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Simulation-Based Optimal Bayesian Design for Sequential Experiments

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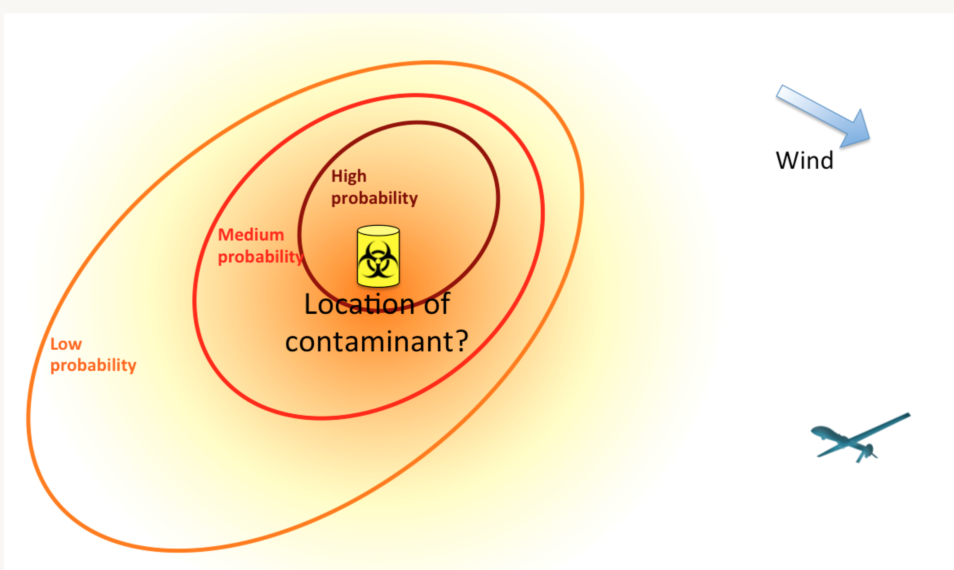
Summary

- *Optimal* design for sequential experiments requires **feedback** and **forward-looking**; batch (open-loop) and greedy (myopic) designs are provably suboptimal
- Optimality is formulated via **dynamic programming (DP)**
- Solving DP is expensive, requiring repeated Bayesian inferences
- Near-optimal policy is found numerically using backward induction coupled with adaptive regression (approximate dynamic programming)
- Fast approximate Bayesian inference is achieved using a transport map transforming the design-data-parameter joint distribution to a Gaussian

Goal: develop computational methods to find optimal policies for a sequence of experiments, accommodating:

- nonlinear models
- non-Gaussian distributions
- continuous variables
- information measure objectives

Motivation



Question: what sequence of measurement locations produces the best inference on the unknown source location?

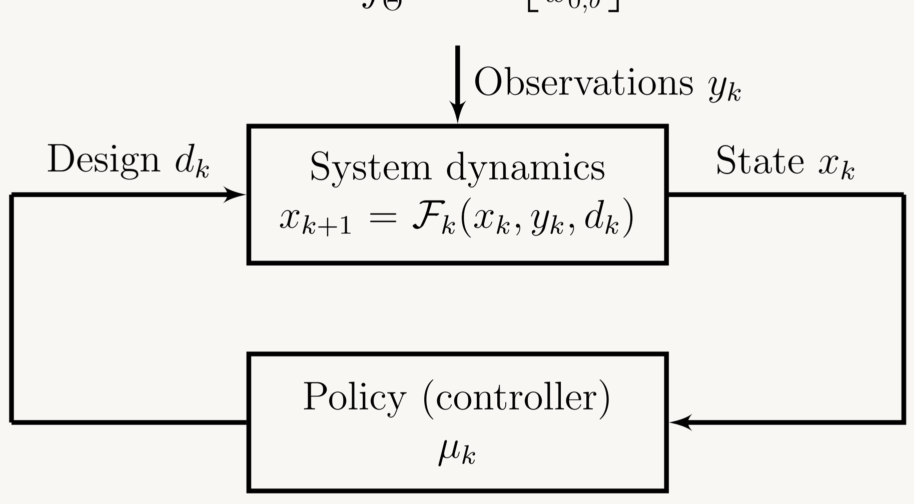
The Optimal Sequential Design Problem

- **Experiment:** $k = 0, \dots, N-1$, total N experiments, $N < \infty$
- **State:** $x_k = [x_{k,b}, x_{k,p}]$ contains all information needed for optimal future designs
  - *Belief state:* $x_{k,b}$ current state of uncertainty (e.g., posterior density $x_{k,b} = f(\theta|d_0, \dots, d_{k-1}, y_0, \dots, y_{k-1})$)
  - *Physical state:* $x_{k,p}$ deterministic variables (e.g., vehicle position)
- **Design:** $d_k = \mu_k(x_k)$; we seek good policy $\pi = \{\mu_0, \mu_1, \dots, \mu_{N-1}\}$
- **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 noise)
- **System dynamics:** $x_{k+1} = \mathcal{F}(x_k, d_k, y_k)$ state evolution
  - *Belief state:* Bayes' theorem

$$x_{k+1,b} = \frac{f(y_k|\theta, d_k) x_{k,b}}{f(y_k|d_0, \dots, d_k, y_0, \dots, y_{k-1})}$$

  - *Physical state:* physical process
- **Stage reward:** $g_k(x_k, y_k, d_k)$ experimental rewards/costs
- **Terminal reward:** $g_N(x_N)$ value of final state (e.g., information gain via Kullback-Leibler divergence)

$$g_N(x_N) = \int_\Theta x_{N,b} \ln \left[\frac{x_{N,b}}{x_{0,b}}\right] d\theta$$



Sequential optimal experimental design (sOED) problem:

Find π^* where

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

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

Approximate Dynamic Prgoramming

- Equivalent problem, different form— **dynamic program (Bellman equations):**

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

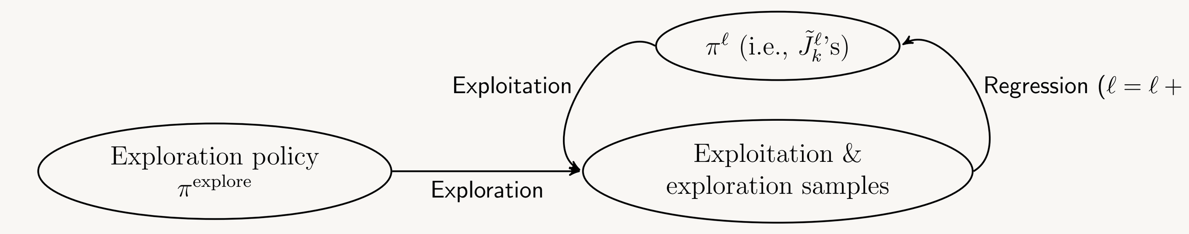
$k = 0, \dots, N-1$; $J_k(x_k)$ are called value functions
  - Optimal policy functions: $d_k^* = \mu_k^*(x_k)$
  - Rich existing work in *approximate dynamic programming*
- Represent policies: **one-step lookahead**

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

  - policy π implicitly parameterized by $\tilde{J}_1(x_1), \dots, \tilde{J}_N(x_N)$
  - if $\tilde{J}_{k+1}(x_{k+1}) = J_{k+1}(x_{k+1})$, then $\mu_k(x_k) = \mu_k^*(x_k)$ is optimal: therefore want $\tilde{J}_{k+1}(x_{k+1})$ close to $J_{k+1}(x_{k+1})$
- Represent $\tilde{J}_k$'s: **linear architecture** $\tilde{J}_k(x_k) = r_k^\top \phi_k(x_k)$; ϕ_k features (selected from heuristics: posterior moments), r_k weights
- Construct $\tilde{J}_k$'s using **approximate value iteration (backward induction with regression):**

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

Start with $\tilde{J}_N(x_N) \equiv g_N(x_N)$, and proceed backwards $k = N-1, \dots, 1$
$\mathcal{P}$ is regression operator
- Efficient regression point selection
  Exploration: random designs, "try something new", regularization
  Exploitation: applies current policy approximation, leverages current understanding of good policy, places more points at frequently-visited states
- Procedure to iteratively adapt regression as $\tilde{J}_k$'s improved

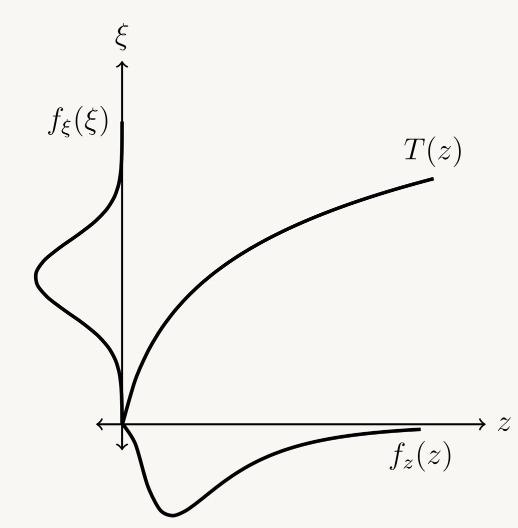


Fast Approximate Bayesian Inference: Transport Maps

- **How to numerically represent belief state (posterior)...**
  - for general non-Gaussian continuous random variables
  - in a finite-dimensional manner
  - to easily perform Bayesian inference repeatedly in evaluating

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

  $\Rightarrow$ potentially MILLIONS of repeated Bayesian inferences
  - Need approach that can quickly perform **many** Bayesian inferences
- **Transport maps:**



  - $\xi \sim$ reference distribution, $z \sim$ target distribution
  - Equivalence in distribution $\xi \overset{i.d.}{=} T(z)$
  - Knothe-Rosenblatt (KR) map: defined by conditional distributions, triangular and monotone, exists and is unique
  - Easy to construct: a benign convex optimization problem
- **Fast approximate inference:** posterior is conditioning the joint distribution

$$f(\theta|y) = \frac{f(y|\theta)f(\theta)}{f(y)} = \frac{f(y,\theta)}{f(y)}$$

For one experiment: KR map from (d, y, θ) to $\xi \sim \mathcal{N}(0, I)$ is:

$$\begin{bmatrix}\xi_1\\ \xi_2\\ \xi_3\end{bmatrix} = \begin{bmatrix}T_d(d)\\ T_{y|d}(d,y)\\ T_{\theta|y,d}(d,y,\theta)\end{bmatrix} = \begin{bmatrix}\Phi^{-1}(F(d))\\ \Phi^{-1}(F(y|d))\\ \Phi^{-1}(F(\theta|y,d))\end{bmatrix}$$

KR map of posterior given realizations d^* and y^* is:

$$T_{\theta|y^*,d^*}(\theta) = \Phi^{-1}(F(\theta|y^*,d^*))$$

This is precisely $T_{\theta|y,d}$ substituted with d^* and y^*: $T_{\theta|y,d}(d^*, y^*, \theta)$!

- Inference for multiple experiments by building a joint distribution map:

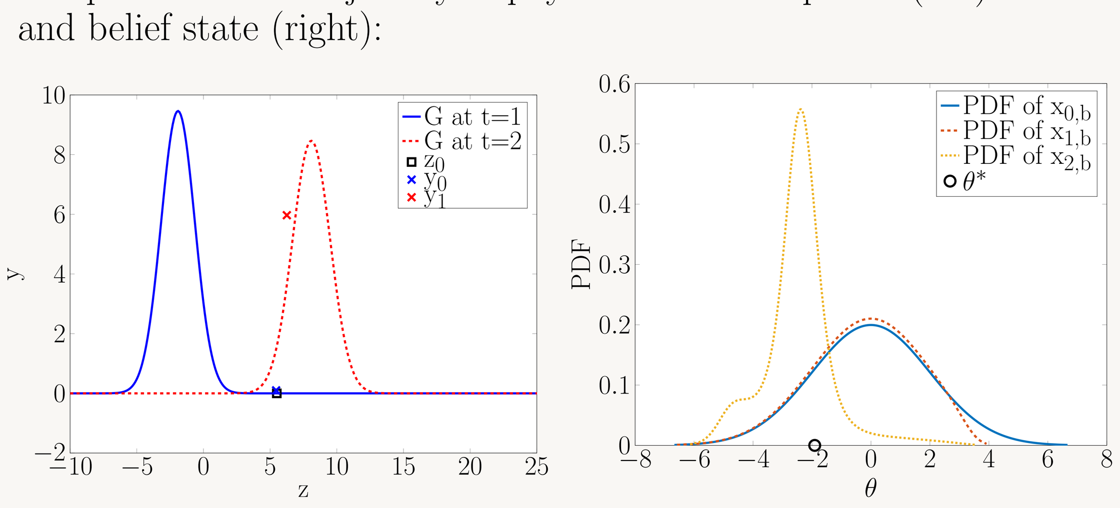
$k=0$	1	2	...
$\xi_{d_0} = T_{d_0}(d_0)$	$\xi_{d_0} = T_{d_0}(d_0)$	$\xi_{d_0} = T_{d_0}(d_0)$	
$\xi_{y_0} = T_{y_0}(d_0, y_0)$	$\xi_{y_0} = T_{y_0}(d_0, y_0)$	$\xi_{y_0} = T_{y_0}(d_0, y_0)$	
$\xi_{\theta_0} = T_{\theta_0}(d_0, y_0, \theta)$	$\xi_{d_1} = T_{d_1}(d_0, y_0, d_1)$	$\xi_{d_1} = T_{d_1}(d_0, y_0, d_1)$	
	$\xi_{y_1} = T_{y_1}(d_0, y_0, d_1, y_1)$	$\xi_{y_1} = T_{y_1}(d_0, y_0, d_1, y_1)$	
	$\xi_{\theta_1} = T_{\theta_1}(d_0, y_0, d_1, y_1, \theta)$	$\xi_{d_2} = T_{d_2}(d_0, y_0, d_1, y_1, d_2)$	
		$\xi_{y_2} = T_{y_2}(d_0, y_0, d_1, y_1, d_2, y_2)$	
		$\xi_{\theta_2} = T_{\theta_2}(d_0, y_0, d_1, y_1, d_2, y_2, \theta)$	

  - Posterior map after Bayesian inference on $k+1$ experiments is the n_θ-dimensional $T_{\theta_k|d_0^*,y_0^*,\dots,d_k^*,y_k^*}(\theta)$
  - Components grouped by the red rectangular boxes are identical; concatenate unique parts and construct overall map in one shot
  - Map constructed using exploration and exploitation samples

Results: Source Inversion in 1D Space

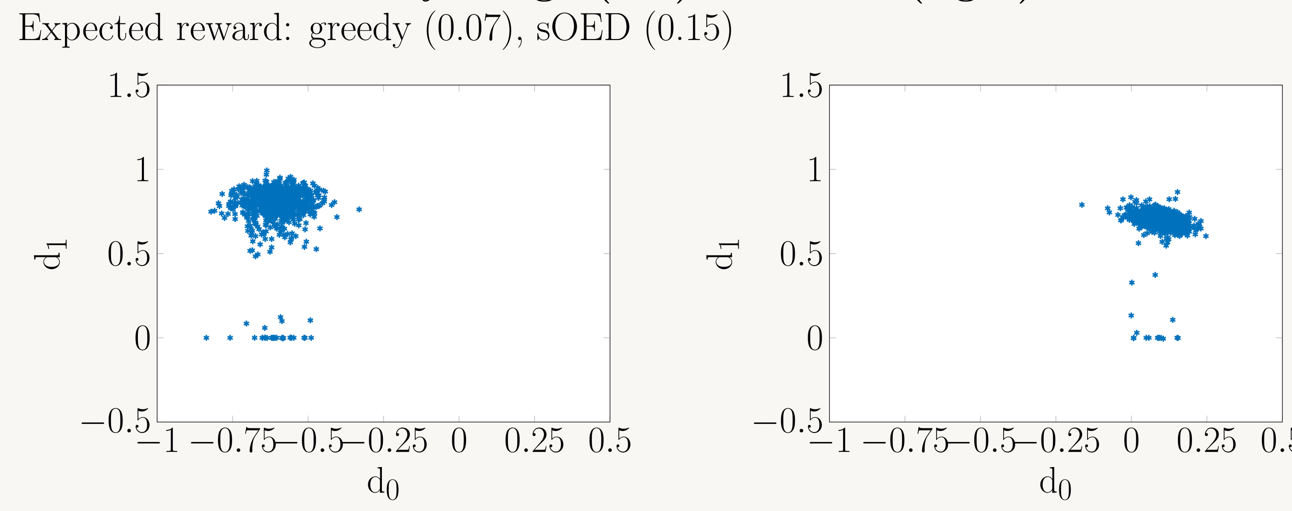
$$y_k = \frac{s}{\sqrt{2\pi}\sqrt{(1.2 + 4Dt)}} \exp\left(-\frac{\|\theta + d_w(t) - z_{k+1}\|^2}{2(1.2 + 4Dt)}\right) + \epsilon_k$$

- 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
- Sample evolution trajectory of physical state and plume (left) and belief state (right):



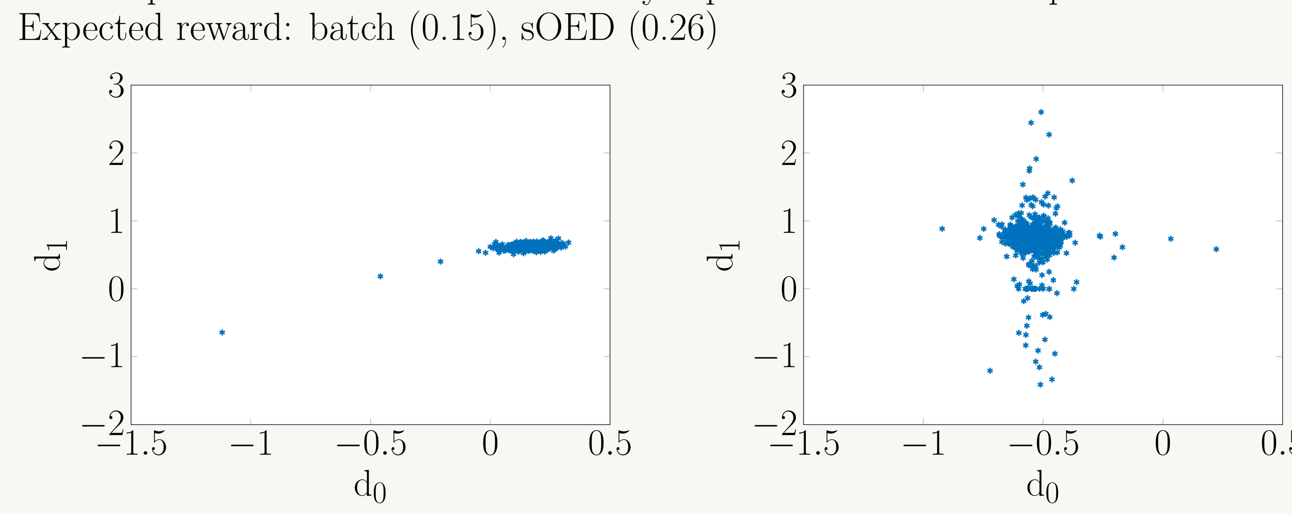
Greedy design (left) vs. sOED (right)

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



Batch design (left) vs. sOED (right)

A more precise instrument available only if posterior variance drops < 3
Expected reward: batch (0.15), sOED (0.26)



Results: Source Inversion in 2D Space

A more challenging problem:

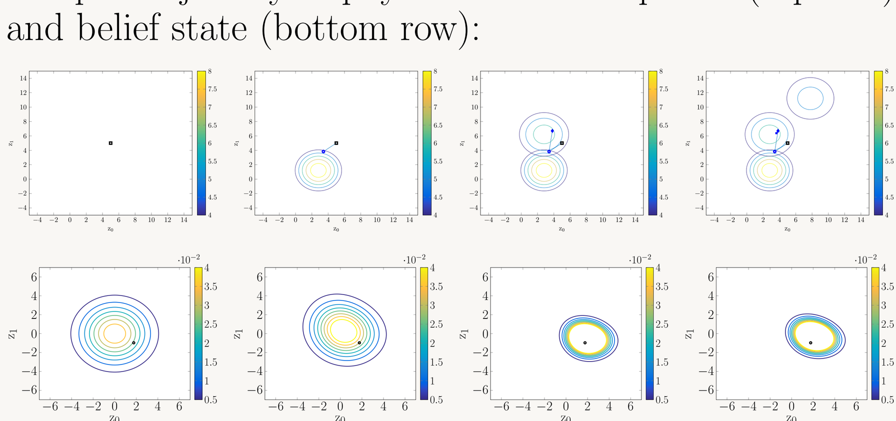
- 3 experiments
- 2D parameter and physical spaces

$$\theta \sim \mathcal{N}\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}2^2 & 0\\ 0 & 2^2\end{bmatrix}\right)$$

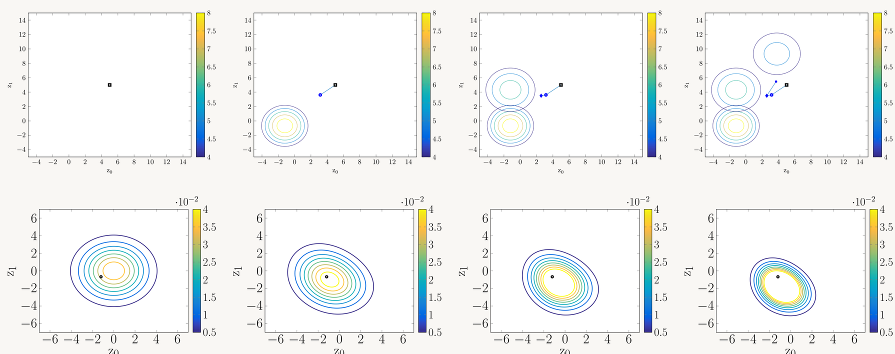
- Starting location = [5, 5]
- 15 dimensional joint distribution map
- Variable wind:
  blows north after experiment 1
  north-east after experiment 2

$\Rightarrow$ **Takeaway:** policy inherently adaptive, selects design based on what occurred so far!

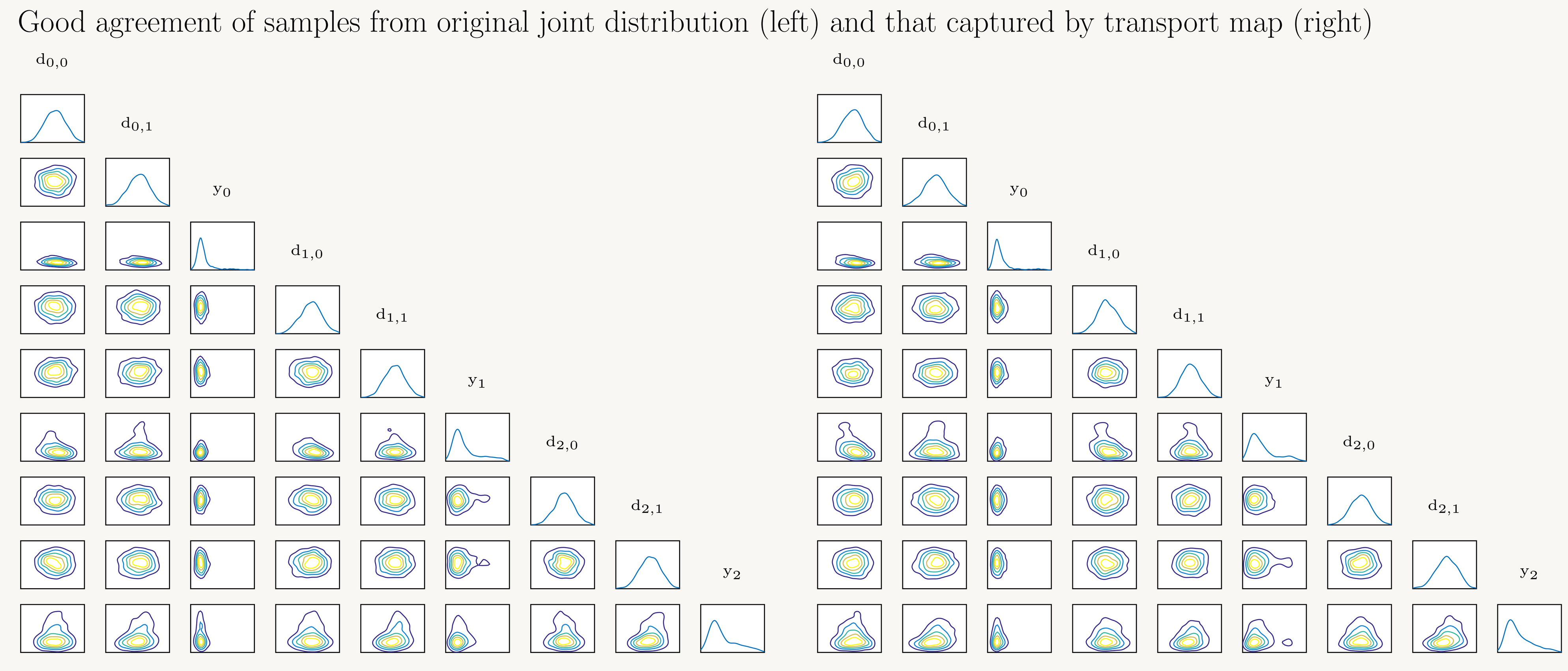
Sample trajectory of physical state and plume (top row) and belief state (bottom row):



Another sample trajectory:



Good agreement of samples from original joint distribution (left) and that captured by transport map (right)



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