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Coupling optimal experimental design and optimal control

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U.S. DEPARTMENT OF ENERGY NNSA

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What is optimal experimental design?

tells us when, where, and how to collect data to maximize information

Digital twin problems

Data

- Physical property information
- Decision making
- Determine control strategies

Limits on data collection

- Feasibility
- Cost
- Inaccessibility

Why is OED challenging?

How to characterize information in data?

Optimization constrained by an **inverse problem** constrained by a **PDE**

Goal: estimate model parameters

$$\underbrace{\pi(\theta|\boldsymbol{y})}_{\text{posterior}} \propto \underbrace{\pi(\boldsymbol{y}\,|\theta)}_{\text{likelihood}}\, \underbrace{\pi_{\text{pri}}(\theta)}_{\text{prior}}$$

$$\pi(\boldsymbol{y}\,|\theta) \propto \exp\left(-\frac{1}{2}\,\|\underbrace{f(\theta)}_{\text{Mathematical Model}} - \boldsymbol{y}\|_{\Gamma}^{2}\right)$$

Model – often expensive to compute partial differential equations (PDEs)

Our approach

minimize uncertainty directly related to prediction and control objectives

Goal oriented OED

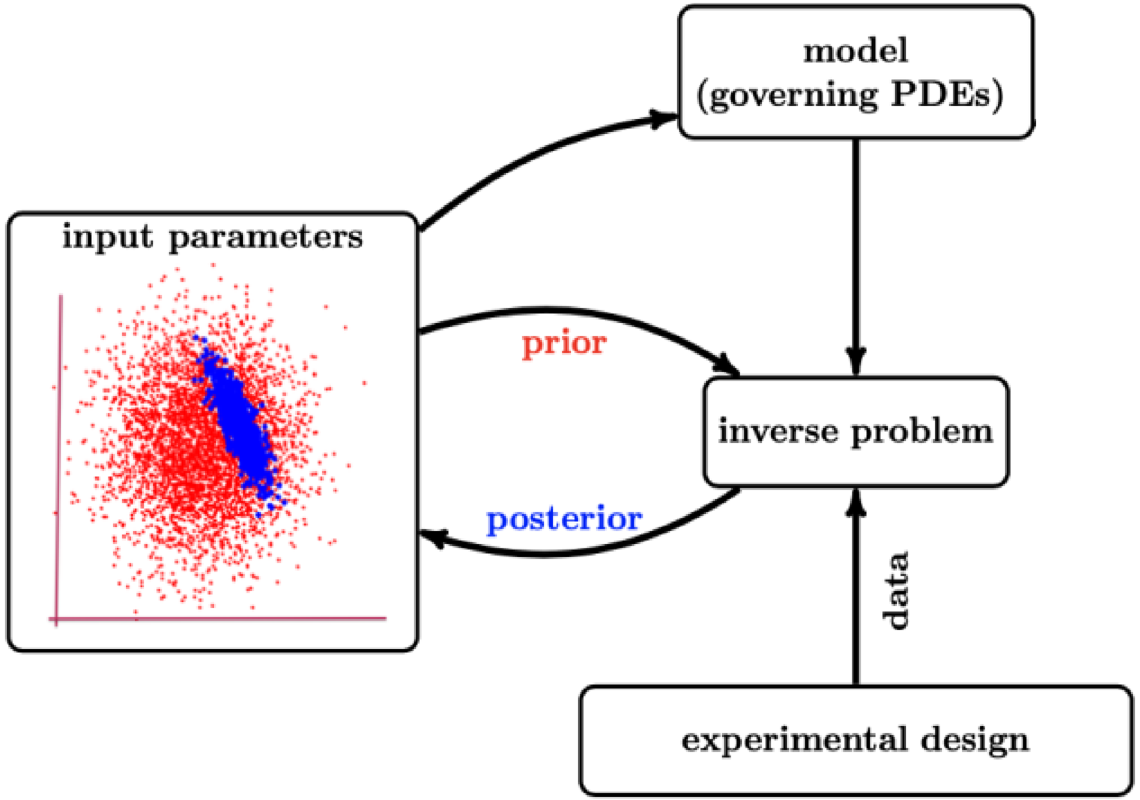


Figure: overview of Bayesian OED‡

‡ A. Alexanderian. Optimal Experimental Design for Bayesian Inverse Problems Governed by PDEs: A Review

Why are goal-oriented approaches beneficial?

Stationary advection-diffusion example

$$-\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{\theta})\nabla u) + b\nabla u = f, \text{ in } \Omega = \ [0,1] \cup [0,1]$$

$$u(\boldsymbol{x}) = 0 \text{ on } \Gamma_D$$

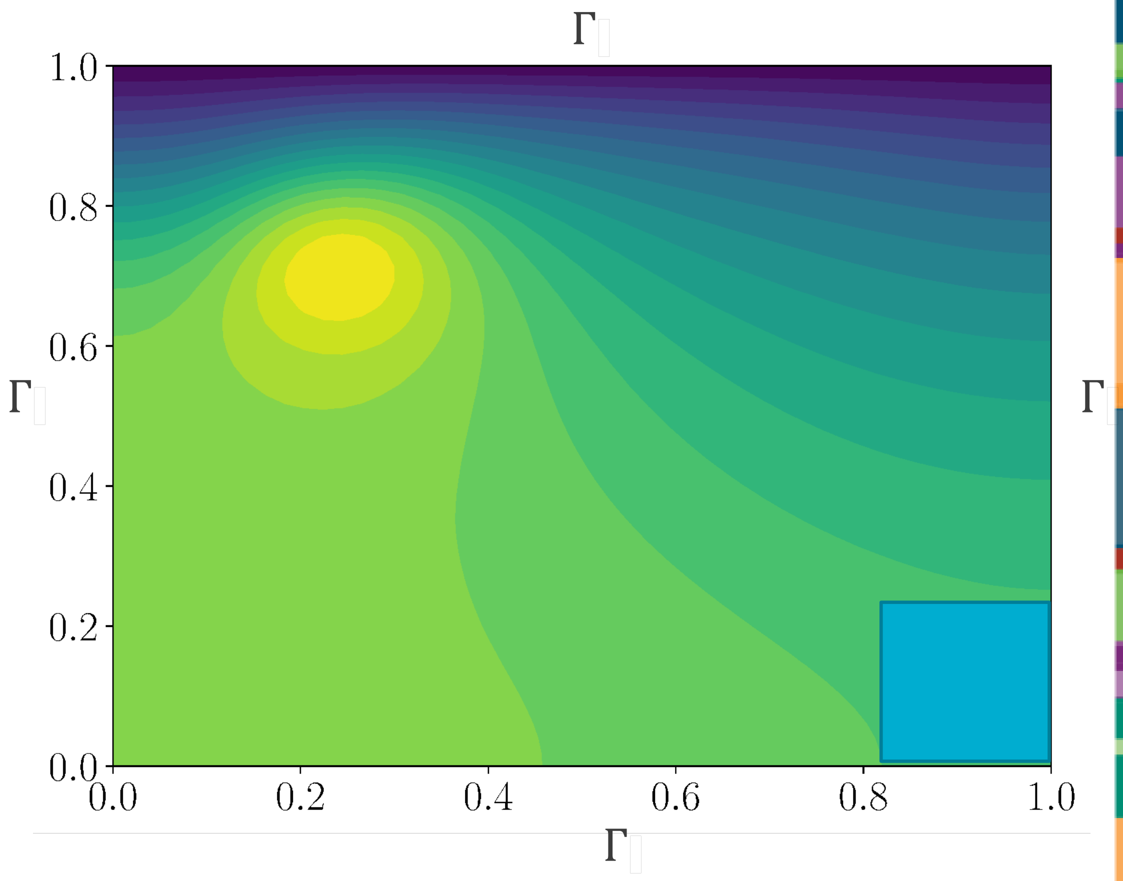
$$\nabla u(\boldsymbol{x}) = 0 \text{ on } \Gamma_N$$

What is the best way to collect data:

Estimate model parameters $\boldsymbol{\theta}$

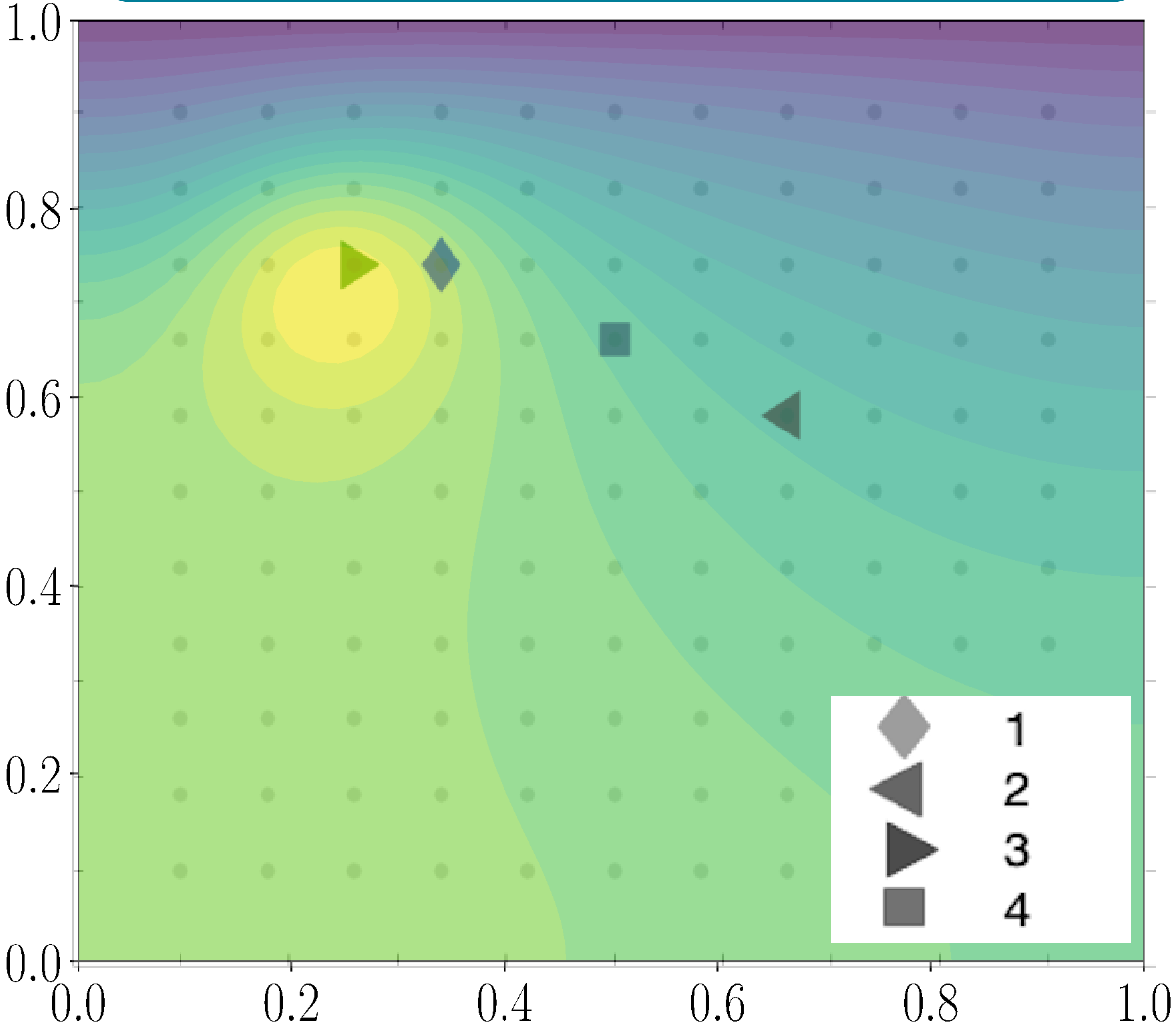
vs.

Improve prediction accuracy in lower right hand corner?

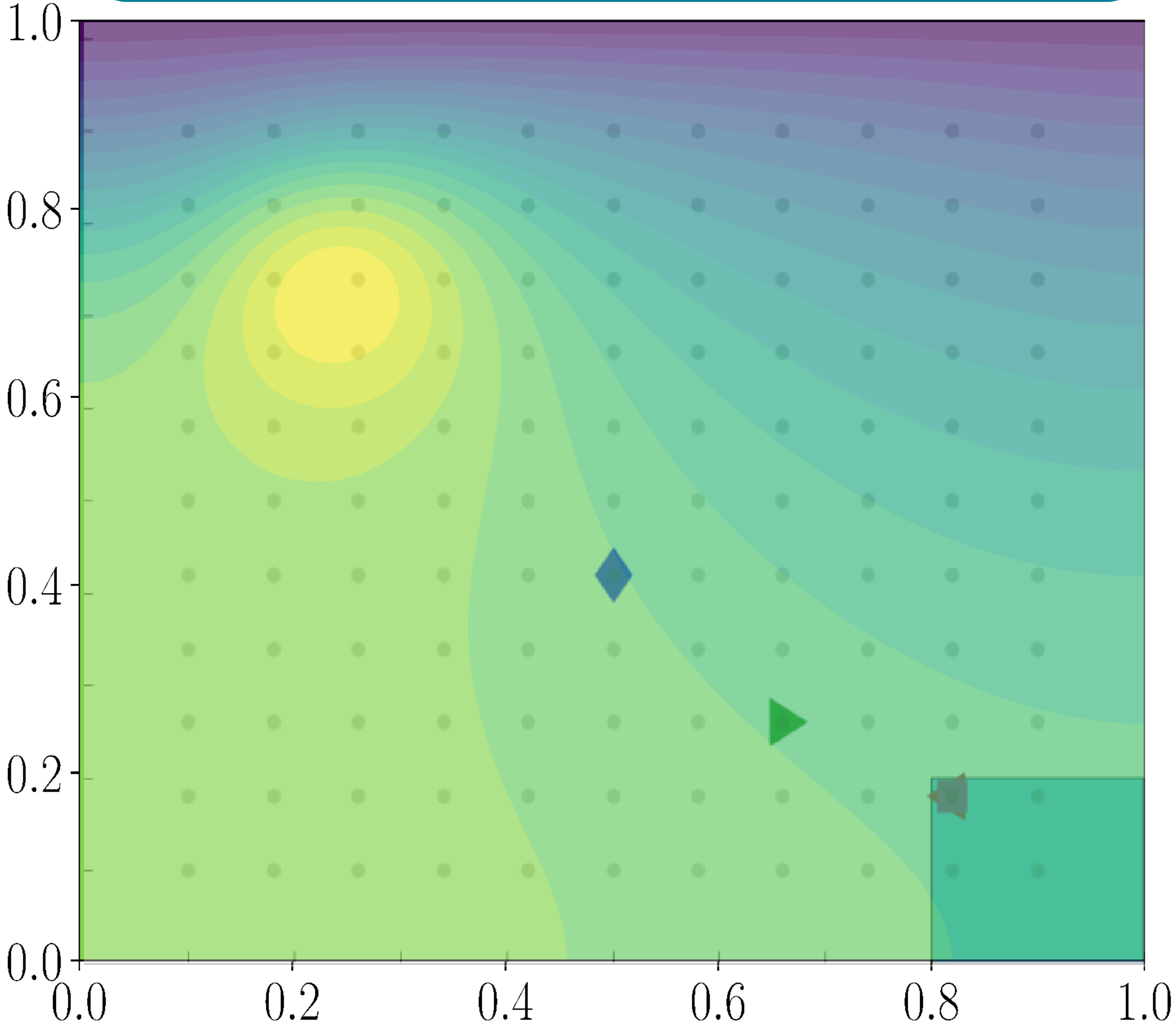


Why are goal-oriented approaches beneficial?

OED for inverse problems



OED for prediction



Experimental design for optimal control problems

What if our goal is to **minimize uncertainty** related to an **optimal control** policy?

analytical expressions for the **objective function** →

- Gaussian prior
- Linear parameter-to-observable map
- Quadratic control objective

Deriving the OED for control objective function

Solution to the OED problem

$$\xi^* = \min_{\xi} U(\xi)$$

Goal: derive $U(\xi)$ for control problems

↓

How to collect data to minimize **uncertainty** in a control objective

1. Define parameter-to-observable map

2. Determine objective function for the inverse problem

3. Determine objective function for the control problem

1. Define parameter-to-observable map

Γ

Γ

$$-\kappa \Delta u(x,y) = z(x,y) \text{ in } \Omega$$

$$u(x,y) = 0 \text{ on } \Gamma_D$$

$$-\kappa \nabla u(x,y) \cdot \boldsymbol{n} = p(x) \text{on } \Gamma_{\mathrm{N}}$$

Γ

Γ

Steady state-advection diffusion

Design – spatial locations for data collection

1. Define parameter-to-observable map

Γ

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Γ Γ

Γ

Steady state-advection diffusion

Control

1. Define parameter-to-observable map

Γ

Γ

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Γ

Γ

Steady state-advection diffusion

Unknown parameter

Assumption – discrete

$$p(x) = \sum_{i=1}^{n_p} p_i \phi_i(x)$$

1. Define parameter-to-observable map

Γ

$$-\kappa\Delta u(x,y) = z(x,y) \text{ in } \Omega$$

$$u(x,y) = 0 \text{ on } \Gamma_D$$

$$-\kappa\nabla u(x,y)\cdot \boldsymbol{n} = p(x) \text{ on } \Gamma_N$$

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Γ

Discretized PDE

$$= \quad + \quad +$$

Parameter-to-observable map

$$= \quad + \quad + \quad +$$

Linear in parameter and control

2. OED objective function – inverse problem

Experimental design goal: minimize uncertainty parameter estimates

OED objective function

$$U(\xi) = \text{trace}\left(\boldsymbol{\Gamma}_{\text{post}}(\xi)\right)$$

Only posterior mean depends on data

and control

$$\boldsymbol{\Gamma}_{\text{post}} = \left(\boldsymbol{F}_2^T \boldsymbol{\Gamma}_{\text{noise}}^{-1} \boldsymbol{F}_2 + \boldsymbol{\Gamma}_{\text{pr}}^{-1}\right)^{-1}$$

$$\boldsymbol{m}_{\text{post}} = \boldsymbol{\Gamma}_{\text{post}}\left(\boldsymbol{F}_2^T \boldsymbol{\Gamma}_{\text{noise}}^{-1} \boldsymbol{y} + \boldsymbol{\Gamma}_{\text{pr}}^{-1} \boldsymbol{m}_{\text{pr}} - \boldsymbol{F}_2^T \boldsymbol{\Gamma}_{\text{noise}}^{-1}(\boldsymbol{F}_1 \boldsymbol{z} + \boldsymbol{\beta})\right)$$

3. Determine objective function for control problem

I. Define the **optimal control** problem and objective

II. Compute the **variance** of the control objective

III. Derive the **objective function**

3.1 Define the **optimal control** problem and objective

Control objective

$$\phi(\mathbf{z}) = \frac{1}{2}\int_{\Omega}(u - \bar{\boldsymbol{u}})^2 dxdy$$

Target concentration

Optimal control Solution

$$\boldsymbol{z}^*(\boldsymbol{p}) = \boldsymbol{F}_3\boldsymbol{p} + \boldsymbol{\beta}_2$$

Optimal control problem

$$z(x,y) = \sum_{k=1}^{n_z} z_k \xi_k(x,y)$$

$$\mathbf{z}^* = \min_{\mathbf{z}} \frac{1}{2}\int_{\Omega}(u - \bar{u})^2 dxdy + \frac{\alpha}{2}\|\mathbf{z}\|_2^2$$

Discretized objective

$$\phi^N(\mathbf{z}^*) = \frac{1}{2}\langle \boldsymbol{F}\boldsymbol{p} + \boldsymbol{c}, \boldsymbol{Q}(\boldsymbol{F}\boldsymbol{p} + \boldsymbol{c})\rangle$$

Quadratic in parameter

3.II Compute the **variance** of the control objective

Since $\boldsymbol{p} \sim \mathcal{N}(\boldsymbol{m}_{\text{post}}, \boldsymbol{\Gamma}_{\text{post}})$ we can analytically compute variance‡

$$\psi(\boldsymbol{y}) := \text{Var}\left[\frac{1}{2}\langle \boldsymbol{F}\boldsymbol{p} + \boldsymbol{c}, \boldsymbol{Q}(\boldsymbol{F}\boldsymbol{p} + \boldsymbol{c})\rangle\right]$$

$$= \frac{1}{2}\text{tr}\left[\left(\widehat{\boldsymbol{A}}\boldsymbol{\Gamma}_{\text{post}}\right)^2\right] + \langle \widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}, \boldsymbol{\Gamma}_{\text{post}}\left(\widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}\right)\rangle$$

‡ https://aalexan3.math.ncsu.edu/articles/moments_quad.pdf

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$$\boldsymbol{m}_{\text{post}} = \boldsymbol{\Gamma}_{\text{post}}\left(\boldsymbol{F}_2^T\boldsymbol{\Gamma}_{\text{noise}}^{-1}\boldsymbol{y} + \boldsymbol{\Gamma}_{\text{pr}}^{-1}\boldsymbol{m}_{\text{pr}} - \boldsymbol{F}_2^T\boldsymbol{\Gamma}_{\text{noise}}^{-1}(\boldsymbol{F}_1\boldsymbol{z} + \boldsymbol{\beta})\right)$$

depends upon the data and control

3.II Compute the **variance** of the control objective

Since $\boldsymbol{p} \sim \mathcal{N}(\boldsymbol{m}_{\text{post}}, \Gamma_{\text{post}})$ we can analytically compute variance‡

$$\psi(\boldsymbol{y}) = \frac{1}{2}\text{tr}\left[\left(\widehat{\boldsymbol{A}}\Gamma_{\text{post}}\right)^2\right] + \left\langle \widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}, \Gamma_{\text{post}}\left(\widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}\right)\right\rangle$$

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Nominal control

$$\boldsymbol{z}^*(\boldsymbol{m}_{pr}) = \boldsymbol{F}_3\boldsymbol{m}_{pr} + \boldsymbol{\beta}_2$$

3.III Derive the **objective function**

OED for control objective function

$$
\begin{aligned}
U(\xi) &= E_{\boldsymbol{p}} E_{\boldsymbol{y}}[\psi(\boldsymbol{y}, \boldsymbol{\theta})] \\
&= E_{\boldsymbol{p}} E_{\boldsymbol{y}}\left[\frac{1}{2}\operatorname{tr}\left[\left(\widehat{\boldsymbol{A}}\boldsymbol{\Gamma}_{\text{post}}\right)^2\right] + \left\langle \widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}, \boldsymbol{\Gamma}_{\text{post}}\left(\widehat{\boldsymbol{A}}\boldsymbol{m}_{\text{post}} + \widehat{\boldsymbol{b}}\right)\right\rangle\right]
\end{aligned}
$$

Design experiments that maximize **information** regarding how well an **optimal control** policy **performs**

Deriving OED for control objective function

- Define parameter-to-observable map
- Derive Bayesian inverse problem solution
- Write OED for inverse problem objective function
- Derive optimal control problem solution
- Define OED in the context of control problem
  - Compute posterior variance
  - Define objective function

OED for the inverse problem

Experimental design goal: determine optimal spatial locations to collect data which minimizes uncertainty in parameter estimates

Goal

$$\xi^* = \min_{\xi} U(\xi)$$

OED objective function

$$U(\xi) = \text{trace}\left(\Gamma_{\text{post}}(\xi)\right)$$

Minimizing the average uncertainty in model parameters – p

2. OED objective function – inverse problem

Assumptions

$\sim (\ _{\text{pr}},\ _{\text{pr}})$ $\sim (\ ,\ _{\text{noise}})$

Bayesian inverse problem solution

$$\Gamma_{\text{post}} = \left(\boldsymbol{F}_2^T \Gamma_{\text{noise}}^{-1} \boldsymbol{F}_2 + \Gamma_{\text{pr}}^{-1}\right)^{-1}$$

Does not depend upon $\boldsymbol{y}$

$$\boldsymbol{m}_{\text{post}} = \Gamma_{\text{post}} \left(\boldsymbol{F}_2^T \Gamma_{\text{noise}}^{-1} \boldsymbol{y} + \Gamma_{\text{pr}}^{-1} \boldsymbol{m}_{\text{pr}} - \boldsymbol{F}_2^T \Gamma_{\text{noise}}^{-1} (\boldsymbol{F}_1 \boldsymbol{z} + \boldsymbol{\beta})\right)$$

Uncertainty in model parameter estimates is characterized by the covariance

Optimal control problem solution

Assumption

$$z(x,y) = \sum_{k=1}^{n_z} z_k \xi_k(x,y)$$

Goal

$$\min_{\boldsymbol{z}} \frac{1}{2}\int_{\Omega} (u - \underbrace{\bar{u}}_{\text{target temperature}})^2 dxdy + \frac{\alpha}{2}\|\boldsymbol{z}\|_2^2$$

target temperature

optimal control can be written as an affine function in $\boldsymbol{p}$

Optimal control Solution

$$\boldsymbol{z}^*(\boldsymbol{p}) = \boldsymbol{F}_3\boldsymbol{p} + \boldsymbol{\beta}_2$$

OED for control problem

Experimental design goal: determine optimal spatial locations to collect data which minimizes the variance (uncertainty) in the control objective at the optimal control

$$\phi(\boldsymbol{z}) = \frac{1}{2}\int_{\Omega}(u - \bar{u})^2 dxdy$$

Discretize and evaluate at optimal control

$$\phi^N(\boldsymbol{z}^*) := \phi(\boldsymbol{p}) = \frac{1}{2}\langle \boldsymbol{F}\boldsymbol{p} + \boldsymbol{c}, \boldsymbol{Q}(\boldsymbol{F}\boldsymbol{p} + \boldsymbol{c})\rangle$$

Quadratic in $\boldsymbol{p}$