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Sandia National Laboratories

Machine learning in the context of inverse, control, and experimental design problems

MACHINE LEARNING & DEEP LEARNING

MLDL

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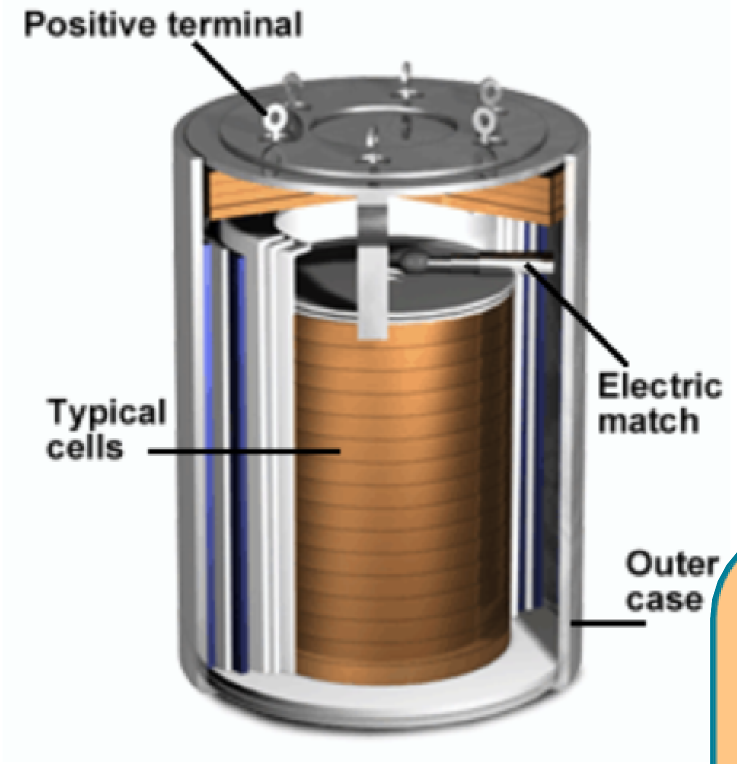
Machine learning in decision making and computational sciences

Digital twin problems

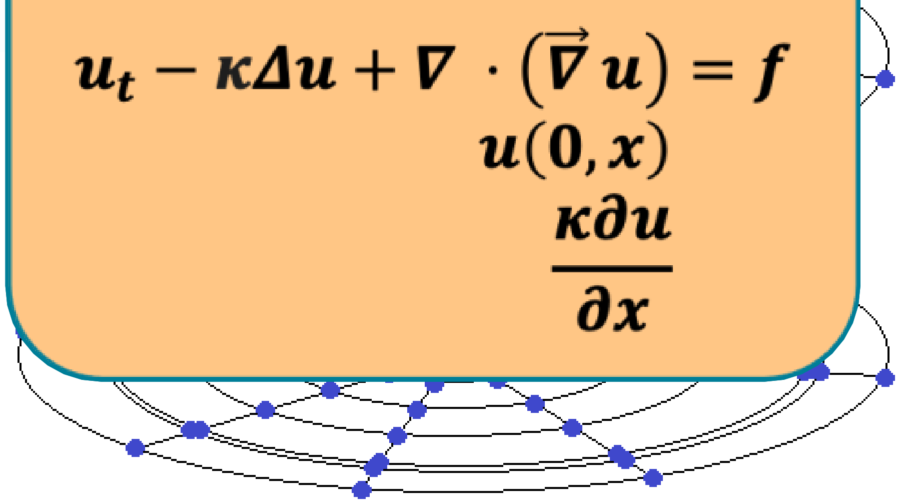


Real-world asset

Mathematical representation

Thermal Energy Model

$$u_t - \kappa \Delta u + \nabla \cdot (\vec{\nabla} u) = f$$
$$u(0, x)$$
$$\frac{\kappa \partial u}{\partial x}$$



Infer properties about the system

Digital twin systems

Make predictions about future scenarios

Decision making

In contrast to classical ML problems

To accomplish these goals we need data

Limited data

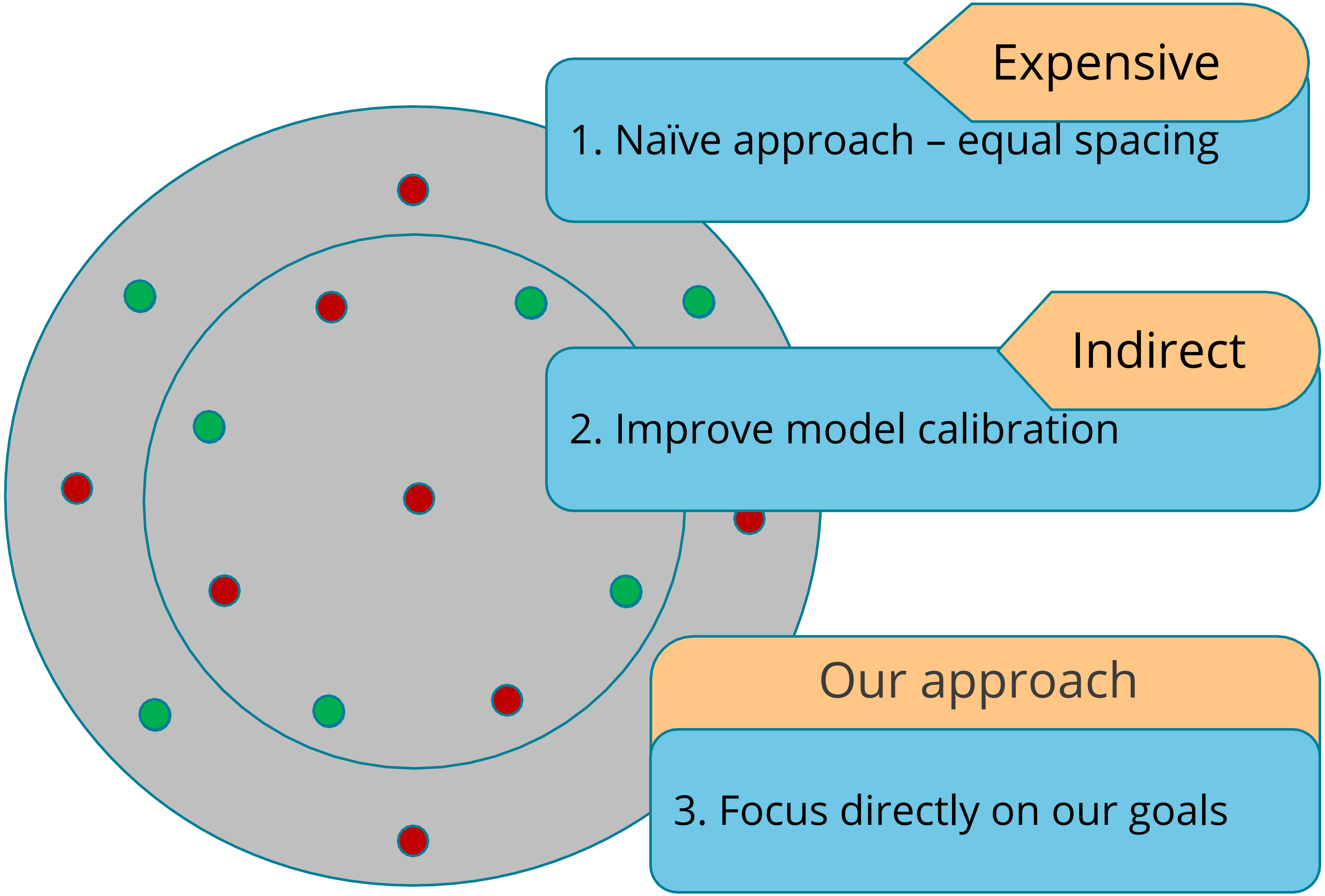
- Indirect measurements
- Limited sensor budget
- Multiple experiments infeasible

Physics constraints

- Complicated multiphysics systems
- Physical interpretability important
- Extrapolation is crucial

Optimal experimental design (OED)

Determine when, where, and how to collect data to maximize information



Sensor locations in battery cell

Bayesian optimal experimental design

Measurement Data

$$\boldsymbol{y} = f(\theta) + \boldsymbol{\eta}$$

- θ – model paran
- f – model
- $\boldsymbol{\eta} \sim \mathcal{N}(0, \boldsymbol{\Gamma})$ – Noi

Goal: estimate model parameters

$$\pi(\theta|\boldsymbol{y}) \propto \pi(\boldsymbol{y}|\theta)\, \pi_{\text{pri}}(\theta)$$

elihood

prior

$$\frac{1}{2}\|f(\theta) - \boldsymbol{y}\|_{\boldsymbol{\Gamma}}^2 \Big)$$

Mathematical Model

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

Model – often expensive to compute partial differential equations PDEs

Goal-oriented Bayesian OED

Determine what data y minimizes uncertainty in predictions

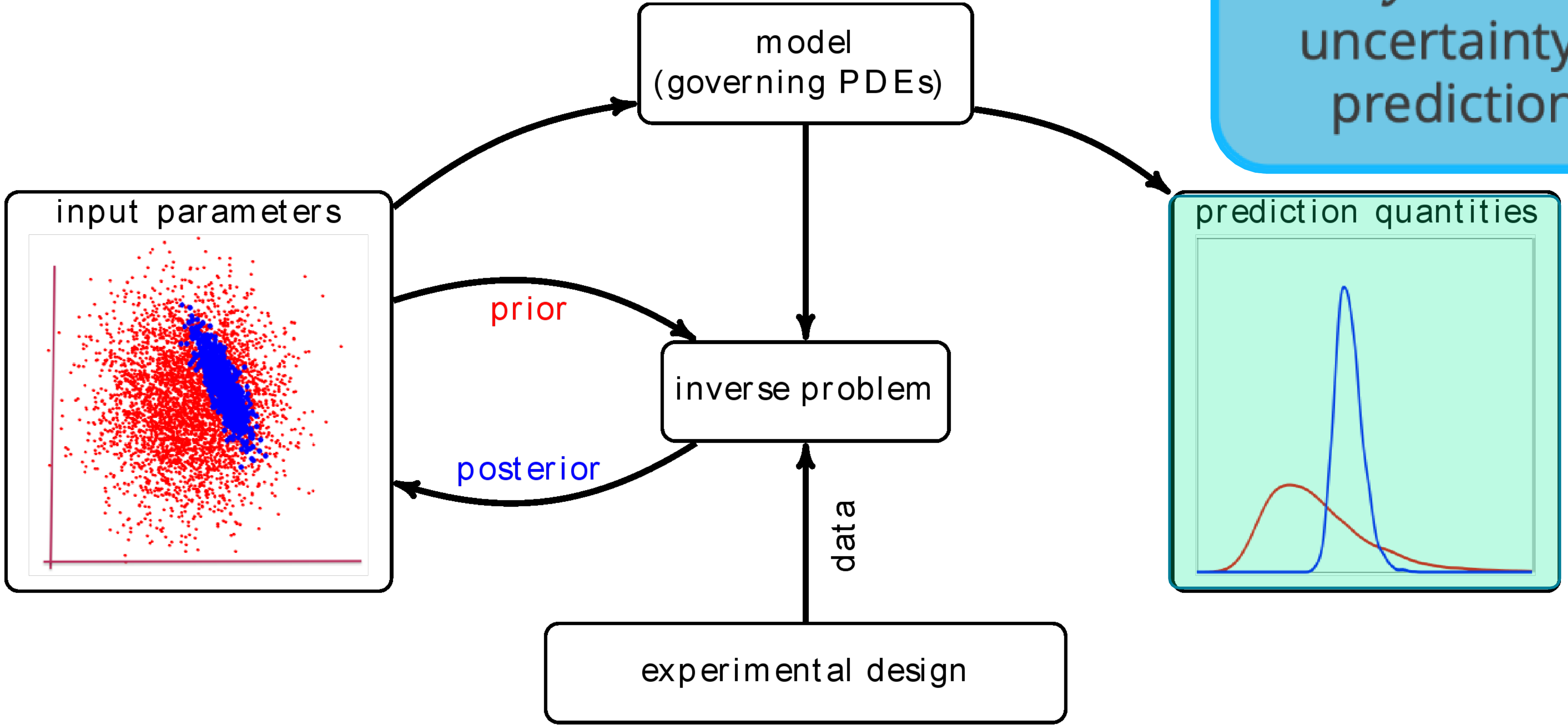


Figure: Overview of Bayesian Optimal Experimental design ‡

† A. Alexanderian, A. Saibaba, and A. Attia. Goal-oriented optimal design of experiments for large-scale Bayesian inverse problems. *Inverse Problems.* 2017
‡ A. Alexanderian. Optimal experimental design for Bayesian inverse problems governed by PDEs: A review. 2020

Design of sensor placement problem

2D stationary advection-diffusion

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

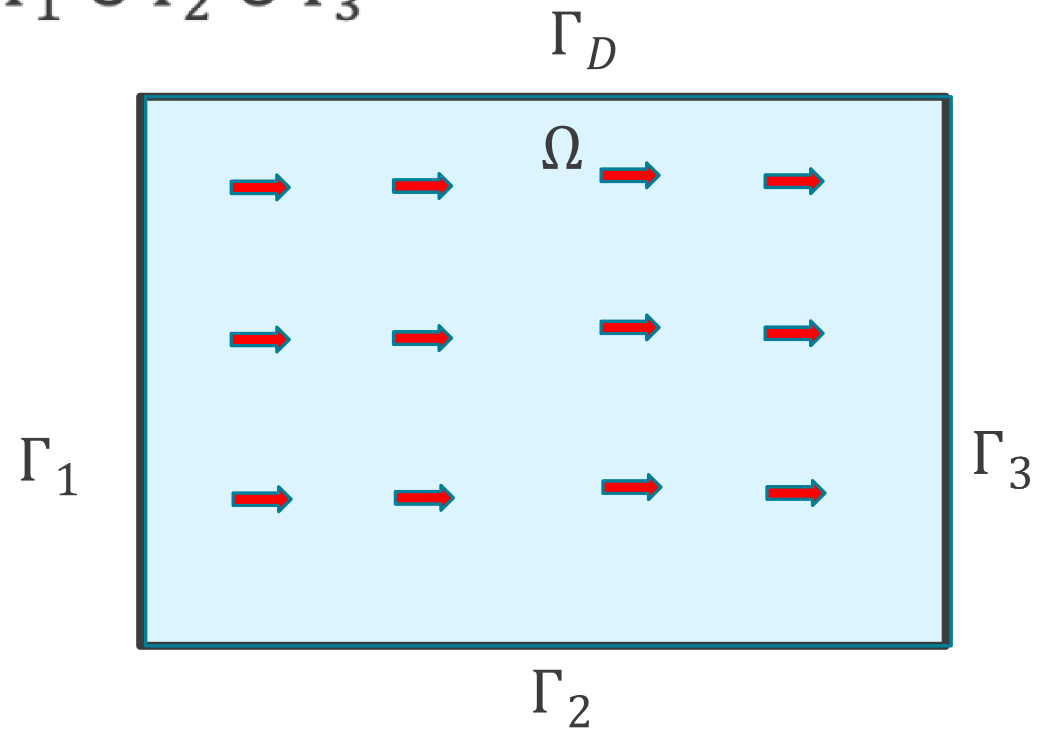
$$u(\boldsymbol{x}) = 0, \qquad \text{on } \Gamma_D$$

$$\nabla u(\boldsymbol{x}) = 0, \qquad \text{on } \Gamma_N = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$$

Source

$$f = \alpha \exp\left[-\frac{1}{\beta^2}\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2\right]$$

- $\alpha = 1$
- $\beta = 0.1$
- $x_0 = [0.25, 0.75]$



Design of sensor placement problem

2D stationary advection-diffusion

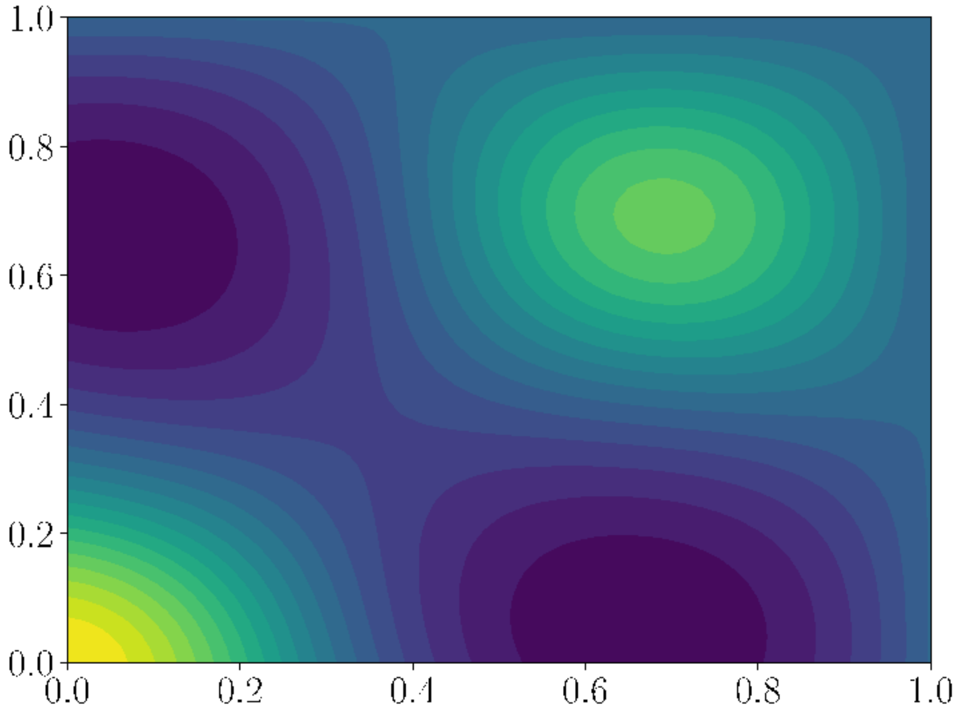
$$
\begin{aligned}
-\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{\theta}) \nabla u) + b \nabla u &= f, && \text{in } \Omega = [0,1] \\
u(\boldsymbol{x}) &= 0, && \text{on } \Gamma_D \\
\nabla u(\boldsymbol{x}) &= 0, && \text{on } \Gamma_N = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3
\end{aligned}
$$

Model is nonlinear in parameters

Diffusion

$$
\begin{aligned}
a(\boldsymbol{x}, \boldsymbol{\theta}) = \; & \exp\big[\theta_1 \sin(x_1 \pi) \sin(x_2 \pi) \\
& + \theta_2 \cos(3/2 x_1 \pi) \cos(3/2 x_2 \pi)\big]
\end{aligned}
$$

$$
\boldsymbol{\theta} = [\theta_1, \theta_2] \in \mathbb{R}^2
$$



Optimal experimental design problem

Where to place sensors to measure concentration to maximize information

Predictions

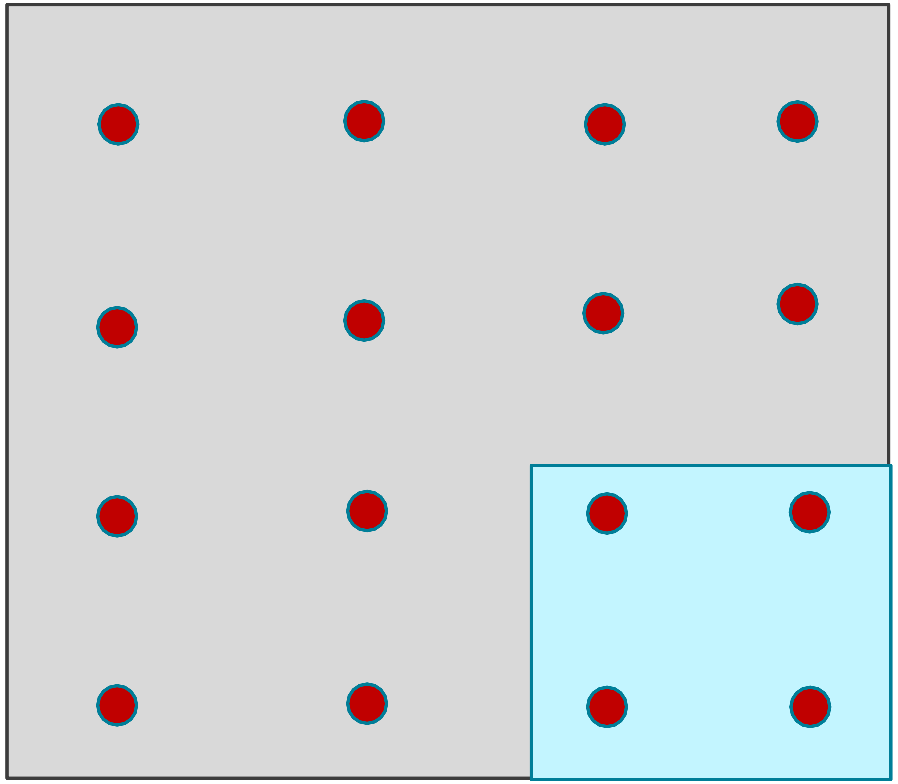


Figure: Sensor locations on a 2D domain measuring contaminant

Design Criterion

$$\psi(\xi, \boldsymbol{y}, \boldsymbol{\theta}) = \mathrm{Var}(u(\boldsymbol{\theta}, \xi)) \qquad \boldsymbol{\theta} \sim \pi(\boldsymbol{\theta} | \boldsymbol{y}, \xi)$$

Penalized uncertainty in our prediction directly

OED objective function

Goal

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

Where

$$U(\xi) = E_{\boldsymbol{\theta}} E_{\boldsymbol{y}} [\psi(\xi, \boldsymbol{y}, \boldsymbol{\theta})]$$

$$\boldsymbol{\theta} \sim \pi_{\text{pri}}(\boldsymbol{\theta})$$

$$\boldsymbol{y} \sim \pi(\boldsymbol{y} \mid \boldsymbol{\theta})$$

Recall

$$\pi(\boldsymbol{y} \mid \theta) \propto \exp\left(-\frac{1}{2} \|\boldsymbol{f}(\theta) - \boldsymbol{y}\|_{\Gamma}^{2}\right)$$

Evaluating objective function requires many evaluations of the **expensive-to-compute model**

One area where **ML surrogates** can be useful

Possible parameter-to-observable map surrogates

Polynomial chaos expansions

- Represents random variables in terms of polynomial functions

Neural networks

- Involves multiple hidden layers in a neural network

Operator inference

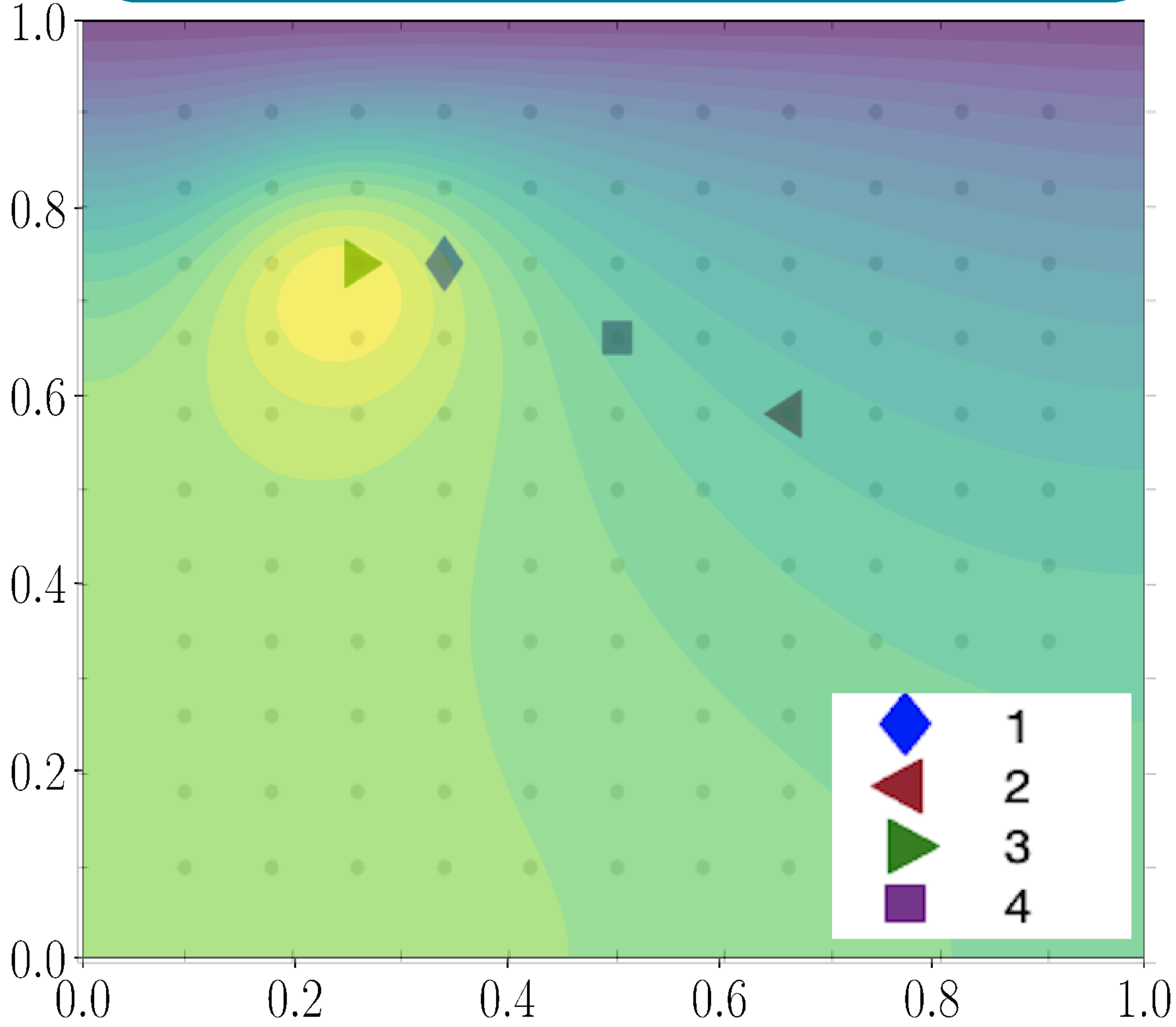
- Linear regression to determine a reduced order model that maintains structure – physical constraints

Gaussian processes

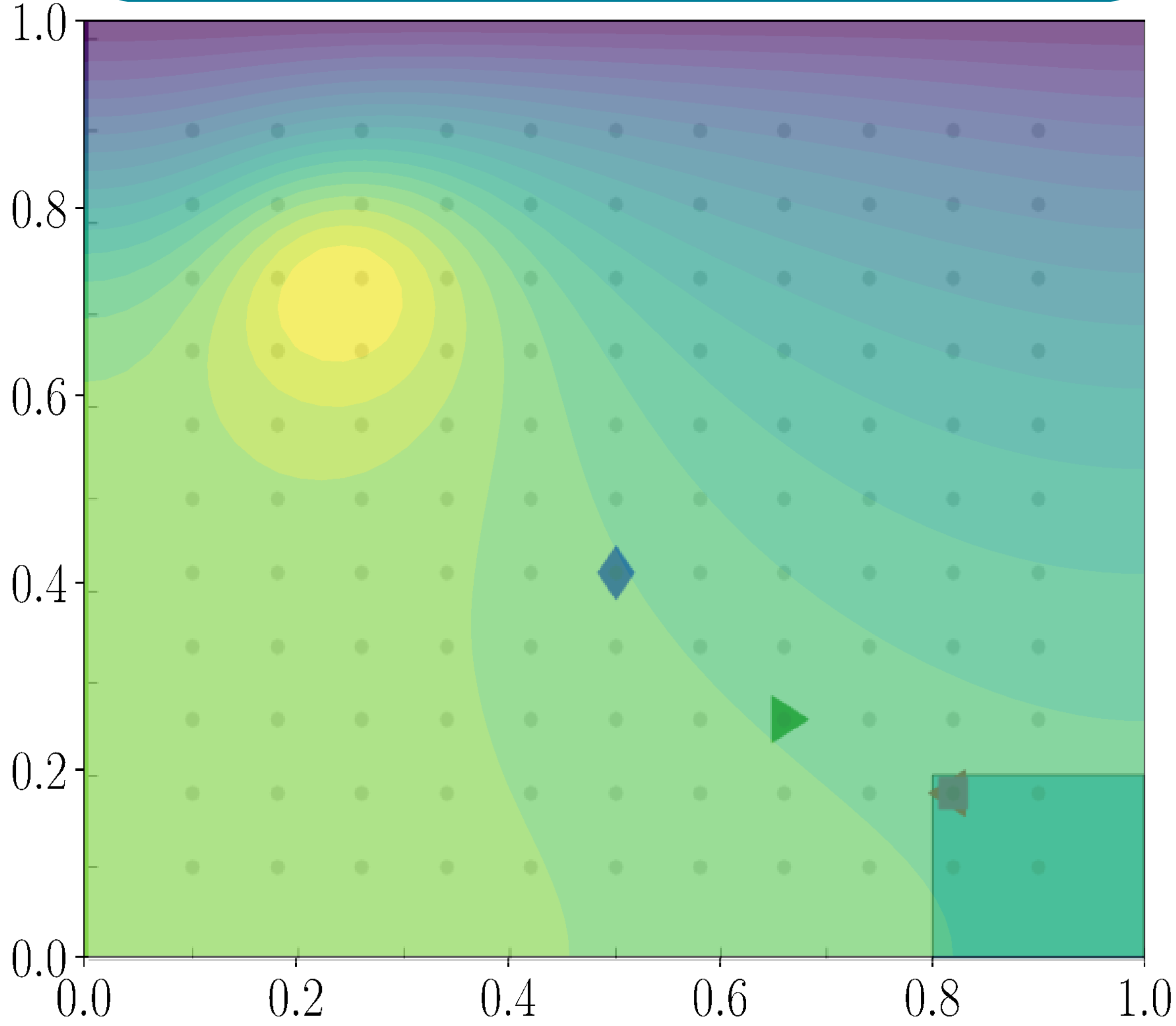
- Models random processes using Gaussian random variables

Benefits of goal-oriented approaches

OED for inverse problems



OED for prediction

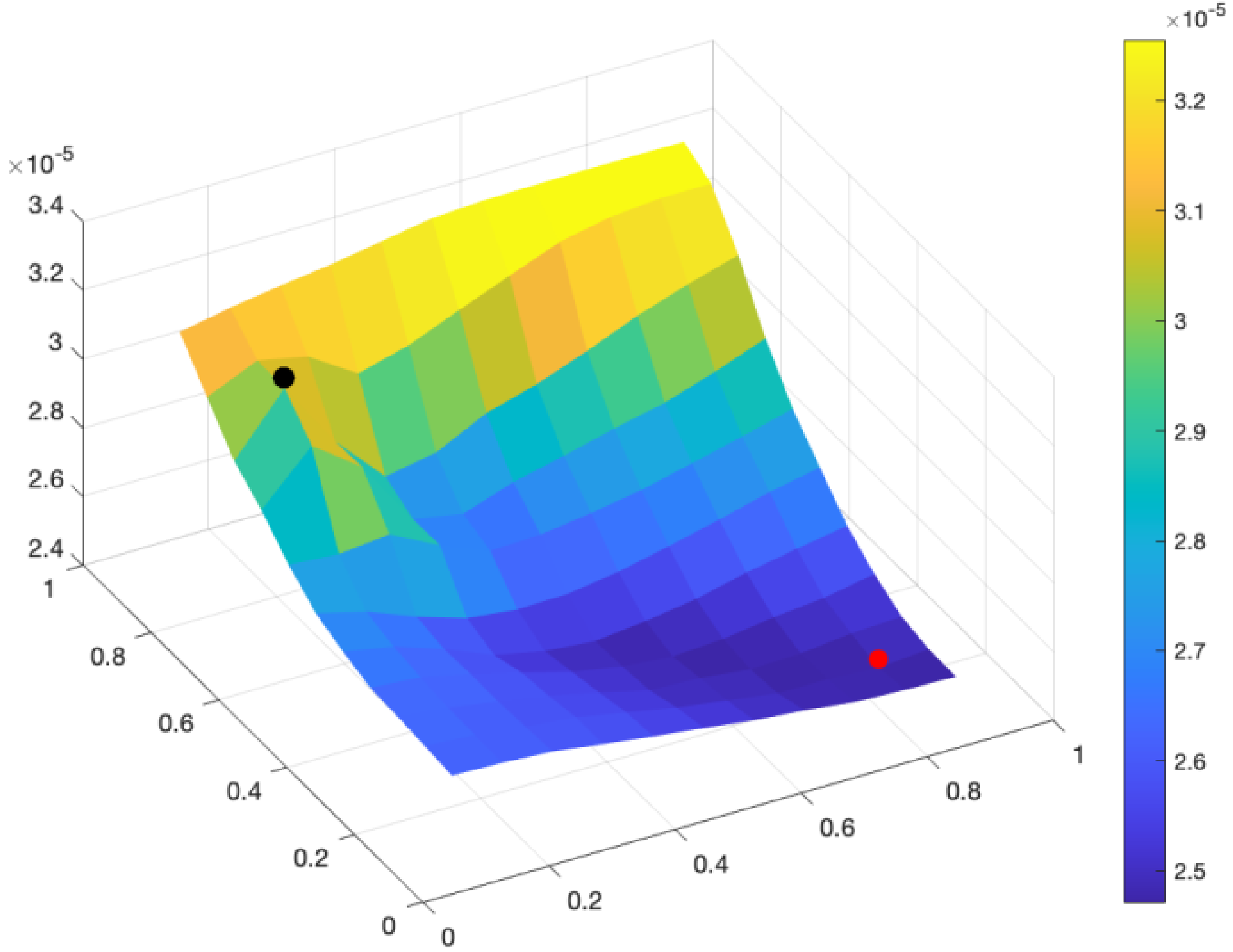


Benefits of goal-oriented approaches

Uncertainty in concentration prediction

Predictions

Parameters



Focusing directly on digital twin **goals improves** experimental **designs**

OED provides one way to maximize the information we **learn** from **data**