \quad \text{in } \Omega \text{ for } t > 0$$

$$p = \psi \quad \text{on } \Gamma_L \cup \Gamma_R$$

$$-\kappa \nabla p \cdot n = 0 \quad \text{on } \Gamma_B \cup \Gamma_T$$

$$\nabla u \cdot n = 0 \quad \text{on } \Gamma_L \cup \Gamma_R \cup \Gamma_B \cup \Gamma_T \text{ for } t > 0$$

$$u = 0 \quad \text{in } \Omega \text{ for } t = 0$$

Permeability Field and Tracer Injection

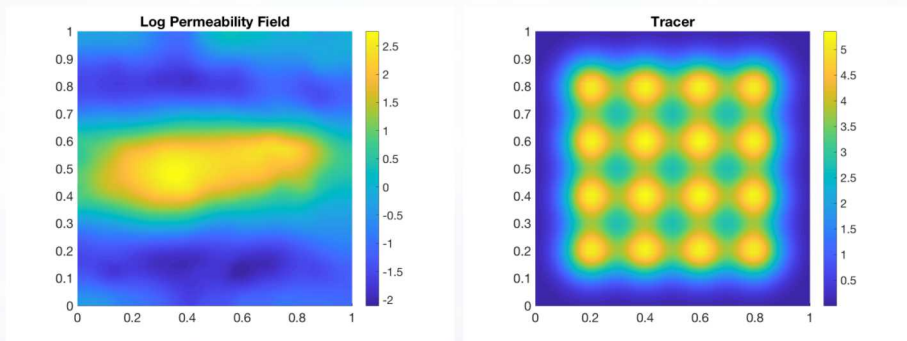


Figure: Left: the log (base 10) of the true permeability field; right: the tracer injection.

- pressure field produces a right to left flow with high velocity around $y = 0.5$
- tracer enters the domain through 16 injection points

Sensitivity Indices

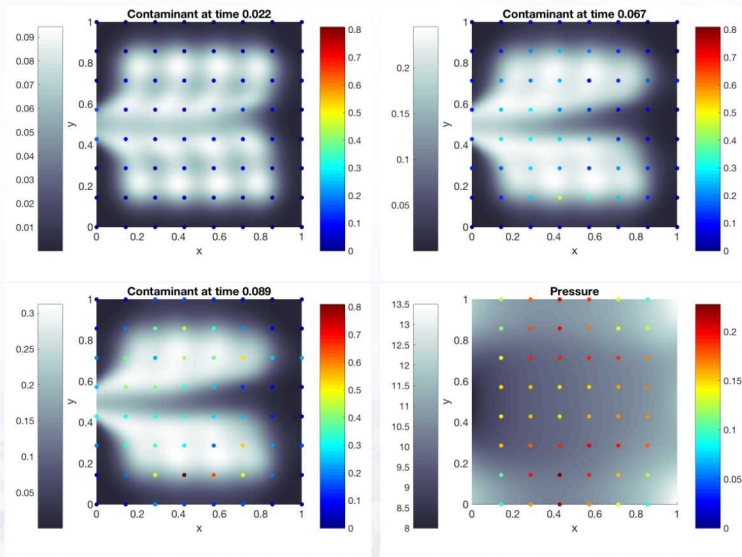


Figure: Sensitivity indices for contaminant and pressure data

Observations and Applications

Observations:

- pressure data is more important in earlier times and tracer concentration data is more important in later times
- spatial structure in both pressure and tracer concentration sensitivities indicate that the most important sensors are
 - those lying in low permeability regions
 - those (moving in time) which measure the contaminant concentration on the back end of the high permeability flow region

Applications:

- provides insight into sensor design and deployment by distinguishing data types and spatiotemporal structure

1 Sensitivity Analysis Framework

- Classical Framework
- Hyper-Differential Sensitivity Analysis (HDSA) Framework

2 Method and Computation

- Overview of the Method
- Computational Considerations

3 Software Design

4 Applications

- Parametric Sensitivity for Optimal Control
- Parametric Sensitivity for Inverse Problems
- Data Source Sensitivity for Inverse Problems
- **Distributional Sensitivity for Stochastic Optimization**

Distributional Robustness for Darcy Flow Control

$$\min_{u,z} \mathbb{E}_\theta \left[\frac{1}{2} \sum_{j=1}^M (\mathcal{P}_j u(\theta) - d_j)^2 \right] + \frac{\alpha}{2} \int_{\Omega} \|z\|^2 dx dy$$

s. t.

$$\nabla \cdot (-\kappa(\theta) \nabla u) = f(z)$$

$$u = \psi$$

$$-\kappa(\theta) \nabla u \cdot n = 0$$

in Ω

on $\Gamma_B \cup \Gamma_T$

on $\Gamma_L \cup \Gamma_R$

Distributional Robustness for Darcy Flow Control

$$\min_{u,z} \sum_{i=1}^N w_i \left(\frac{1}{2} \sum_{j=1}^M (\mathcal{P}_j u_i - d_j)^2 \right) + \frac{\alpha}{2} \int_{\Omega} \|z\|^2 dx dy$$

s.t. for $i = 1, 2, \dots, N$

$$\nabla \cdot (-\kappa(\theta_i) \nabla u_i) = f(z)$$

$$u_i = \psi$$

$$-\kappa(\theta_i) \nabla u_i \cdot n = 0$$

in Ω

on $\Gamma_B \cup \Gamma_T$

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Distributional Robustness for Darcy Flow Control

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$$-\kappa(\theta_i) \nabla u_i \cdot n = 0$$

in Ω

on $\Gamma_B \cup \Gamma_T$

on $\Gamma_L \cup \Gamma_R$

State and Target

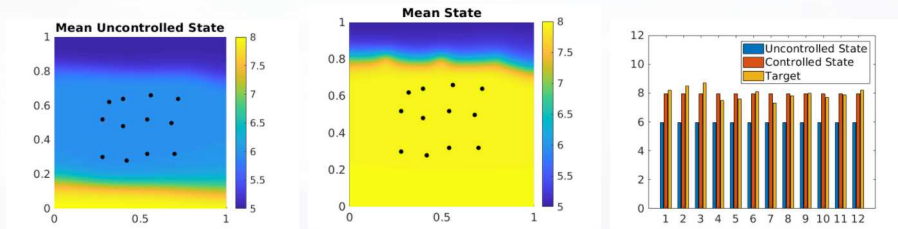


Figure: Left: uncontrolled mean state; center: controlled mean state; right: comparison of mean states with the target data. The black dots correspond to the locations of the target wells.

- control injection wells to get desired pressure at production wells
- uncertainty in the permeability field

Control and Sensitivity

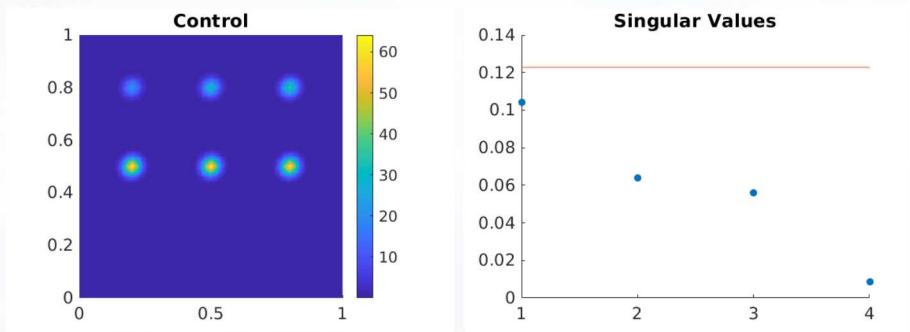


Figure: Left: optimal risk neutral control strategy; right: singular values of the sensitivity operator. The horizontal line above the singular values indicates the norm of the optimal controller.

- control strategy is parameterized by gaussian sources at 6 locations
- leading singular value is 85% of the magnitude of the optimal controller norm

Observations and Applications

Observations:

- a 10% relative perturbation of the weights produces approximately a 8.5% perturbation of the optimal controller

Applications:

- the control strategy is not robust to uncertainty in the distribution of the permeability field
- ongoing work explores how additional information may be leveraged from the singular vector or sensitivity indices to direct practitioners in such cases

Summary

- defined derivative-based local sensitivity indices for the solution of optimization problems with respect to auxiliary parameters
- identified computational challenges and proposed to use a randomized generalized eigenvalue solver to identify low rank structure and parallelize computation
- highlighted the software design and abstraction
- shown the versatility of the approach in various use cases
- presented numerical results and inferences made using HDSA for multi-physics problems

Questions?

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