Hyper-Differential Sensitivity Analysis of Inverse Problems Governed by PDEs

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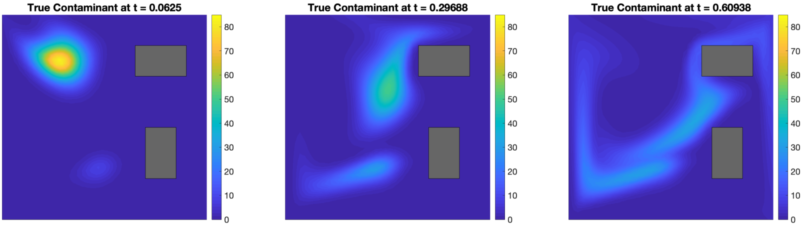
Motivation



Considerations

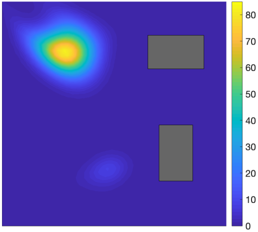
- Multiple sources of uncertainty
- Experimental and model
- Solution sensitivity
- Relative importance

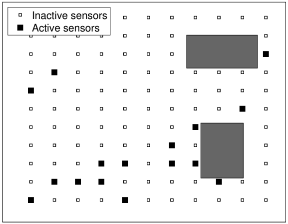
Inverse Problems

Inverse problems reconstruct uncertain parameters using measurement data.

Forward Problem

Inverse Problem





Complementary Parameters

Consider a PDE-constrained inverse problem of the following form:

$$\min_{m \in \mathcal{M}} J(m, \theta_e, \theta_a) := \frac{1}{2} \| \mathcal{Q} u(m, \theta_a) - \boldsymbol{y}(\theta_e) \| + \mathcal{R}(m)$$

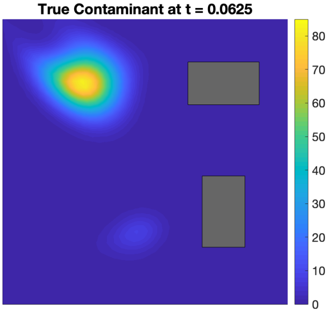
where $r(u(m, \theta_a), m, \theta_a) = 0$

- $\boldsymbol{y}$ - measurement data
- $\mathcal{R}$ - regularization operator
- r - governing equations
- $\mathcal{Q}$ - observation operator
- u - state variable
- m - inversion parameter
- θ_e - experimental parameters
- θ_a - auxiliary parameters

Complementary parameters: $\theta = (\theta_e, \theta_a)$

Hyper-Differential Sensitivity Analysis

Goal: Determine the sensitivity of the solution of a deterministic inverse problem to perturbations of complementary parameters.



Applications

- Augment experimental designs
- Important measurements
- Sensor error tolerances
- Optimal Experimental Design Under Uncertainty

Joseph Hart, Bart van Bloemen Waanders, and Roland Herzog. Hyper-differential sensitivity analysis of uncertain parameters in PDE-constrained optimization. International Journal of Uncertainty Quantification, 2020.

Sensitivity Operator

- Given nominal parameters $\bar{\theta}$, J has a local minimum $\bar{m}^* = m^*(\bar{\theta})$
- Optimality Condition: in a neighborhood of $(\bar{m}^*, \bar{\theta})$

$$J_m(m^*(\theta), \theta) = 0$$

- Differentiate through the optimality condition to obtain the sensitivity operator:

$$\mathcal{D} = -\mathcal{H}^{-1}\mathcal{B}$$

  - $\mathcal{H} := J_{m,m}(\bar{m}^*, \bar{\theta})$ is Hessian of J with respect to m
  - $\mathcal{B} := J_{m,\theta}(\bar{m}^*, \bar{\theta})$ is the Fréchet derivative of J_m with respect to θ
  - Use adjoint based gradient/Hessian computation
- Change in the solution of the inverse problem when the nominal parameter values are perturbed in the direction $\tilde{\theta}$:

$$\mathcal{D}\tilde{\theta} = \left[\nabla_\theta m^*\right](\tilde{\theta})$$

Kerstin Brandes and Roland Griesse. Quantitative stability analysis of optimal solutions in PDE-constrained optimization. Journal of Computational and Applied Mathematics, 2007.

Sensitivity Indices

Pointwise sensitivity indices

$$S_i^k = \frac{\|\mathbf{D}\boldsymbol{e}_i^k\|_{\mathbf{M}}}{\|\boldsymbol{e}_i^k\|_{\boldsymbol{\Theta}}}$$

- change in the solution of the inverse problem with respect to a perturbation of the i^{th} element of the k^{th} parameter

Generalized sensitivity indices

$$S^k = \max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \frac{\|\mathbf{D}\mathbf{T}_k\boldsymbol{\theta}\|_{\mathbf{M}}}{\|\boldsymbol{\theta}\|_{\boldsymbol{\Theta}}}$$

- maximum change in the solution with respect to a norm-1 perturbation of the k^{th} parameter

Model Problem

Forward problem

$$
\begin{aligned}
-\nabla \cdot (e^m \nabla p) &= 0 \quad \text{in } \Omega \\
c_t - \nabla \cdot \left(\epsilon \nabla c\right) + \nabla \cdot \left(\boldsymbol{v} c\right) &= g \quad \text{in } [0,T] \times \Omega, \quad \text{with} \quad \boldsymbol{v} = -e^m \nabla p \\
p &= p_1 \quad \text{on } \Gamma_1 \\
p &= p_2 \quad \text{on } \Gamma_3 \\
\nabla p \cdot n &= 0 \quad \text{on } \Gamma_0 \cup \Gamma_2 \\
\nabla c \cdot n &= 0 \quad \text{on } [0,T] \times \{\Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \Gamma_3\} \\
c(0,x) &= 0 \quad \text{in } \Omega
\end{aligned}
$$

- Inversion Parameter: log-permeability field m
- Auxiliary Parameters: diffusivity constant ϵ, fluid source g, BCs p_1 and p_2
- Experimental Parameters: concentration and pressure data measurements

Model Problem

$$
\begin{aligned}
-\nabla \cdot (e^{m} \nabla p) &= 0 \quad \text{in } \Omega \\
c_t - \nabla \cdot \Big(\epsilon \nabla c\Big) + \nabla \cdot \big(\boldsymbol{v} c\big) &= g \quad \text{in } [0,T] \times \Omega, \qquad \text{with} \qquad \boldsymbol{v} = -e^{m} \nabla p \\
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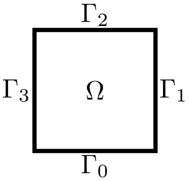
$$



Inverse Problem

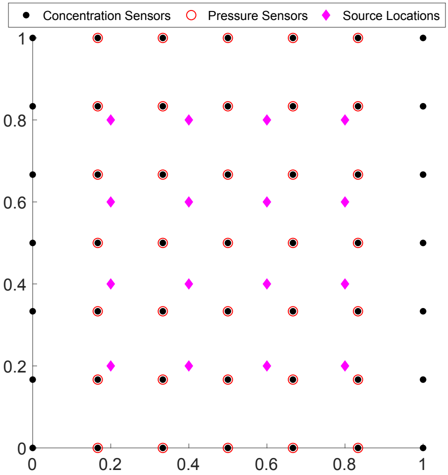
Inverse problem

$$\min_{m\in\mathcal{M}} J(m,\theta_e,\theta_a) := \frac{1}{2}\|\mathcal{Q}_p p(m,\theta_a) - \boldsymbol{y}_p(\theta_e)\|^2_{\mathbf{W}_p} + \frac{1}{2}\|\mathcal{Q}_c c(m,\theta_a) - \boldsymbol{y}_c(\theta_e)\|^2_{\mathbf{W}_c} + \frac{\alpha}{2}\int_\Omega \|\nabla m\|_2^2 \, dx$$

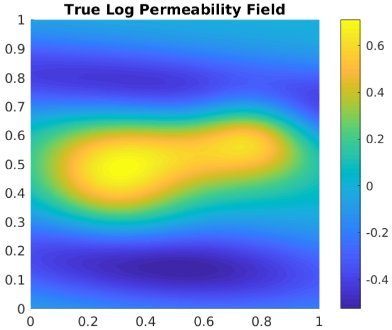
where c and p solve

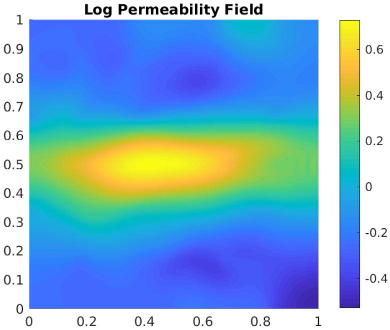
$$\begin{aligned}
-\nabla\cdot(e^m\nabla p) &= 0 && \text{in } \Omega \\
c_t - \nabla\cdot\left(\epsilon\nabla c\right) + \nabla\cdot\left(\boldsymbol{v}c\right) &= g && \text{in } [0,T]\times\Omega, \quad \text{with} \quad \boldsymbol{v} = -e^m\nabla p \\
p &= p_1 && \text{on } \Gamma_1 \\
p &= p_2 && \text{on } \Gamma_3 \\
\nabla p\cdot n &= 0 && \text{on } \Gamma_0\cup\Gamma_2 \\
\nabla c\cdot n &= 0 && \text{on } [0,T]\times\{\Gamma_0\cup\Gamma_1\cup\Gamma_2\cup\Gamma_3\} \\
c(0,x) &= 0 && \text{in } \Omega
\end{aligned}$$

Experimental Setup

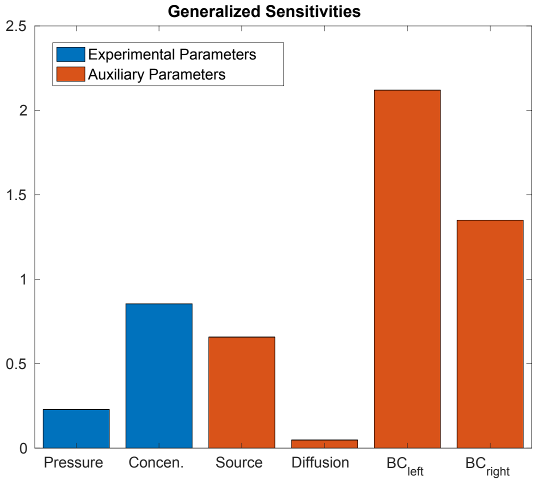


Inverse Problem Solution

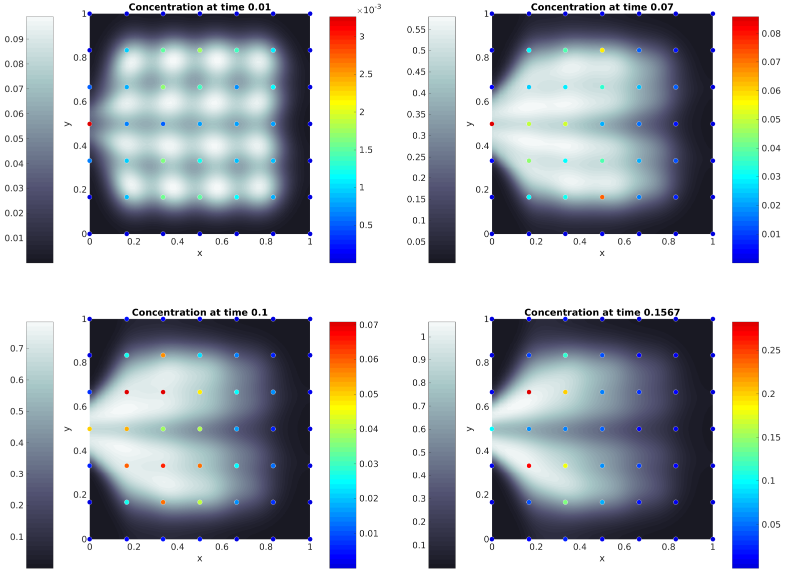




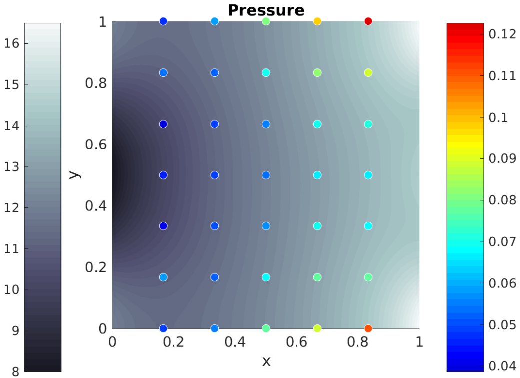
Generalized Sensitivity Indices



Concentration Sensitivity Indices



Pressure Sensitivity Indices



HDSA: Next Steps

Completed Work

- Formulate HDSA in the context of deterministic inverse problems
- Define pointwise and generalized sensitivity indicies
- Both experimental and auxiliary parameters
- Paper: Isaac Sunseri, Joseph Hart, Bart van Bloemen Waanders, and Alen Alexandarian. Hyper-Differential Sensitivity Analysis for Inverse Problems Constrained by Partial Differential Equations. *Inverse Problems*, 36(12), 2020.

Future Work

- How do we define sensitivity of the solution of a Bayesian inverse problem?
- Posterior distributions would be difficult or impossible to derive directly
- Consider the sensitivity of measures of the posterior

Bayesian HDSA

Consider

$$
\begin{aligned}
\frac{\partial y(x,t)}{\partial t} &= e^m \frac{\partial^2 y(x,t)}{\partial x^2}, && x \in (0,\pi), t \in (0,1) \\
y(0,t) &= y(\pi,t) = 0, && t \in (0,1) \\
y(x,0) &= \sin(x) + e^\theta \sin(2x), && x \in (0,\pi).
\end{aligned}
$$