SAND2017-8268C

Sequential Optimal Experimental Design using Transport Maps

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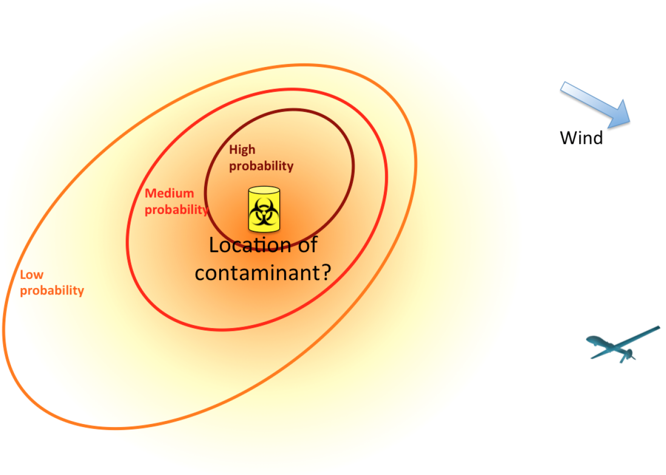
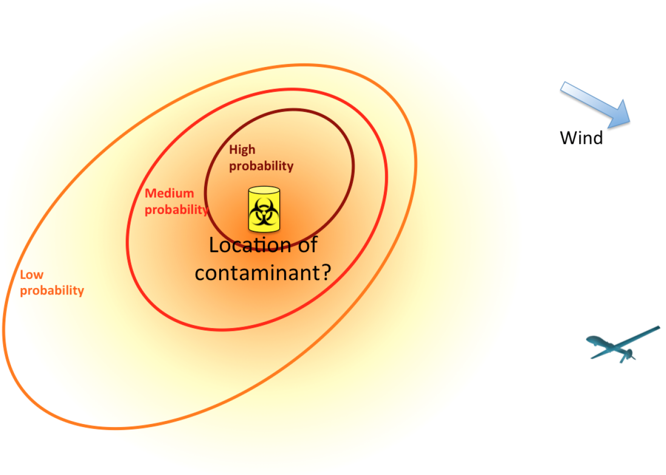
August 2, 2017

Planning measurements: batch (non-sequential) design



Planning measurements: sequential design



Sequential experimental design is relatively less developed

Batch experimental design:

- Linear: Fisher information matrix (e.g., A-, D-optimal)
- Nonlinear: advances beyond linearization and Gaussianization
- Information-based experimental design [Lindley 56]

Greedy (myopic) design:

- Repeated application of batch design [Solonen 12, Drovandi 14, Kim 14]
- But it is *not optimal*

Dynamic programming:

- Fully optimal description (has 1. feedback, 2. forward looking)
- Very difficult to tackle generally
- Thus far limited to discrete variables, special problem and solution structures, simple objectives [Carlin, Bradley 98, Brockwell 03, Berry 02]

Objective and scope

Objective:

Illustrate mathematical framework and numerical tools to find optimal sequential experimental designs in a computationally feasible manner

Scope:

- Use models to guide real experiments (simulation-based OED)
- Finite number of experiments
- Nonlinear and expensive physical models
- Continuous parameter, design, and data spaces of multiple dimensions
- Bayesian treatment of uncertainty
- Non-Gaussian distributions
- Information measure objective (design for parameter inference)

Core components of general sequential design formulation

Experiment: $k = 0, \ldots, N-1$, total N experiments; $N < \infty$

State: $x_k = [x_{k,b},\, x_{k,p}]$ all information needed for optimal future designs

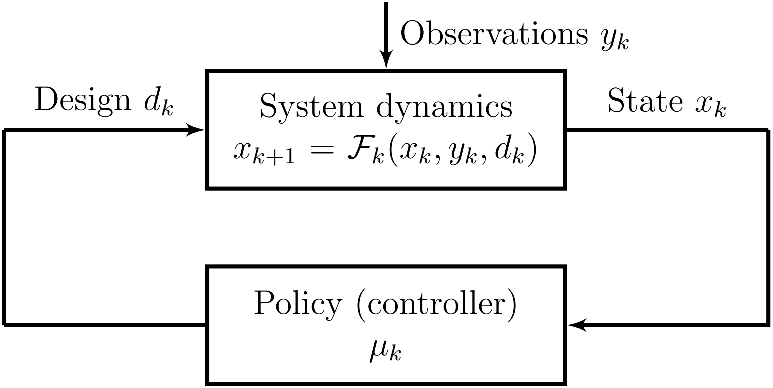
- *Belief state*: $x_{k,b}$ current state of uncertainty
- *Physical state*: $x_{k,p}$ deterministic design-relevant variables

Design: $d_k = \mu_k(x_k)$
seek good *policy* $\pi \equiv \{\mu_0, \mu_1, \ldots, \mu_{N-1}\}$

Observations: y_k distributed according to likelihood $f(y_k|\theta, d_k)$
(e.g., $y_k = G(\theta, d_k) + \epsilon$, with ϵ Gaussian)

System dynamics: $x_{k+1} = \mathcal{F}_k(x_k, y_k, d_k)$ state evolution

Sequential design exhibits a closed-loop behavior



The sOED problem: find optimal policy that maximizes the expected total reward

Stage reward: $g_k(x_k, y_k, d_k)$ **Terminal reward:** $g_N(x_N)$

The sequential optimal experimental design (sOED) problem:

Find π^* where

$$\pi^* = \underset{\pi=\{\mu_0,\ldots,\mu_{N-1}\}}{\operatorname{argmax}} \mathbb{E}_{y_0,\ldots,y_{N-1}|\pi} \left[\sum_{k=0}^{N-1} g_k\left(x_k, y_k, \mu_k(x_k)\right) + g_N\left(x_N\right) \right]$$

$$\begin{aligned} s.t. \qquad & x_{k+1} = \mathcal{F}_k(x_k, y_k, d_k), \forall k \\ & \mu_k(x_k) \in \mathcal{D}_k, \forall x_k, k \end{aligned}$$

Difficult to solve directly, involves optimization of a functional

The sOED problem in dynamic programming (DP) form

Re-express using Bellman's Principle of Optimality [Bellman 53]

Dynamic programming form (Bellman equations): (e.g., [Bertsekas 05])

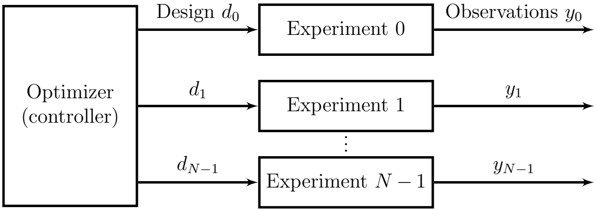
$$\begin{aligned} J_k(x_k) &= \max_{d_k \in \mathcal{D}_k} \mathbb{E}_{y_k|x_k,d_k}\left[g_k(x_k,d_k,y_k) + J_{k+1}\left(\mathcal{F}_k(x_k,d_k,y_k)\right)\right] \\ J_N(x_N) &= g_N(x_N) \end{aligned}$$

$k = 0, \ldots, N-1$; $J_k(x_k)$ are value functions

- A set of smaller tail subproblems
- Optimal policy functions implicitly in argmax: $d_k^* = \mu_k^*(x_k)$
- "Curse of dimensionality": exponential scenario growth from recursion
- Large body of approximate methods: *approximate dynamic programming* (e.g., [Bertsekas 96, Kaelbling 96, Sutton 98, Powell 11])

Batch (non-sequential) design is a special case of the sOED problem, and thus suboptimal

- Has no feedback
- Designs all experiments concurrently as a batch
- Finds optimal *designs* (vectors) rather than a policy



$$\left\{d_0^*, \ldots, d_{N-1}^*\right\} = \underset{d_0,\ldots,d_{N-1}}{\operatorname{argmax}} \mathbb{E}_{y_0,\ldots,y_{N-1}|d_{0:N-1}} \left[\sum_{k=0}^{N-1} g_k\left(x_k, y_k, d_k\right) + g_N\left(x_N\right) \right]$$

Greedy (myopic) design is a special case of the sOED problem (DP form), and thus suboptimal

- Uses feedback
- Considers the *next experiment* only
- Has no future effects

$$
\begin{aligned}
J_k(x_k) &= \max_{d_k \in \mathcal{D}_k} \mathbb{E}_{y_k|x_k,d_k}\left[g_k(x_k, y_k, d_k) + \cancel{J_{k+1}\left(\mathcal{F}_k(x_k, d_k, y_k)\right)} \right] \\
J_N(x_N) &= g_N(x_N)
\end{aligned}
$$

subject to $x_{k+1} = \mathcal{F}_k(x_k, y_k, d_k)$

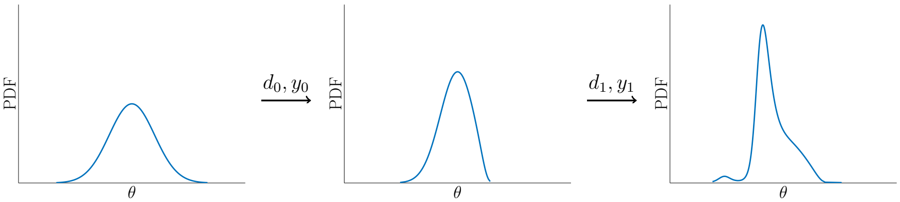
Sequential Bayesian inference

For the k-th experiment:

$$\overbrace{f(\theta|y_k, d_k, I_k)}^{posterior} = \frac{\overbrace{f(y_k|\theta, d_k, I_k)}^{likelihood}\overbrace{f(\theta|I_k)}^{prior}}{\underbrace{f(y_k|d_k, I_k)}_{evidence}}$$

θ — parameters to infer
I_k — information from previous experiments, $I_k \equiv \{d_0, y_0, \dots, d_{k-1}, y_{k-1}\}$

Conceptually: belief state is posterior random variable $x_{k,b} = \theta|I_k$



Information gain objective for parameter inference

We choose to use total information gain at end of all experiments (Kullback-Leibler (KL) divergence from final posterior to prior)

$$\begin{aligned} g_k(x_k, d_k, y_k) &= \text{reflects experimental cost} \\ g_N(x_N) &= D_{KL}(f(x_{N,b}) || f(x_{0,b})) = \int_{\mathcal{H}} f(x_{N,b}) \ln\left[\frac{f(x_{N,b})}{f(x_{0,b})}\right] d\theta \end{aligned}$$

Corresponding system dynamics:

- *Belief state*: Bayes' Theorem

$$f(x_{k+1,b}) = \frac{f(y_k|\theta, d_k, I_k) f(x_{k,b})}{f(y_k|d_k, I_k)}$$

- *Physical state*: physical process

Represent a policy using one-step lookahead form

One-step lookahead policy representation: (e.g., [Bertsekas 05])

$$\mu_k(x_k) = \underset{d_k \in \mathcal{D}_k}{\operatorname{argmax}} \, \mathbb{E}_{y_k|x_k,d_k} \left[g_k(x_k, y_k, d_k) + \tilde{J}_{k+1} \left(\mathcal{F}_k \left(x_k, y_k, d_k \right) \right) \right]$$

Approximate value functions using **linear architecture**:

$$\tilde{J}_k(x_k) = r_k^\top \phi_k(x_k)$$

ϕ_k features (selected from heuristics), r_k weights

Approximate value iteration (backward induction with regression):

$$\tilde{J}_k(x_k) = \mathcal{P} \left\{ \max_{d_k \in \mathcal{D}_k} \mathbb{E}_{y_k|x_k,d_k} [g_k(x_k, d_k, y_k) + \tilde{J}_{k+1} \left(\mathcal{F}_k(x_k, d_k, y_k) \right)] \right\}$$

Start with $\tilde{J}_N(x_N) \equiv g_N(x_N)$, and proceed backwards $k = N-1, \ldots, 1$

$\mathcal{P}$: regression operator, samples from **exploration** and **exploitation**

Belief state representation

Conceptually: belief state is posterior random variable

How to numerically represent it . . .

- for general non-Gaussian continuous random variables
- in a finite-dimensional manner
- to easily perform Bayesian inference repeatedly in evaluating

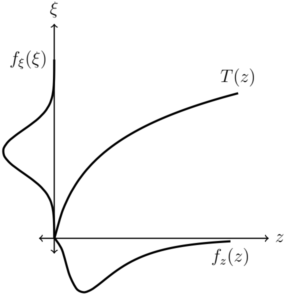
$$\tilde{J}_k(x_k) = \mathcal{P}\left\{ \max_{d_k \in \mathcal{D}_k} \mathbb{E}_{y_k|x_k,d_k}\left[g_k(x_k, d_k, y_k) + \tilde{J}_{k+1}\left(\mathcal{F}_k(x_k, d_k, y_k)\right)\right]\right\}$$

Traditional approaches:

- Gaussian approximation and model linearization
- Gridding or functional approximation of its PDF or CDF
- Non-parametrics (with particle filter, MCMC)

Often expensive and some do not scale well to multiple dimensions. We seek an approach that can quickly perform **many** Bayesian inferences.

Transport map transforms *distributions* (e.g., [Villani 08])



- $\xi \sim$ reference distribution, $z \sim$ target distribution
- Equivalence in distribution $\xi \overset{i.d.}{=} T(z)$
- Knothe-Rosenblatt (KR) map: defined by conditional distributions, is triangular and monotone, exists and is unique [Rosenblatt 52, Carlier 10]
- Easy to construct from samples: convex optimization problem
- Target *joint* distribution for fast approx Bayesian inference

Final algorithm

1. **Set parameters**
2. **Initial exploration**
3. **Make joint map**
4. Iterate to refine . . .
   (a) **Exploration**
   (b) **Exploitation**
   (c) **Approximate value iteration**
5. **Extract final policy parameterization**

1D source inversion problem: problem settings

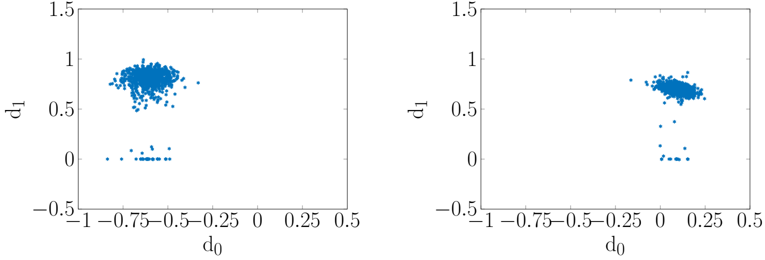
$$y_k = \frac{s}{\sqrt{2\pi}2\sqrt{(0.3+Dt)}} \exp\left(-\frac{\|\,\theta + d_w(t) - z_{k+1}\,\|^2}{2(4)\,(0.3+Dt)}\right) + \epsilon_k$$

- 2 experiments
- $\theta \sim \mathcal{N}(0, 2^2)$ starting location: 5.5
- Strong wind blows to the right after first experiment
- Quadratic movement penalty

1D source inversion problem: case 1 advantages of sOED over greedy design

Greedy design does not account for future wind conditions

Expected reward: greedy (0.07), sOED (0.15)



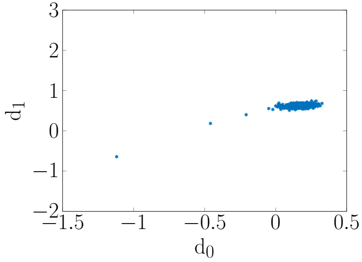
greedy design sOED

1D source inversion problem: case 2 advantages of sOED over batch design

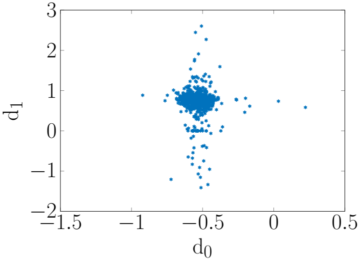
A more precise instrument available only if prior variance < 3

Batch design does not have feedback

Expected reward: batch (0.15), sOED (0.26)



batch design

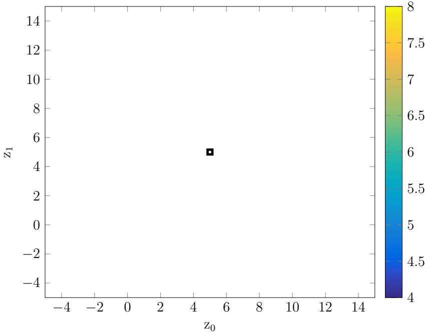


sOED

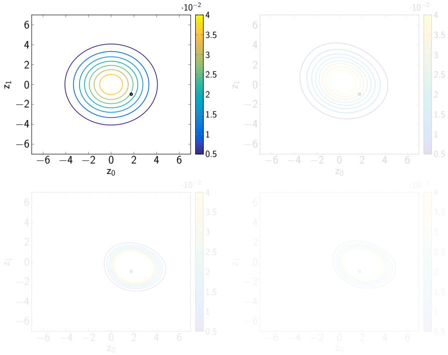
2D source inversion problem: trajectory example #1

An example scenario:

physical state and plume



belief states



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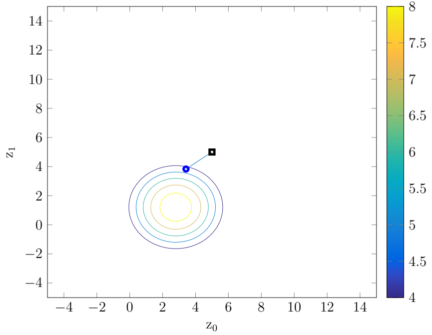

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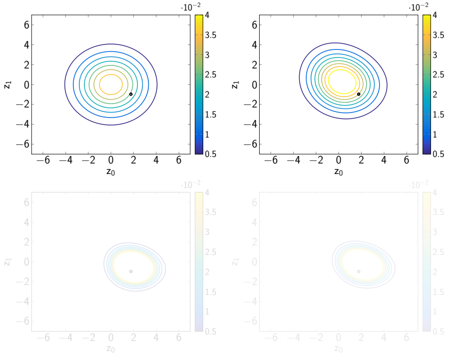

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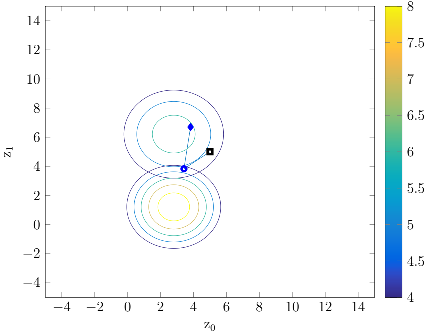

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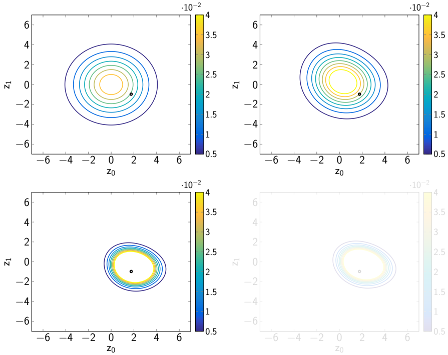

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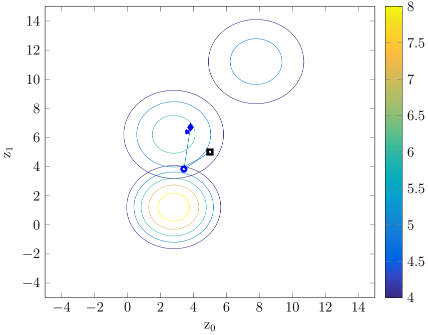
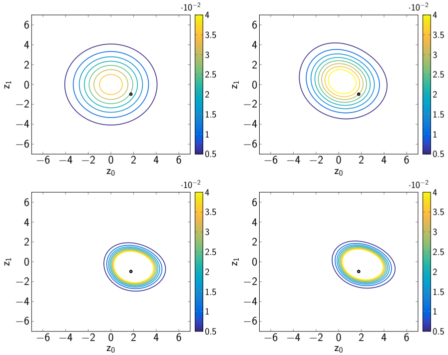


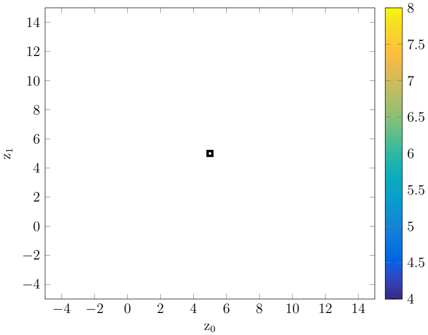
belief states



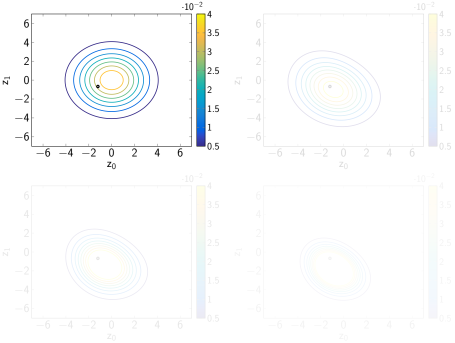
2D source inversion problem: trajectory example #2

Another example scenario:

physical state and plume



belief states



2D source inversion problem: trajectory example #2

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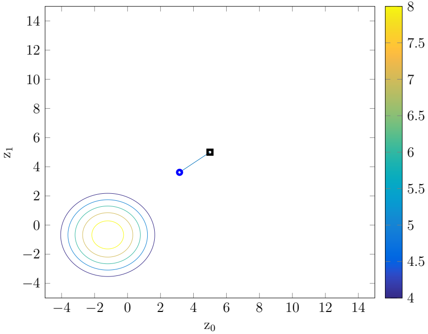
physical state and plume



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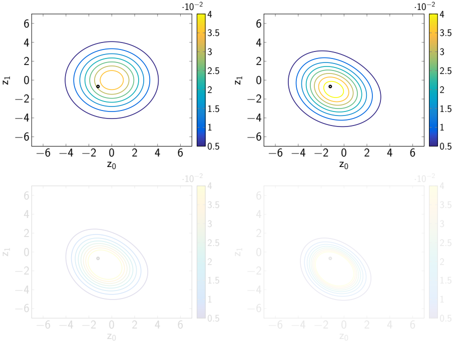

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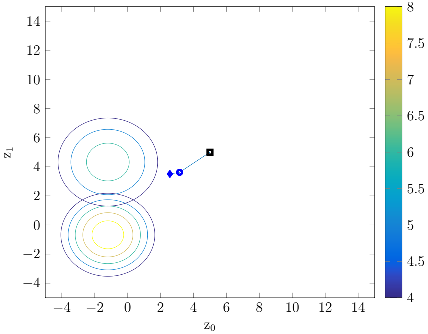

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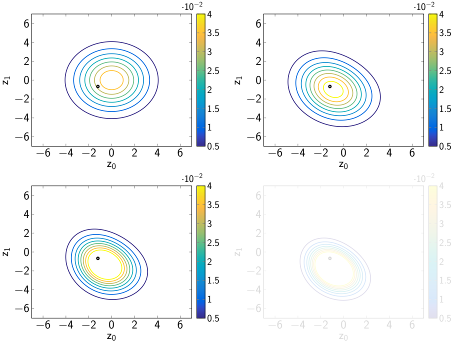

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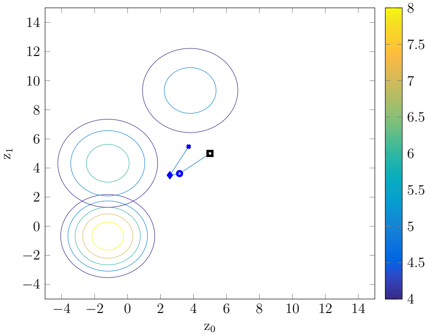

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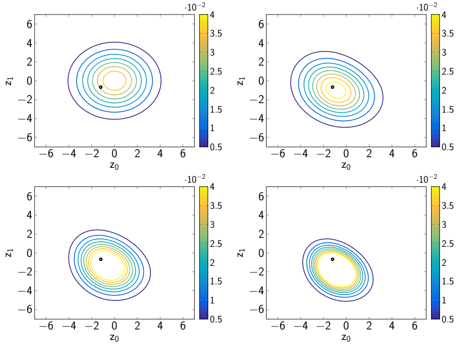

Conclusions

- Formulated the sequential optimal experimental design (sOED) problem rigorously (has 1. feedback, 2. forward looking)
  - best achievable in theory
  - difficult to solve in practice

  (future work: tradeoffs)

- Developed new numerical methods to solve the sOED problem in a computationally-feasible manner, using
  - approximate dynamic programming
  - transport maps

- Demonstrated computational effectiveness on realistic applications

Huan & Marzouk, "Sequential Bayesian Optimal Experimental Design via Approximate Dynamic Programming," *arXiv: 1604.08320*, 2016.

Acknowledgment

- Sandia National Laboratories[1]
- Massachusetts Institute of Technology
- Defense Advanced Research Projects Agency (DARPA)
- Air Force Office of Scientific Research (AFOSR) Computational Mathematics Program

[1]Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energys National Nuclear Security Administration under contract DE-NA-0003525.

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