Sandia National Laboratories

Risk-Aware Bayesian Goal-Oriented Optimal Experimental Design (OED)

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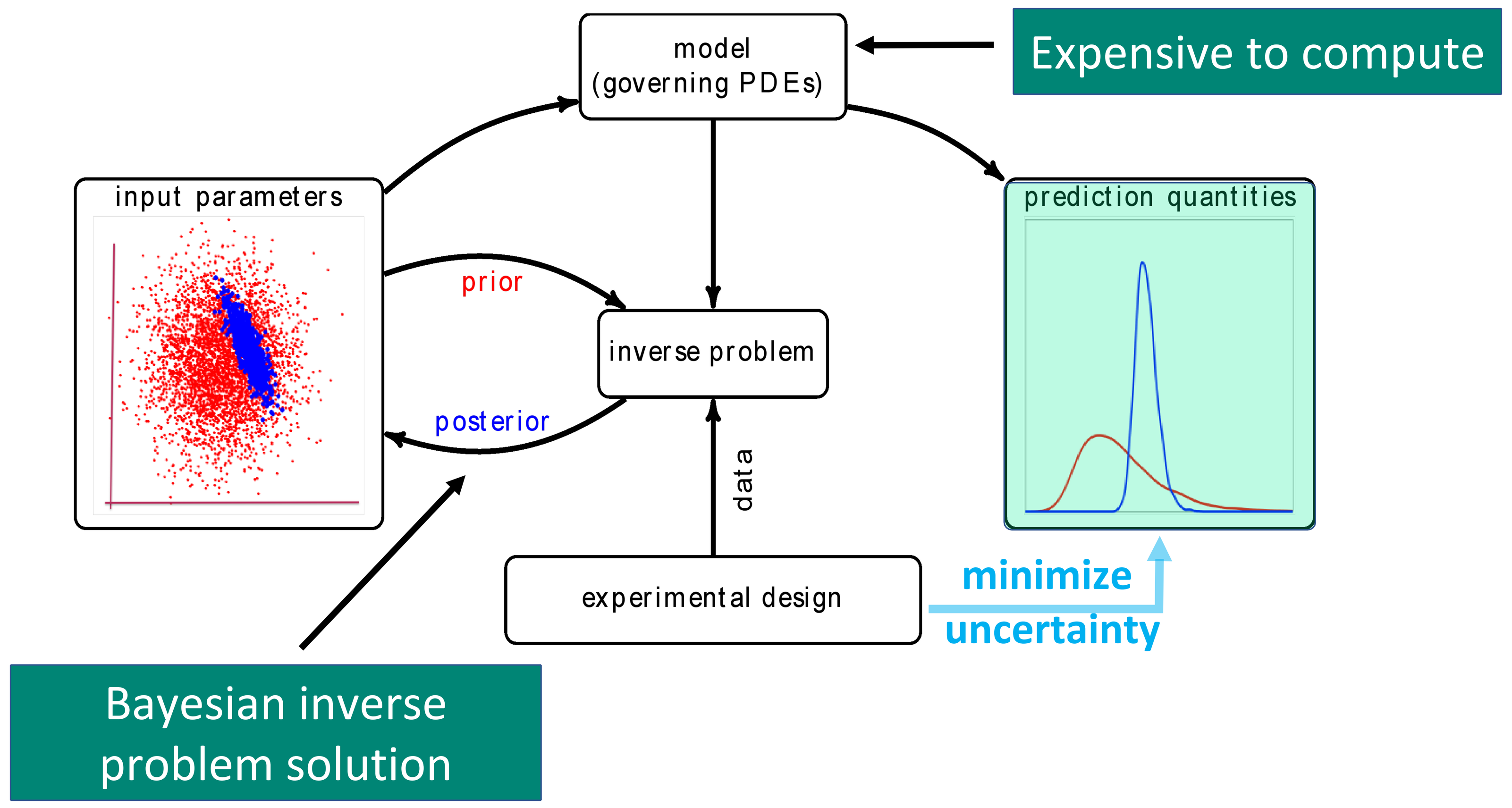
Problems	Goals
Collecting experimental data is expensive	Develop a framework for risk-aware OED
Standard OED doesn't account for risk	Determine optimal sensors to measure contaminant transport

Goal-oriented optimal experimental design (GOOED)



Risk: Statistics used to characterize random variables

$\mathcal{R}[X] \coloneqq \mathrm{AVaR}_p[\ ]$

$= \frac{1}{1-p}\int_{p-quantile}^{\infty} x\,\pi(x)dx$

Our approach

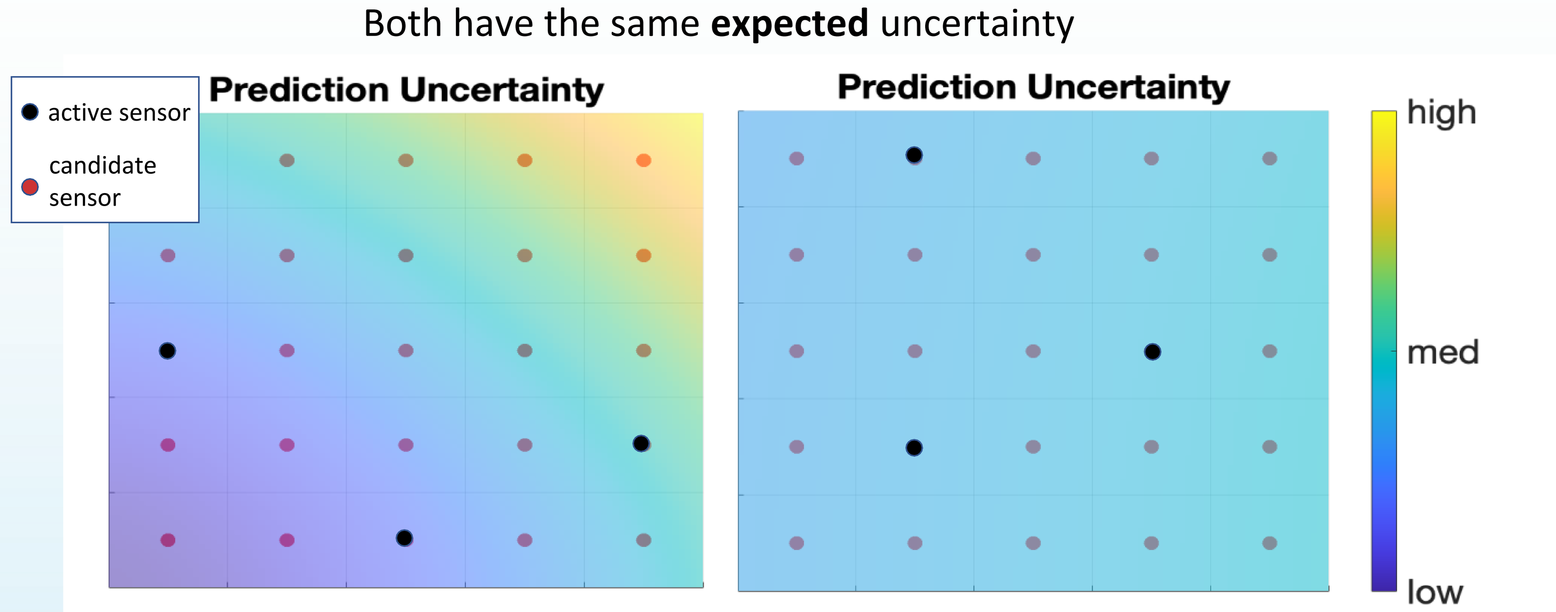
Controls risk averseness

G-optimal: $\mathcal{R}[X] \coloneqq \sup[X]$

I-optimal: $\mathcal{R}[X] \coloneqq E[X]$

Classical

Prediction uncertainty for two design strategies
Both have the same **expected** uncertainty



Bayesian GOOED problem

Determine optimal design

$$\xi^* = \arg\min_{\xi\in\Xi} \mathcal{R}_{\nu_x}\left[\mathcal{R}_y[D[q(\boldsymbol{\theta})]]\right]$$

where

- $\mathcal{R}$ – risk measure
- D – deviation measure characterizing uncertainty

Fundamental risk quadrangle

- $y \sim \pi(y\,|\,\xi)$
- $\sim$ post(| ,)
- q – QoI map
- ν_x – measure over QoI space

Risk measures **generalize** the OED problem

Rockafellar, R.T, and Uryasev, S., The fundamental risk quadrangle in risk management, optimization and statistical estimation, *Surveys in Operations Research and Management Science*, 2013

Steady state advection-diffusion: Modeling the concentration of a contaminant over a 2D domain

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

Diffusion:

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

Nonlinear parameter-to-observable map

Quantities-of-interest

Scalar:

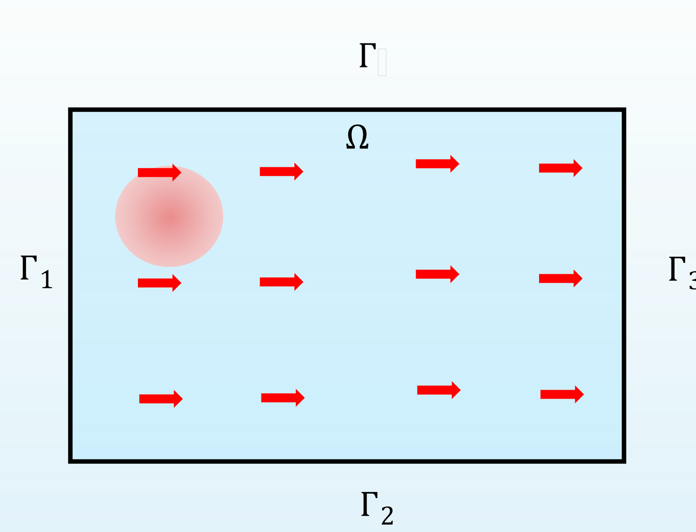
$$q(\boldsymbol{\theta}) \coloneqq \int_{\Omega_s} u(\boldsymbol{x},\boldsymbol{\theta})dx$$

Average concentration in a subdomain

Vector:

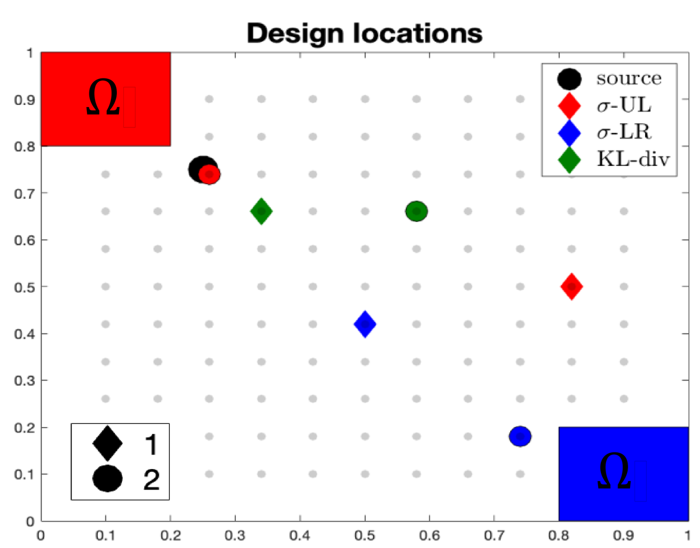
$$u(\boldsymbol{x},\boldsymbol{\theta}),\quad \in\Omega\ \subseteq\Omega$$

Concentration across the domain



Results

Goal-oriented scalar QoI vs. Standard OED



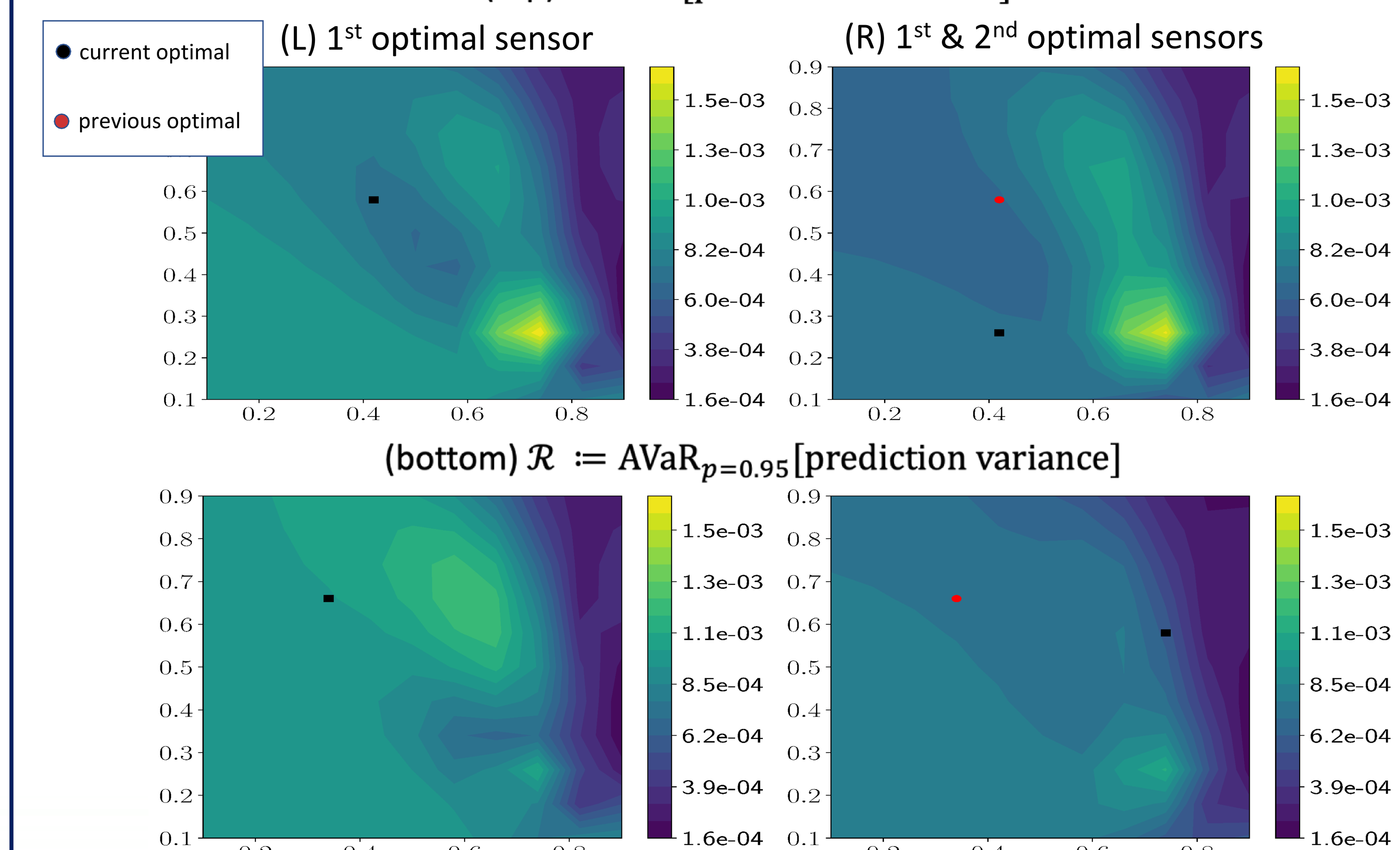
Optimal designs corresponding to minimizing:

- Standard deviation of the average concentration in the upper right versus lower left corner
- KL-divergence on model parameters

Correspondence between **design location** and **QoI location**

Risk-averse vs. risk-neutral approaches for vector QoI

Optimal designs and corresponding prediction variances
(top) $\mathcal{R} \coloneqq E[\text{prediction variance}]$



Risk-averse approach **reduces** maximum prediction **variance**

Conclusions

Goal-oriented OED approaches lead to decreased uncertainty in a QoI compared to standard OED approaches

Generalizing the OED problem using risk measures allows for more flexibility in accounting for risk

RISE

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