Enabling and interpreting hyper-differential sensitivity analysis for Bayesian inverse problems

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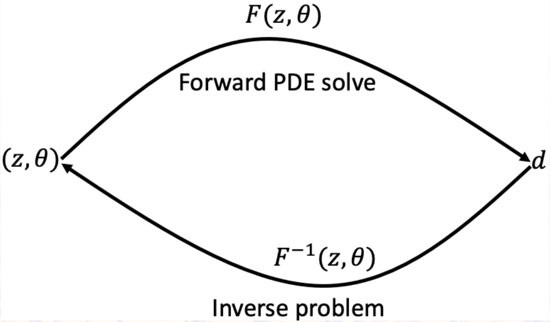
Inverse problems

Find parameters (z, θ) such that

$$F(z, \theta) = \mathcal{Q}(u(z, \theta)) \approx \boldsymbol{d}$$

where

- $\boldsymbol{d}$ are sparse and noisy observations of a state variable $u(z, \theta)$.
- $u(z, \theta)$ is the solution of a PDE and $\mathcal{Q}$ is the observation operator.



The joint Bayesian formulation

- Assume a prior distribution for $(\boldsymbol{z}, \boldsymbol{\theta}) \sim N((\boldsymbol{z}_{\text{prior}}, \boldsymbol{\theta}_{\text{prior}}), \Gamma_{\text{prior}})$.
- Assume that $\boldsymbol{d} = F(\boldsymbol{z}^\star, \boldsymbol{\theta}^\star) + \epsilon$ where $\epsilon \sim N(0, \Gamma_{\text{noise}})$.
- The joint posterior probability density function (PDF) is

$$\pi_{\text{post}}(\boldsymbol{z}, \boldsymbol{\theta}) \propto \pi_{\text{like}}(\boldsymbol{d} | \boldsymbol{z}, \boldsymbol{\theta}) \pi_{\text{prior}}(\boldsymbol{z}, \boldsymbol{\theta})$$

where

- π_{like} is the likelihood function,
- π_{prior} is the prior PDF.

Analyzing properties of $\pi_{\text{post}}(\boldsymbol{z}, \boldsymbol{\theta})$ provide a wealth of information, but may be computationally intractable.

The conditional Bayesian formulation

- The posterior probability density function (PDF) for $\boldsymbol{z}$ given $\boldsymbol{\theta} = \boldsymbol{\theta}_{\text{prior}}$ is

$$\pi_{\text{post}}(\boldsymbol{z}|\boldsymbol{\theta}_{\text{prior}}) \propto \pi_{\text{like}}(\boldsymbol{d}|\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}})\pi_{\text{prior}}(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}}).$$

- The maximum a posteriori probability (MAP) point(s) for $\pi_{\text{post}}(\boldsymbol{z}|\boldsymbol{\theta}_{\text{prior}})$ are local minima of

$$\min_{\boldsymbol{z} \in \mathbb{R}^m} J(\boldsymbol{z}; \boldsymbol{\theta}_{\text{prior}}) := M(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}}) + R(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}})$$

where $M(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}})$ and $R(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}})$ are the negative log likelihood and prior.

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- How does fixing $\boldsymbol{\theta} = \boldsymbol{\theta}_{\text{prior}}$ influence the analysis for $\boldsymbol{z}$?

1. Bayesian inverse problems
2. Hyper-differential sensitivity analysis (HDSA)
3. The Bayesian interpretation of HDSA
4. Enabling HDSA for ill-posed problems
5. Numerical Results

Post optimality sensitivity analysis

$$\min_{\boldsymbol{z} \in \mathbb{R}^m} J(\boldsymbol{z}; \boldsymbol{\theta}_{\text{prior}}) := M(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}}) + R(\boldsymbol{z}, \boldsymbol{\theta}_{\text{prior}})$$

- Let $\boldsymbol{z}^\star$ denote a local minimum when $\boldsymbol{\theta} = \boldsymbol{\theta}_{prior}$ is fixed,

$$\nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star, \boldsymbol{\theta}_{\text{prior}}) = 0 \qquad \text{and} \qquad \nabla_{\boldsymbol{z},\boldsymbol{z}} J(\boldsymbol{z}^\star, \boldsymbol{\theta}_{\text{prior}}) \succ 0$$

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- The implicit function theorem gives

$$\mathcal{G} : \mathcal{N}(\boldsymbol{\theta}_{\text{prior}}) \to \mathcal{N}(\boldsymbol{z}^\star),$$

defined on neighborhoods of $\boldsymbol{\theta}_{\text{prior}}$ and $\boldsymbol{z}^\star$, such that

$$\nabla_{\boldsymbol{z}} J(\mathcal{G}(\boldsymbol{\theta}),\boldsymbol{\theta}) = 0 \qquad \forall \boldsymbol{\theta} \in \mathcal{N}(\boldsymbol{\theta}_{\text{prior}})$$

Post optimality sensitivity analysis

$$\mathcal{G} : \mathcal{N}(\boldsymbol{\theta}_{\text{prior}}) \to \mathcal{N}(\boldsymbol{z}^\star)$$

- $\mathcal{G}$ associates parameters $\boldsymbol{\theta}$ with the corresponding MAP points for $\boldsymbol{z}$ given $\boldsymbol{\theta}$
- Further, $\mathcal{G}$ is differentiable at $\boldsymbol{\theta}_{\text{prior}}$ and its Jacobian is given by

$$\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}}) = -\mathcal{H}^{-1}\mathcal{B} \in \mathbb{R}^{m \times n}$$

- $\mathcal{H} = \nabla_{\boldsymbol{z},\boldsymbol{z}} J$ and $\mathcal{B} = \nabla_{\boldsymbol{z},\boldsymbol{\theta}} J$ are second derivatives of the objective $J(\boldsymbol{z}, \boldsymbol{\theta})$

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- HDSA efficiently interrogates $\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}})$ using adjoint-based derivative calculations and matrix-free linear algebra.

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1. What is the Bayesian interpretation of $\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}})$?

2. Can I still compute/interpret $\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}})$ for ill-posed problems where the optimizer may struggle to solve the MAP point estimation problem to optimality (satisfaction of the first order optimality condition)?

The linear case

Theorem

If $F(\boldsymbol{z},\boldsymbol{\theta}) = A\boldsymbol{z} + B\boldsymbol{\theta}$ *then the posterior is Gaussian with covariance*

$$\Sigma_{post} = \begin{pmatrix} \Sigma_{\boldsymbol{z},\boldsymbol{z}} & \Sigma_{\boldsymbol{z},\boldsymbol{\theta}} \\ \Sigma_{\boldsymbol{\theta},\boldsymbol{z}} & \Sigma_{\boldsymbol{\theta},\boldsymbol{\theta}} \end{pmatrix}$$

and the post-optimality sensitivity is given by

$$\mathcal{G}'(\boldsymbol{\theta}_{prior}) = \Sigma_{\boldsymbol{z},\boldsymbol{\theta}}\Sigma_{\boldsymbol{\theta},\boldsymbol{\theta}}^{-1}.$$

- The post-optimality sensitivity is a correlation between $\boldsymbol{z}$ and $\boldsymbol{\theta}$.

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- Connection between optimization/analysis and Bayesian statistics.
- Local correlation for nonlinear inverse problems (Laplace approximation).

Handling ill-posedness

- For ill-posed inverse problems, $\mathcal{H}$ may be ill-conditioned yielding high sensitivity as a result of lacking information/data.
- Analyzing $\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}})$ results in sensitivities dominated by what the data does not tell you.

[2] T. Cui, J. Martin, Y. M. Marzouk, A. Solonen, and A. Spantini, Likelihood-informed dimension reduction for nonlinear inverse problems, Inverse Problems, 30 (2014), pp. 1–28.

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Proposed Approach: Compute sensitivities

$$\mathcal{P}\mathcal{G}'(\boldsymbol{\theta}_{\text{prior}}) = -\mathcal{P}\mathcal{H}^{-1}\mathcal{B}$$

where $\mathcal{P}$ projects onto the likelihood informed subspace [2] defined by the leading eigenvectors of

$$\mathcal{H}_M \boldsymbol{v}_j = \lambda_j \mathcal{H}_R \boldsymbol{v}_j.$$

The eigenvalues

$$\lambda_j = \frac{\boldsymbol{v}_j^T \mathcal{H}_M \boldsymbol{v}_j}{\boldsymbol{v}_j^T \mathcal{H}_R \boldsymbol{v}_j}$$

measure the ratio of the likelihood and prior in the direction of $\boldsymbol{v}_j$.

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Failure to satisfy the first order optimality condition?

It may not be practical to solve the MAP point estimation problem

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to optimality if ill-conditioning yields slow convergence.

- Early iterations refine features which are well informed by the data.
- Ill-conditioning may yield slow convergence in the uniformed subspace.

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Question: HDSA assumes satisfaction of the optimality criteria. What can I do when converging the optimization is impractical/unnecessary?

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- Assume that $\boldsymbol{z}^\star$ is an approximation of the MAP point but

$$\nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star, \boldsymbol{\theta}_{\text{prior}}) \neq 0.$$

- Find a minimum norm perturbation $\tilde{R}$ so that $\nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{\text{prior}}) + \nabla_{\boldsymbol{z}} \tilde{R}(\boldsymbol{z}^\star) = 0$,

$$\min_{\tilde{R} \in Q} ||\tilde{R}||_{L^1(\mu)}$$
$$\text{s.t. } \nabla_{\boldsymbol{z}} \tilde{R}(\boldsymbol{z}^\star) = -\nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{\text{prior}})$$

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$$\text{s.t. } \nabla_{\boldsymbol{z}} \tilde{R}(\boldsymbol{z}^\star) = -\nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{\text{prior}})$$

- Judicious linear algebra gives a closed form solution

$$\tilde{R}(\boldsymbol{z}) = \frac{\alpha}{2}||\boldsymbol{g}||_2 - (\boldsymbol{z} - \boldsymbol{z}^\star)^T \boldsymbol{g} + \frac{1}{2}(\boldsymbol{z} - \boldsymbol{z}^\star)^T \frac{1}{\alpha||\boldsymbol{g}||_2} \boldsymbol{g}\boldsymbol{g}^T (\boldsymbol{z} - \boldsymbol{z}^\star),$$

where $\boldsymbol{g} = \nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{\text{prior}})$.

The perturbed MAP point problem

$$\min_{\boldsymbol{z} \in \mathbb{R}^m} J(\boldsymbol{z}; \boldsymbol{\theta}_{\text{prior}}) + \tilde{R}(\boldsymbol{z})$$

- $\boldsymbol{z}^\star$ satisfies the first order optimality condition.
- Post-optimality sensitivities are well defined for this perturbed problem.

The perturbed MAP point problem

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Some important questions:

- What is the Bayesian interpretation of $\tilde{R}$?
- How does the perturbation influence the sensitivities?

A perturbed Gaussian prior

- What is the Bayesian interpretation of $\tilde{R}$?
- How does the perturbation influence the sensitivities?

Theorem

The perturbed inverse problem has a Gaussian prior with mean

$$\tilde{\boldsymbol{z}}_{prior} = \boldsymbol{z}_{prior} + \frac{\alpha - (\boldsymbol{z}^\star - \boldsymbol{z}_{prior})^T \boldsymbol{s}}{\alpha - \boldsymbol{v}^T \boldsymbol{s}} \boldsymbol{v}$$

and covariance

$$\tilde{\Gamma}_{prior} = \Gamma_{prior} - \frac{1}{||\boldsymbol{g}||_2} \frac{1}{\alpha - \boldsymbol{v}^T \boldsymbol{s}} \boldsymbol{v}\boldsymbol{v}^T$$

where

$$\boldsymbol{g} = \nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{prior}), \qquad \boldsymbol{s} = -\frac{\boldsymbol{g}}{||\boldsymbol{g}||_2}, \qquad \text{and} \qquad \boldsymbol{v} = \Gamma_{prior} \boldsymbol{g}.$$

The perturbation shifts the mean and reduces uncertainty in the direction $\boldsymbol{v}$.

Difference in sensitivities

- What is the Bayesian interpretation of $\tilde{R}$?
- How does the perturbation influence the sensitivities?

Theorem

The quantities

$$S(\overline{\boldsymbol{\theta}}) = \left|\left|\mathcal{P}\mathcal{H}^{-1}\mathcal{B}\overline{\boldsymbol{\theta}}\right|\right|_{W_z} \qquad \text{and} \qquad \tilde{S}(\overline{\boldsymbol{\theta}}) = \left|\left|\mathcal{P}\tilde{\mathcal{H}}^{-1}\tilde{\mathcal{B}}\overline{\boldsymbol{\theta}}\right|\right|_{W_z}$$

satisfy

$$\frac{|\tilde{S}(\overline{\boldsymbol{\theta}}) - S(\overline{\boldsymbol{\theta}})|}{\left|\left|\mathcal{H}^{-1}\mathcal{B}\overline{\boldsymbol{\theta}}\right|\right|_{W_z}} \leq \frac{||\mathcal{P}\boldsymbol{n}||_{W_z}}{\boldsymbol{s}^T\boldsymbol{n} + \alpha},$$

where

$$\boldsymbol{g} = \nabla_{\boldsymbol{z}} J(\boldsymbol{z}^\star; \boldsymbol{\theta}_{prior}), \qquad \boldsymbol{s} = -\frac{\boldsymbol{g}}{||\boldsymbol{g}||_2}, \qquad \text{and} \qquad \boldsymbol{n} = -\mathcal{H}^{-1}\boldsymbol{g}.$$

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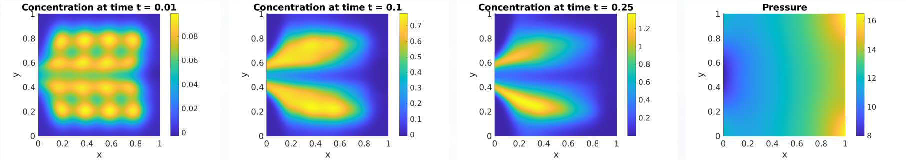
Subsurface permeability inversion



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

$$c_t-\nabla\cdot\Big(\epsilon(\boldsymbol{\theta})\nabla c\Big)+\nabla\cdot\big(-e^{\kappa}\nabla pc\big)=g(\boldsymbol{\theta}) \qquad \text{in } [0,T]\times\Omega$$

$$p=p_1(\boldsymbol{\theta}) \qquad \text{on } \Gamma_1$$

$$p=p_2(\boldsymbol{\theta}) \qquad \text{on } \Gamma_3$$

$$e^{\kappa}\nabla p\cdot n=0 \qquad \text{on } \Gamma_0\cup\Gamma_2$$

$$\nabla c\cdot n=0 \qquad \text{on } [0,T]\times\{\Gamma_0\cup\Gamma_1\cup\Gamma_2\cup\Gamma_3\}$$

$$c(0,x)=0 \qquad \text{in } \Omega$$

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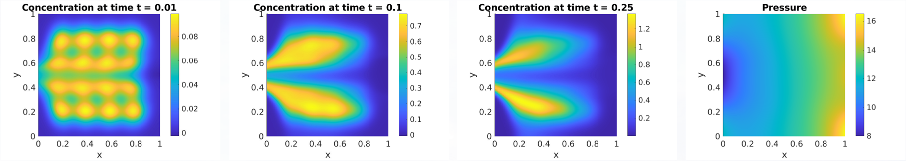

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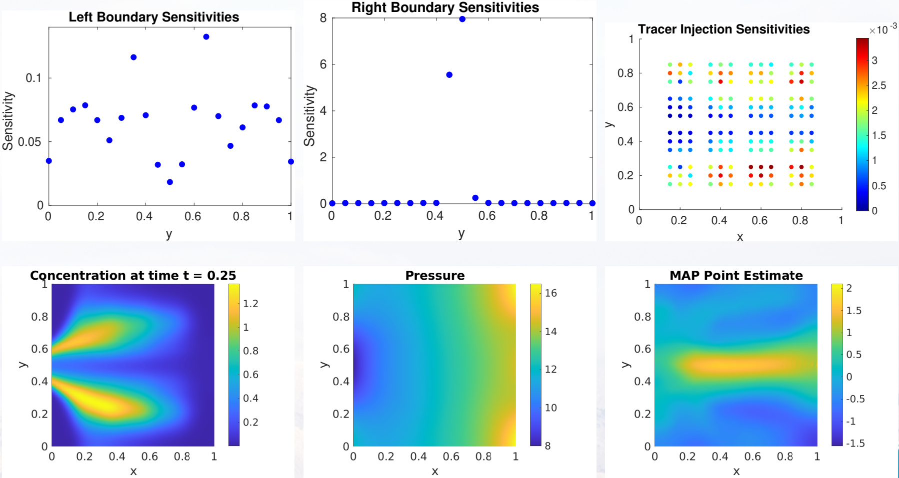
Sensitivities



Summary

- Established the Bayesian interpretation of post-optimality sensitivity analysis.
- Addressed ill-posedness by projecting on likelihood informed subspaces.
- Theoretically justified HDSA when optimization fails to converge.
- Provided strong error bounds establishing the robust of the analysis.

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