

## Motivation

First Consider a PDE model:

$$\begin{aligned}
 -\nabla \cdot (c^m \nabla u) &= f && \text{in } \Omega \\
 c^m \nabla u \cdot n &= 0 && \text{on } \Gamma_1 \cup \Gamma_3 \\
 c^m \nabla u \cdot n &= \beta(T_m - u) && \text{on } \Gamma_2 \\
 c^m \nabla u \cdot n &= s && \text{on } \Gamma_4
 \end{aligned}$$

models heat flow across a conductive surface

Inverse Problems: There is some unknown parameter of interest that we seek to infer using knowledge of our governing model and data measurements  $y$ .

- inversion parameter:  $m(x)$  - spatially varying log-conductivity
- auxiliary parameters :  $\beta$  - heat transfer coef. of medium  
 $s(x)$  - boundary source term  
 $f(x)$  - heat source in domain
- experimental parameters:  $y$  - data measurements
- complementary parameters: auxiliary + experimental parameters

Frequentist Perspective: Solve inverse problem to obtain an estimate of the inversion parameter  $m^*$ .

Bayesian Perspective: Solve inverse problem to obtain a posterior distribution of the inversion parameter.

HDSA: We use derivative based sensitivity analysis to determine the sensitivity of the solution of the inverse problem to perturbations of the complementary parameters.

- informs experimental priorities
  - sensor design
  - estimating auxiliary parameters
- dimension reduction for OEDUV
- insight into the inverse problem

## HDSA for Bayesian Nonlinear Inverse Problems

Data Model:  $y = f(m, \theta) + \eta$

- $f$ : param-to-observable map
- $\Theta$ : complementary params
- $\eta$ : additive Gaussian noise,  $\eta \sim N(0, \Gamma_n)$

Data likelihood:  $\pi_{\text{like}}(y|m) \propto \exp(-\frac{1}{2}(f(m, \theta) - y)^T \Gamma_n^{-1} (f(m, \theta) - y))$

- distribution of data  $y$ , given  $m$

Prior Distribution:  $\mu_{\text{pr}} = N(m_{\text{pr}}, C_{\text{pr}})$

- prior knowledge of  $m$

MAP point:

$$J(m, \theta) = \underbrace{\frac{1}{2} \langle Q_u - y, \Gamma_n^{-1} (Q_u - y) \rangle}_{m_{\text{MAP}} = \underset{m}{\operatorname{arg\,min}} J(m, \theta)} + \underbrace{\frac{1}{2} \langle A(m - m_{\text{pr}}), A(m - m_{\text{pr}}) \rangle}_{A = \Gamma_{\text{pr}}^{-1/2}}, \quad A = \Gamma_{\text{pr}}^{-1/2}$$

Sensitivity of the MAP point:

apply implicit function theorem to  $J_m$

results in a continuously differentiable mapping

$$\tilde{F}: N(\theta^*) \rightarrow N(m^*)$$

We define our sensitivity operator

$$D = \tilde{F}'_{\theta}(\theta^*) = -H^{-1}B \quad \text{where}$$

$$H = J_{m, \theta}(m^*, \theta^*), \quad B = J_{m, \theta}(m^*, \theta^*)$$

We interpret  $D\bar{\theta}$  as the sensitivity of the MAP point when the comp. params are perturbed in the direction  $\bar{\theta}$ .

Pointwise Sensitivity Indices: compare within parameters

$$S_k^i = \frac{\|D e_k^i\|_M}{\|e_k^i\|_\Theta}$$

Generalized Sensitivity Indices: compare across parameters

$$S_k = \max_{\Theta} \frac{\|DT_k\Theta\|_M}{\|\Theta\|_\Theta}$$

Measures of Posterior Uncertainty

Bayes Risk: approximate by sample averaging

$$\hat{\Psi}_R(\Theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} \|m_{MAP}(y_i, \Theta) - m_i\|^2 \text{ where}$$

$$y_i = f(m_i, \Theta) + \eta_i, \quad \underbrace{m_i}_{\text{prior draws}}$$

$$\hat{\Psi}_{\text{risk}}(\Theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} \langle m_{MAP}(y_i, \Theta), m_{MAP}(y_i, \Theta) \rangle - 2 \langle m_{MAP}(y_i, \Theta), m_i \rangle + \langle m_i, m_i \rangle$$

$$\begin{aligned} \frac{d}{d\Theta_j} \hat{\Psi}_{\text{risk}}(\Theta^*) &= \frac{1}{n_s} \sum_{i=1}^{n_s} 2 \left\langle \frac{d}{d\Theta_j} m_{MAP}(y_i, \Theta^*), m_{MAP}(y_i, \Theta^*) \right\rangle - 2 \left\langle \frac{d}{d\Theta_j} m_{MAP}(y_i, \Theta^*), m_i \right\rangle \\ &= \frac{1}{n_s} \sum_{i=1}^{n_s} 2 \langle D_j^i, m_{MAP}(y_i, \Theta^*) \rangle - 2 \langle D_j^i, m_i \rangle, \quad j=1, 2, \dots, p \end{aligned}$$

\* note that  $D_j^i$  is the  $j^{\text{th}}$  column of sens. op.  $D^i$  which depends on the  $i^{\text{th}}$  sample draw.

let  $D_j^R = \frac{d}{d\Theta_j} \hat{\Psi}_{\text{risk}}(\Theta^*)$  and  $D^R = \begin{bmatrix} D_1^R \\ \vdots \\ D_p^R \end{bmatrix} = \nabla_{\Theta} \hat{\Psi}_R(\Theta^*)$ , then  $D^R \bar{\Theta}$  can be

interpreted as the sens. of  $\hat{\Psi}_R$  wrt a perturbation of the params in the direction  $\bar{\Theta}$ .

\* Note that building  $D^R$  requires building  $n_s$  sens. op.  $D^i = -H^{-1}B$ , i.e. many Hessian solves.