

Sensitivity Analysis of the Information Gain in Infinite-Dimensional Bayesian Linear Inverse Problems

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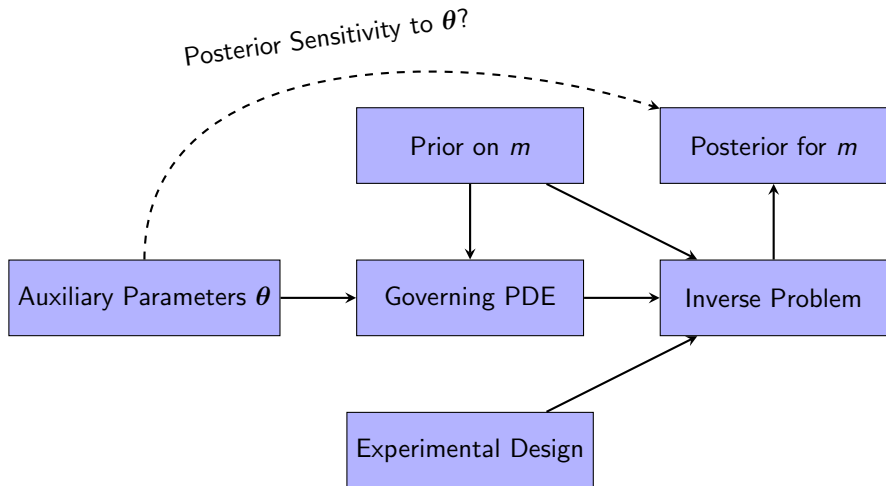
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- 1 Bayesian Inverse Problems Preliminaries
- 2 The Information Gain
- 3 Hyper Differential Sensitivity Analysis (HDSA) for the Information Gain
 - Eigenvalue Sensitivities
 - Post-Optimal Sensitivity Analysis
- 4 Numerical Results

Bayesian Inverse Problems Framework



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$m \in \mathcal{M}$ is the inversion parameter and $\theta \in \Theta$ are the auxiliary parameters.

Governing PDE Model

For some appropriate function space \mathcal{V} , we consider the abstract weak PDE:

$$\mathcal{A}(p, u, \theta) + \mathcal{C}(p, m, \theta) + \mathcal{D}(p, \theta) = 0, \quad \forall p \in \mathcal{V}$$

- $u \in \mathcal{V}$ is the *state variable*.
- $p \in \mathcal{V}$ is the *adjoint variable*.
- $m \in \mathcal{M}$ is the (potentially infinite dimensional) *inversion parameter*.
- $\theta \in \Theta$ are the (potentially infinite dimensional) *auxiliary parameters*.

Goal

Assuming some measurement data \mathbf{y} obeys the above PDE, infer a probability distribution for m and quantify its sensitivity with respect to θ .

- Let $\mathcal{F} : \mathcal{M} \rightarrow \mathbb{R}^{N_{\text{obs}}}$ be the *parameter-to-observable* map.

Bayesian Inversion in Infinite Dimensions

Theorem (Bayes Theorem in Infinite Dimensions)

$$\frac{d\mu_{\text{post}}^{\mathbf{y}}}{d\mu_{\text{pr}}} \propto \pi_{\text{like}}(\mathbf{y}|m)$$

- Gaussian Prior $m \sim \mathcal{N}(m_{\text{pr}}, \Gamma_{\text{prior}})$.
- Additive Gaussian noise

$$\mathbf{y} = \mathcal{F}(m) + \boldsymbol{\eta}, \quad \boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \Gamma_{\text{noise}})$$

- Assuming \mathcal{F} linear:

$$\mu_{\text{post}}^{\mathbf{y}} = \mathcal{N}(m_{\text{post}}, C_{\text{post}})$$

where:

$$m_{\text{post}} = C_{\text{post}} \left(\mathcal{F}^* \Gamma_{\text{noise}}^{-1} \mathbf{y} + \Gamma_{\text{prior}}^{-1} m_{\text{pr}} \right)$$

$$C_{\text{post}} = \left(\mathcal{F}^* \Gamma_{\text{noise}}^{-1} \mathcal{F} + \Gamma_{\text{prior}}^{-1} \right)^{-1}$$

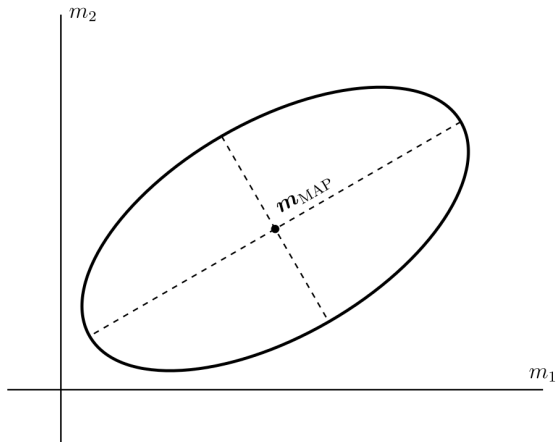


Figure: The confidence region corresponding to bivariate Gaussian posterior.

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Kullback-Leibler Divergence of the Posterior from the Prior

$$D_{\text{kl}}(\mu_{\text{post}}^{\mathbf{y}} || \mu_{\text{pr}}) := \int_{\mathcal{M}} \log \left[\frac{d\mu_{\text{post}}^{\mathbf{y}}}{d\mu_{\text{pr}}} \right] d\mu_{\text{post}}^{\mathbf{y}}$$

- Informally: information gained when updating beliefs to $\mu_{\text{post}}^{\mathbf{y}}$ from μ_{pr} .
- Averaging this over experimental data is the D-optimal design criteria
- In the linear inverse problem setting, possess an analytic expression

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S. Kullback and R. A. Leibler. "On Information and Sufficiency". In: *The Annals of Mathematical Statistics* 22.1 (Mar. 1951), pp. 79–86. DOI: [10.1214/aoms/1177729694](https://doi.org/10.1214/aoms/1177729694)

Adjoint-Based Framework

More generally, m_{post} can be inferred by solving the PDE-constrained optimization problem:

$$\begin{aligned}\mathcal{J}(m, \theta) &:= \frac{1}{2} \|\mathcal{F}(\theta)(m) - \mathbf{y}\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \|m - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2 \\ &= \frac{1}{2} \|\mathcal{Q}u - \mathbf{y}\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \|m - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2\end{aligned}$$

- u is given by the forward model.
- $\mathbf{y} \in \mathbb{R}^{N_{\text{obs}}}$ where N_{obs} is the number of data points.
- $\mathcal{Q} : \mathcal{V} \rightarrow \mathbb{R}^{N_{\text{obs}}}$ is an observation operator.

Gradient and Hessian action implicitly defined by PDEs

Lagrangian Enforcing PDE-Constraints

$$\mathcal{L}(u, p, m) := \frac{1}{2} \|\mathcal{Q}u - \mathbf{y}\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \|m - m_0\|_{C_0^{-1}}^2 + \mathcal{A}(p, u, \theta) + \mathcal{C}(p, m, \theta) + \mathcal{D}(p, \theta)$$

Take variations with respect to (u, p, m) and set to zero to find:

Gradient System

$$\begin{cases} \mathcal{G}(m)(\tilde{m}) = \mathcal{C}(p, \tilde{m}, \theta) + \langle m - m_0, \tilde{m} \rangle_{C_0^{-1}} \\ \langle \mathcal{Q}u - \mathbf{y}, \mathcal{Q}\tilde{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\tilde{u}, p, \theta) = 0, & \forall \tilde{u} \in \mathcal{V} \\ \mathcal{A}(\tilde{p}, u, \theta) + \mathcal{C}(\tilde{p}, m, \theta) + \mathcal{D}(\tilde{p}, \theta) = 0, & \forall \tilde{p} \in \mathcal{V} \end{cases}$$

Gradient and Hessian action implicitly defined by PDEs

(Meta)-Lagrangian constraining Gradient System

$$\begin{aligned}\mathcal{L}^H(u, p, m, \hat{u}, \hat{p}, \hat{m}) &= \mathcal{C}(p, \hat{m}, \theta) + \langle m - m_0, \hat{m} \rangle_{\mathcal{C}_0^{-1}} \\ &\quad + \langle \mathcal{Q}u - \mathbf{y}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{u}, p, \theta) \\ &\quad + \mathcal{A}(\hat{p}, u, \theta) + \mathcal{C}(\hat{p}, m, \theta) + \mathcal{D}(\hat{p}, \theta)\end{aligned}$$

Take variations with respect to (u, p, m) and set to zero to find:

Implicit Hessian Action

$$\begin{cases} \mathcal{H}(\hat{m}, \tilde{m}) = \mathcal{C}(\hat{p}, \tilde{m}, \theta) + \langle \tilde{m}, \hat{m} \rangle_{\mathcal{C}_0^{-1}} \\ \langle \mathcal{Q}\tilde{u}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{p}, \tilde{u}, \theta) = 0, & \forall \tilde{u} \in \mathcal{V} \\ \mathcal{A}(\tilde{p}, \hat{u}, \theta) + \mathcal{C}(\tilde{p}, \hat{m}, \theta) = 0, & \forall \tilde{p} \in \mathcal{V} \end{cases}$$

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$$\begin{aligned}\mathcal{L}^H(u, p, m, \hat{u}, \hat{p}, \hat{m}) &= \mathcal{C}(p, \hat{m}, \theta) + \cancel{\langle m - m_0, \hat{m} \rangle_{C_0^{-1}}} \\ &+ \langle \mathcal{Q}u - \mathbf{y}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{u}, p, \theta) \\ &+ \mathcal{A}(\hat{p}, u, \theta) + \mathcal{C}(\hat{p}, m, \theta) + \mathcal{D}(\hat{p}, \theta)\end{aligned}$$

Take variations with respect to (u, p, m) and set to zero to find:

Implicit Data-Misfit Hessian

$$\begin{cases} \mathcal{H}_m(\hat{m}, \tilde{m}) = \mathcal{C}(\hat{p}, \tilde{m}, \theta) + \cancel{\langle \tilde{m}, \hat{m} \rangle_{C_0^{-1}}} \\ \langle \mathcal{Q}\tilde{u}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{p}, \tilde{u}, \theta) = 0, & \forall \tilde{u} \in \mathcal{V} \\ \mathcal{A}(\tilde{p}, \hat{u}, \theta) + \mathcal{C}(\tilde{p}, \hat{m}, \theta) = 0, & \forall \tilde{p} \in \mathcal{V} \end{cases}$$

Information Gain for Linear Bayesian Inverse Problems

Definition (Explicit KL-Divergence)

For linear Bayesian inverse problems, the KL-Divergence has explicit form

$$\Phi_{\text{KL}} = \frac{1}{2} \left[\log \det(\tilde{\mathcal{H}}_m + \mathcal{I}) - \text{tr} \left(\tilde{\mathcal{H}}_m (\mathcal{I} + \tilde{\mathcal{H}}_m)^{-1} \right) + \|m_{\text{post}} - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2 \right]$$

where

$$\tilde{\mathcal{H}}_m = \Gamma_{\text{prior}}^{1/2} \mathcal{H}_m \Gamma_{\text{prior}}^{1/2}$$

is the prior-preconditioned data-misfit Hessian

For local sensitivity, we want to compute $\frac{\partial}{\partial \theta_j} \Phi_{\text{KL}}$ for every j .

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Q: How do we differentiate this expression?

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Low Rank Approximations

Definition ($\tilde{\mathcal{H}}_m$ Low-Rank Approximation)

Let $\{(\lambda_i, \psi_i)\}_{i=1}^r$ be the dominant eigenpairs of $\tilde{\mathcal{H}}_m$, then:

$$\tilde{\mathcal{H}}_m \phi \approx \sum_{i=1}^r \lambda_i \langle \psi_i, \phi \rangle \psi_i$$

is a low rank approximation of $\tilde{\mathcal{H}}_m$.

Definition (Kullback-Leibler Divergence Low-Rank Approximation)

$$\hat{\Phi}_{\text{KL}} := \frac{1}{2} \sum_{j=1}^r \left[\log(\lambda_j + 1) - \frac{\lambda_j}{1 + \lambda_j} \right] + \frac{1}{2} \left\| m_{\text{post}} - m_{\text{pr}} \right\|_{\Gamma_{\text{prior}}^{-1}}^2$$

Hyper Differential Sensitivity Analysis

Q: How do we differentiate this expression?

$$\hat{\Phi}_{\text{KL}}(\boldsymbol{\theta}) = \underbrace{\frac{1}{2} \sum_{j=1}^r \left[\log(\lambda_j(\boldsymbol{\theta}) + 1) - \frac{\lambda_j(\boldsymbol{\theta})}{1 + \lambda_j(\boldsymbol{\theta})} \right]}_{(1)} + \underbrace{\frac{1}{2} \|m_{\text{post}}(\boldsymbol{\theta}) - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2}_{(2)}$$

- (1): Eigenvalue Sensitivities
- (2): Post-Optimal Sensitivity Analysis

Adjoint-Based Eigenvalue Sensitivities

Q: How do we differentiate this expression?

$$\hat{\phi}_{\text{KL}}^{(1)}(\boldsymbol{\theta}) := \sum_{j=1}^k \frac{1}{2} \left[\log(\lambda_j(\boldsymbol{\theta}) + 1) - \frac{\lambda_j(\boldsymbol{\theta})}{1 + \lambda_j(\boldsymbol{\theta})} \right]$$

Recall: Structure around \mathcal{H}_m

Assuming dominant eigenpairs are not repeated, \mathcal{H}_m satisfies the eigenproblem

$$\mathcal{H}_m(\psi_i, \phi) = \lambda_i \langle \phi, \psi_i \rangle_{\Gamma_{\text{prior}}^{-1}} \quad \text{and} \quad \langle \psi_i, \psi_i \rangle_{\Gamma_{\text{prior}}^{-1}}$$

for every $\phi \in \mathcal{M}$ and $i = 1, \dots, r$. Likewise, it has implicit structure

$$\begin{cases} \mathcal{H}_m(\hat{m}, \tilde{m}) = \mathcal{C}(\hat{p}, \tilde{m}, \boldsymbol{\theta}) \\ \langle \mathcal{Q}\tilde{u}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{p}, \tilde{u}, \boldsymbol{\theta}) = 0, & \forall \tilde{u} \in \mathcal{V} \\ \mathcal{A}(\tilde{p}, \hat{u}, \boldsymbol{\theta}) + \mathcal{C}(\tilde{p}, \hat{m}, \boldsymbol{\theta}) = 0, & \forall \tilde{p} \in \mathcal{V} \end{cases}$$

Adjoint-Based Eigenvalue Sensitivities

Lagrangian Constraining \mathcal{H}_m and Eigenproblem

$$\begin{aligned} & \mathcal{L}^\lambda (\{\psi_i\}_{i=1}^r, \{\hat{u}_i\}_{i=1}^r, \{\hat{p}_i\}_{i=1}^r, \{\gamma_i^*\}_{i=1}^r, \{\hat{u}_i^*\}_{i=1}^r, \{\hat{p}_i^*\}_{i=1}^r; \theta) \\ &= \frac{1}{2} \sum_{i=1}^r \left[\log(1 + \mathcal{C}(\hat{p}_i, \psi_i; \theta)) - \frac{\mathcal{C}(\hat{p}_i, \psi_i; \theta)}{1 + \mathcal{C}(\hat{p}_i, \psi_i; \theta)} \right] \\ &+ \sum_{i=1}^r \left[\mathcal{A}(\hat{p}_i^*, \hat{u}_i; \theta) + \mathcal{C}(\hat{p}_i^*, \psi_i; \theta) + \mathcal{A}(\hat{p}_i, \hat{u}_i^*; \theta) + \langle \mathcal{Q}\hat{u}_i^*, \mathcal{Q}\hat{u}_i \rangle_{\Gamma_{\text{noise}}^{-1}} \right] \\ &+ \sum_{i=1}^r \gamma_i^* \left[\langle \psi_i, \psi_i \rangle_{\Gamma_{\text{prior}}^{-1}} - 1 \right] \end{aligned}$$

Adjoint-Based Eigenvalue Sensitivities

Resulting Expressions

With Lagrange multipliers

$$\hat{u}_i^* = \frac{\lambda_i}{2(1 + \lambda_i)^2} \hat{u}(\psi_i) \quad \text{and} \quad \hat{p}_i^* = \frac{\lambda_i}{2(1 + \lambda_i)^2} \hat{p}(\psi_i)$$

We can take derivatives of $\hat{\Phi}_{\text{KL}}^{(1)}$ with the expression:

$$\mathcal{L}_{\theta_j}^\lambda = \sum_{i=1}^r \left[\frac{C(\hat{p}_i, \psi_i; \boldsymbol{\theta})}{2(1 + C(\hat{p}_i, \psi_i; \boldsymbol{\theta}))^2} C_{\theta_j}(\hat{p}_i, \psi_i; \boldsymbol{\theta}) + \mathcal{A}_{\theta_j}(\hat{p}_i^*, \hat{u}_i; \boldsymbol{\theta}) + C_{\theta_j}(\hat{p}_i^*, \psi_i; \boldsymbol{\theta}) + \mathcal{A}_{\theta_j}(\hat{p}_i, \hat{u}_i^*; \boldsymbol{\theta}) \right]$$

Post-Optimal Sensitivity Analysis

Q: How do we differentiate this expression?

$$\hat{\Phi}_{\text{KL}}^{(2)}(\boldsymbol{\theta}) := \frac{1}{2} \|m_{\text{post}}(\boldsymbol{\theta}) - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2$$

Post-Optimal Sensitivity Analysis

Q: How do we differentiate this expression?

$$\hat{\Phi}_{\text{KL}}^{(2)}(\boldsymbol{\theta}) := \frac{1}{2} \|m_{\text{post}}(\boldsymbol{\theta}) - m_{\text{pr}}\|_{\Gamma_{\text{prior}}^{-1}}^2$$

Post-Optimal Sensitivity Analysis

Previous work demonstrated that

$$\frac{\partial}{\partial \theta_j} m_{\text{post}}(\boldsymbol{\theta}) = \mathcal{H}^{-1}(\boldsymbol{\theta}) \mathcal{B}_j(\boldsymbol{\theta})$$

where $\mathcal{B}_j : \Theta_j \rightarrow \mathcal{E}$ is the operator describing the Frechet derivative of the gradient \mathcal{G} with respect to θ_j evaluated at m_{post} , i.e. $\mathcal{B} := J_{m, \theta_j}(m_{\text{post}}, \boldsymbol{\theta})$. Thus

$$\frac{d}{d\theta_j} \hat{\Phi}_{\text{KL}}^{(2)}(\boldsymbol{\theta}) = 2 \langle m_{\text{post}} - m_{\text{pr}}, \frac{d}{d\theta_j} m_{\text{post}} \rangle_{\Gamma_{\text{prior}}^{-1}} = -2 \langle m_{\text{post}} - m_{\text{pr}}, \mathcal{H}^{-1} \mathcal{B}_j \rangle_{\Gamma_{\text{prior}}^{-1}}$$

Isaac Sunseri et al. "Hyper-differential sensitivity analysis for nonlinear Bayesian inverse problems". In: *International Journal for Uncertainty Quantification*

Accepted (2023)

Post-Optimal Sensitivity Analysis

Lagrangian Constraining Gradient System

$$\begin{aligned}\mathcal{L}^{(2)}(u, p, m, \hat{u}, \hat{p}, \hat{m}, \theta) &= \langle m - m_0, \hat{m} \rangle_{C_0^{-1}} + \mathcal{C}(p, \hat{m}, \theta) \\ &\quad + \langle \mathcal{Q}u - \mathbf{y}, \mathcal{Q}\hat{u} \rangle_{\Gamma_{\text{noise}}^{-1}} + \mathcal{A}(\hat{u}, p, \theta) \\ &\quad + \mathcal{A}(\hat{p}, u, \theta) + \mathcal{C}(\hat{p}, m, \theta) + \mathcal{D}(\hat{p}, \theta)\end{aligned}$$

Derivative of $\hat{\Phi}^{(2)}$ with respect to θ_j

$$\mathcal{L}_{\theta_j}^{(2)} = \mathcal{B}_j(\hat{m}, \theta) := \mathcal{C}_{\theta_j}(p, \hat{m}; \theta) + \mathcal{A}_{\theta_j}(p, \hat{u}; \theta) + \mathcal{C}_{\theta_j}(p, \hat{m}; \theta) + \mathcal{A}_{\theta_j}(\hat{p}, u; \theta) + \mathcal{D}_{\theta_j}(\hat{p}; \theta)$$

Putting it all together

Local Information Gain Sensitivity with respect to θ_j

$$\frac{d}{d\theta_j} \hat{\Phi}_{\text{KL}} = \sum_{i=1}^r \left[\frac{c(\hat{\rho}_i, \psi_i; \theta)}{2(1+c(\hat{\rho}_i, \psi_i; \theta))^2} \mathcal{C}_{\theta_j}(\hat{\rho}_i, \psi_i; \theta) + \mathcal{A}_{\theta_j}(\hat{\rho}_i^*, \hat{u}_i; \theta) + \mathcal{C}_{\theta_j}(\hat{\rho}_i^*, \psi_i; \theta) + \mathcal{A}_{\theta_j}(\hat{\rho}_i, \hat{u}_i^*; \theta) \right] \\ - 2 \langle m_{\text{post}} - m_{\text{pr}}, \mathcal{H}^{-1} \mathcal{B}_j \rangle_{\Gamma_{\text{prior}}^{-1}}$$

where

$$\mathcal{B}_j(\hat{m}, \theta) := \mathcal{C}_{\theta_j}(p, \hat{m}; \theta) + \mathcal{A}_{\theta_j}(p, \hat{u}; \theta) + \mathcal{C}_{\theta_j}(p, \hat{m}; \theta) + \mathcal{A}_{\theta_j}(\hat{\rho}, u; \theta) + \mathcal{D}_{\theta_j}(\hat{\rho}; \theta)$$

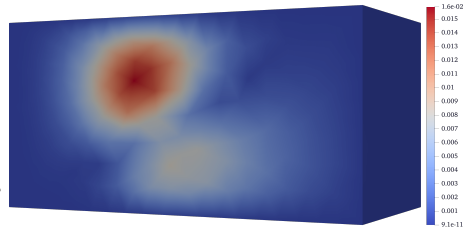
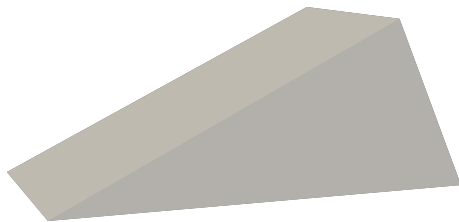
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Fault-Slip Inversion

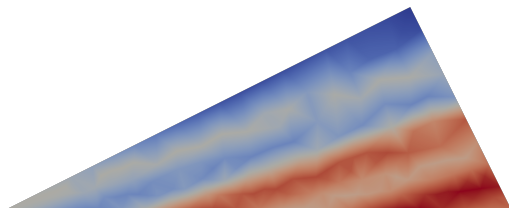
Governing PDE

$$\begin{aligned} -\nabla \cdot [\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \lambda \nabla \cdot \mathbf{u} \mathbf{I}] &= \mathbf{0} && \text{in } \Omega, \\ \boldsymbol{\sigma}(\mathbf{u}) \mathbf{n} &= \mathbf{0} && \text{on } \Gamma_t, \\ \mathbf{u} + \beta_k \boldsymbol{\sigma}(\mathbf{u}) \mathbf{n} &= \mathbf{0} && \text{on } \Gamma_k, \\ \mathbf{u} + \beta_s \boldsymbol{\sigma}(\mathbf{u}) \mathbf{n} &= \mathbf{h} && \text{on } \Gamma_s, \\ \mathbf{u} \cdot \mathbf{n} &= 0 && \text{on } \Gamma_b, \\ \delta \mathbf{T}(\boldsymbol{\sigma}(\mathbf{u}) \mathbf{n}) + \mathbf{T} \mathbf{u} &= \mathbf{m} && \text{on } \Gamma_b. \end{aligned}$$

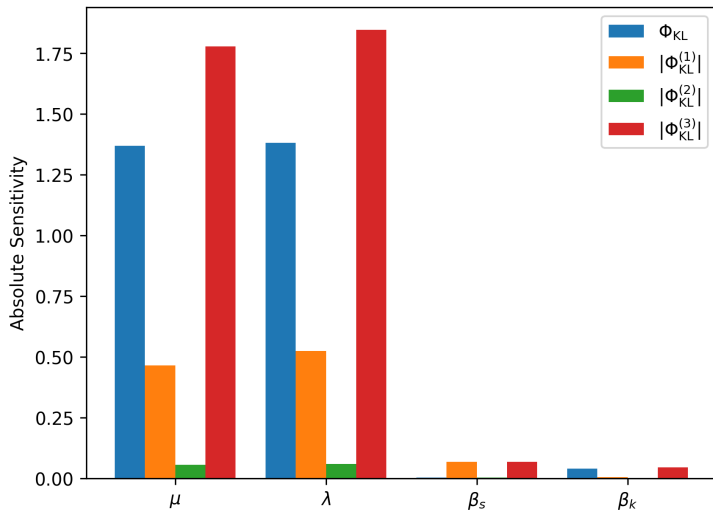


KL-Expansions in the Láme Parameters

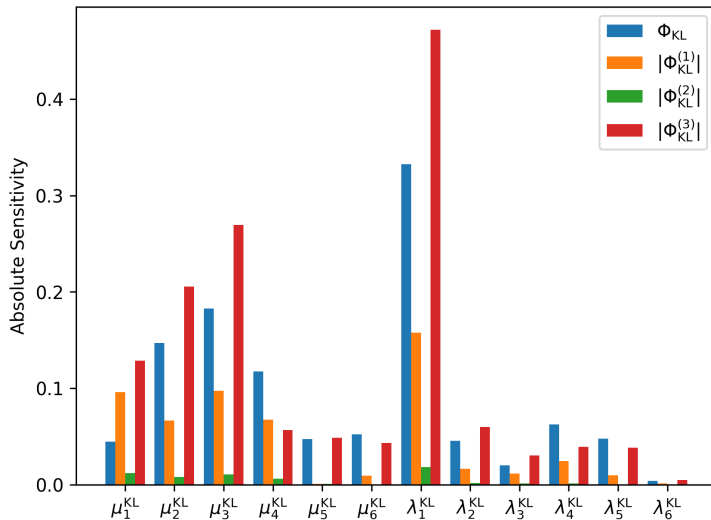
$$\lambda(x, \omega) = \bar{\lambda} + \sum_{i=1}^{\infty} \sqrt{\gamma_i} e_i(x) \xi_i^\lambda(\omega) \quad \text{and} \quad \mu(x, \omega) = \bar{\mu} + \sum_{i=1}^{\infty} \sqrt{\gamma_i} e_i(x) \xi_i^\mu(\omega)$$



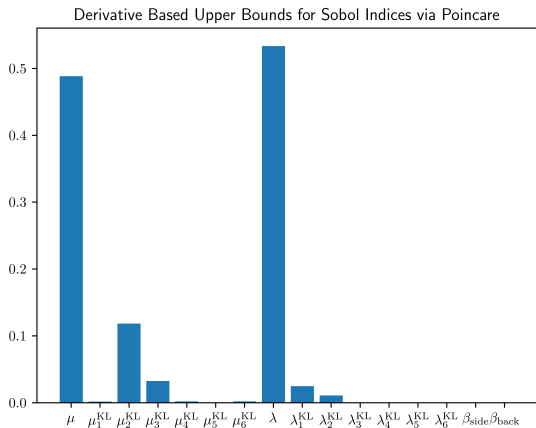
Sensitivity Results



Sensitivity Results



Derivative-Based Sobol Index Upper Bounds



$$S_i^{\text{tot}} \leq \frac{C(F_i)}{V} \int \left(\frac{\partial}{\partial \theta_i} \Phi_{\text{KL}}(\boldsymbol{\theta}) \right)^2 dF(\boldsymbol{\theta})$$

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Sergey Kucherenko and Bertrand Iooss. "Derivative-Based Global Sensitivity Measures". In: (2016). Ed. by Roger Ghanem, David Higdon, and Houman Owhadi, pp. 1–24. DOI: 10.1007/978-3-319-11259-6_36-1

Conclusion

In summary,

- Exact expressions scalable to infinite-dimensional parameters
- Feasible to use to perform global sensitivity analysis
- Only requires variational derivatives of the weak form with respect to θ .

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