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AIRBO

Efficient Robust Bayesian Optimization for Arbitrary Uncertain Inputs

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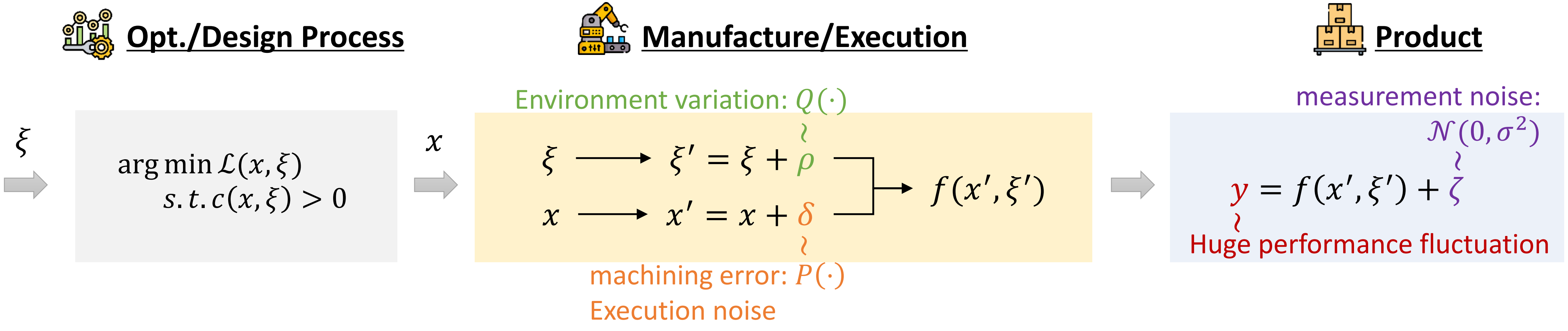
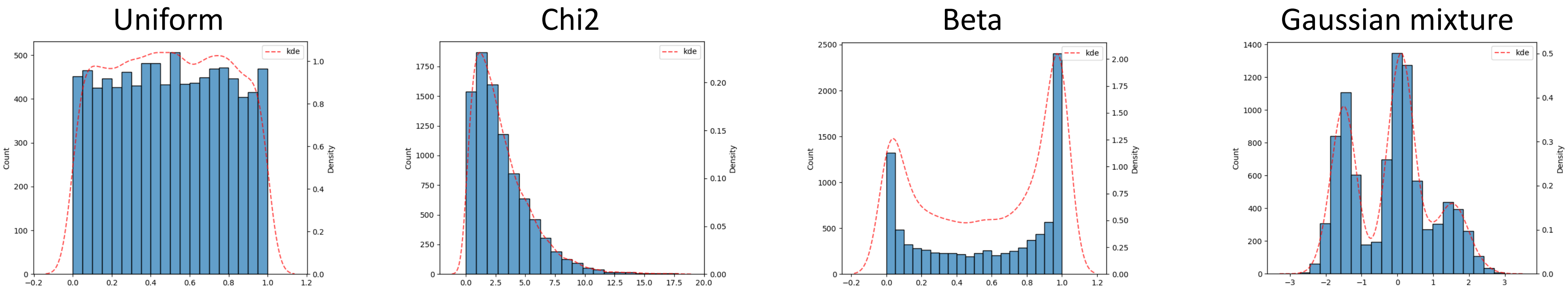
Problem

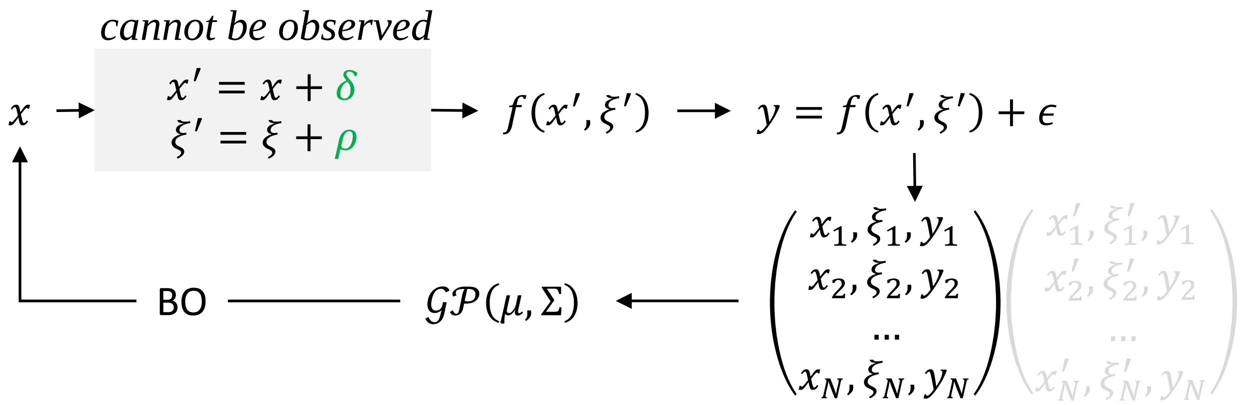


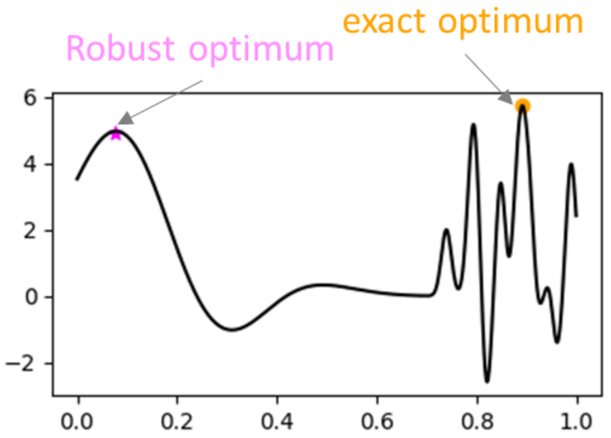
Moreover, depending on the source of randomness, the input uncertainty can be quite complex…



Formulation

➢Robust BO





Objective: Robust optimum

$$\arg\min_{x} \int\int f(x + \delta, \xi + \rho)\, d_\rho\, d_\delta$$

$$s.t.\ C(x') \leq 0$$

➢In this work,

- The input uncertainty can follow arbitrary complex distribution.
- Assume that we can samples from input distribution, which can be done via statistical learning.

Intuition

➢Weight interpretation of $\mathcal{GP}$ [1]

- Starts from Bayesian linear model: $y = x^T w + \zeta, \quad \zeta \sim \mathcal{N}(0, \sigma^2)$

$w \sim \mathcal{N}(0, \Sigma_p)$

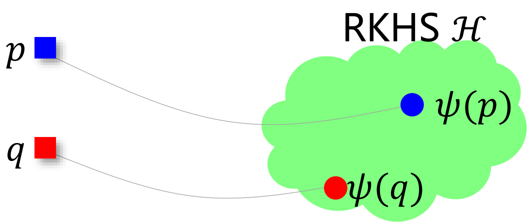
- Posterior:

$$f_* | x_*, X, y \sim \mathcal{N}\left(\phi^T(x_*)\Sigma_p\phi(X)(A + \sigma_n^2 I)^{-1} y,\ \phi^T(x_*)\Sigma_p\phi(x_*) - \phi^T(x_*)\Sigma_p\phi(X)(A + \sigma_n^2 I)^{-1}\phi^T(X)\Sigma_p\phi(x_*)\right)$$

- Apply Kernel to project into feature space

$k(x, x') = \phi^T(x)\Sigma_p\phi(x') = \psi(x) \cdot \psi(x')$

- GP posterior: $f_* | x_*, X, y \sim \mathcal{N}\left(K(X_*, X)(K(X, X) + \sigma_n^2 I)^{-1} y,\ K(X_*, X_*)(K(X, X) + \sigma_n^2 I)^{-1} K(X, X_*)\right)$



The core steps of GP are:

1) project the input x to a high-dim. feature embedding $\psi(x)$

2) compare them in the RKHS defined by the kernel.

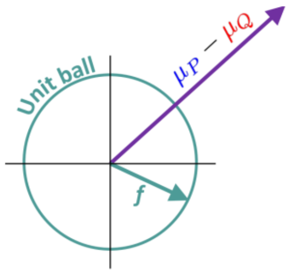
Considering the input uncertainty, how to compare the uncertain inputs?

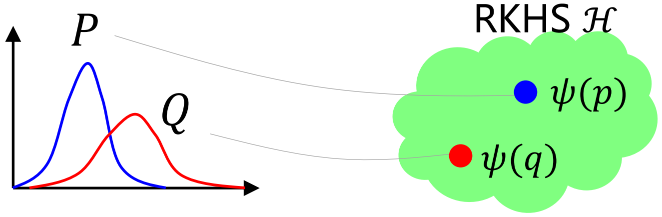
[1] Christopher KI Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*. Vol. 2. 3. MIT press Cambridge, MA, 2006

MMD-based Kernel for Arbitrary Uncertain Inputs

- In general, the Integral Probabilistic Metric (IPM) serves our purpose.
- MMD ⇔ Measuring distance btw prob. distributions in RKHS[*]

$$
\begin{aligned}
\mathrm{MMD}(P,Q) &= \sup_{||g||\le 1} [\mathbb{E}_{X\sim P} g(X) - \mathbb{E}_{Y\sim Q} g(Y)] \\
&= \sup_{||g||\le 1} [\langle g, \mathbb{E}_P \psi(X)\rangle_{\mathcal{G}} - \langle g, \mathbb{E}_Q \psi(Y)\rangle_{\mathcal{G}}] \\
&= \sup_{||g||\le 1} [\langle g, \mu_P\rangle_{\mathcal{G}} - \langle g, \mu_Q\rangle_{\mathcal{G}}] \\
&= \sup_{||g||\le 1} \langle g, \mu_P - \mu_Q\rangle_{\mathcal{G}} \\
&= \langle g^*, \mu_P - \mu_Q\rangle_{\mathcal{G}} \\
&= ||\mu_P - \mu_Q|| \ (\text{the supremum is achieved when } g^* = \frac{\mu_P - \mu_Q}{||\mu_P - \mu_Q||})
\end{aligned}
$$





- MMD-based kernel to propagate input uncertainty to posterior
  - MMD kernel: $\hat{k}(P,Q) = \exp\big(\alpha MMD^2(P,Q,k)\big)$
  - For the MMD estimation, we employ a compositional rational quadratic kernel:

$$k(x,x') = \sum_{\alpha_i \in \mathcal{S}} \left(1 + \frac{(x-x')^2}{2\alpha_i l_i^2}\right)^{-\alpha_i}, \mathcal{S} = \{0.2, 0.5, 1,2,5\}$$

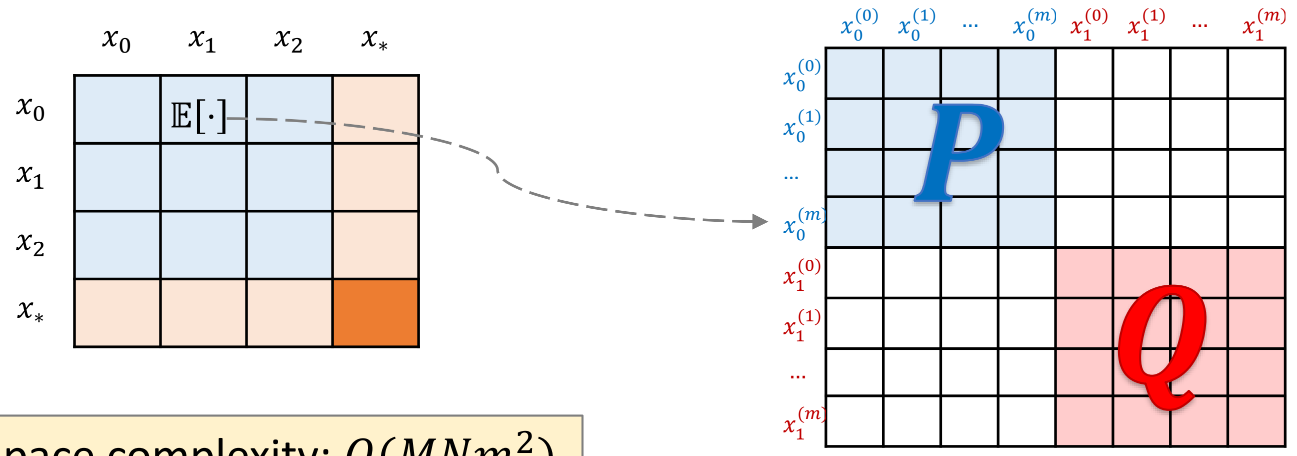
[*] Arthur Gretton, Dougal Sutherland, and Wittawat Jitkrittum. "Interpretable comparison of distributions and models". In NeurIPS *[Tutorial]* (2019)

High Estimation Complexity of MMD

- The empirical Estimation of MMD requires further sampling m samples from the input uncertainty[*]:

$$MMD^2(P,Q) = \mathbb{E}_{u,u' \sim P\otimes P}[k(u,u')] + \mathbb{E}_{v,v' \sim Q\otimes Q}[k(v,v')] - 2\mathbb{E}_{u,v \sim P\otimes Q}[k(u,v)]$$

- This consumes a huge GPU memory and hinders its ability of parallel computation:



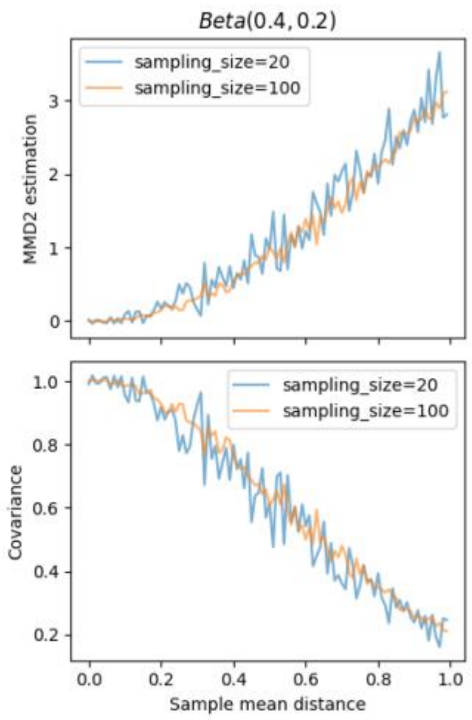
Space complexity: $O(MNm^2)$

M: #training samples
N: #testing samples
m: #sampling size

[*] Note here we only need samples from the input distribution, but not their target function values

Stable MMD Estimation vs. Inference Complexity

- Insufficient sampling results in a highly-varied posterior.
- A larger sample size can occupy significant GPU memory and reduce the ability of parallel computing.



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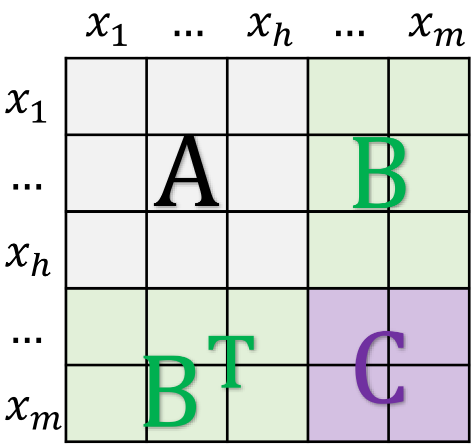
Accelerating Posterior Inference via Nyström Approximation

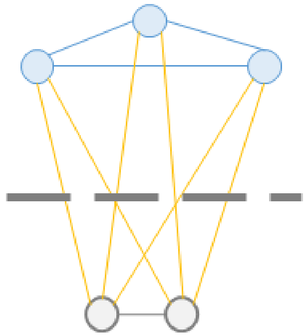
➢Nyström MMD estimator for efficient posterior inference



$C = B^T A^{-1} B$

$$\tilde{\mathrm{MMD}}^2(P,Q) = \mathbb{E}_{X,X'\sim P\otimes P}[k(X,X')] + \mathbb{E}_{Y,Y'\sim Q\otimes Q}[k(Y,Y')] - 2\mathbb{E}_{X,Y\sim P\otimes Q}[k(X,Y)]$$
$$\approx \frac{1}{m^2}\mathbf{1}_m^T U \mathbf{1}_m + \frac{1}{m^2}\mathbf{1}_m^T V \mathbf{1}_m - \frac{2}{m^2}\mathbf{1}_m^T W \mathbf{1}_m$$
$$\approx \frac{1}{m^2}\mathbf{1}_m^T U_{mh} U_h^+ U_{mh}^T \mathbf{1}_n + \frac{1}{m^2}\mathbf{1}_m^T V_{mh} V_h^+ V_{mh}^T \mathbf{1}_m - \frac{2}{m^2}\mathbf{1}_m^T W_{mh} W_h^+ W_{mh}^T \mathbf{1}_m,$$

where $U = K(X,X')$, $V = K(Y,Y')$, $W = K(X,Y)$ are the kernel matrices, $\mathbf{1}_m$ represents a m-by-1 vector of ones, m defines the sampling size and h controls the sub-sampling size.



Empirical estimator
Space complexity: $O(MNm^2)$

⇨

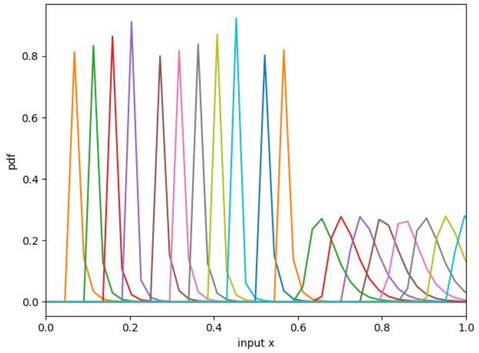
Nystrom estimator
Space complexity: $O(MNmh)$

$h \ll m$
For 1D Gaussian,
$m = 1000, h = 10$

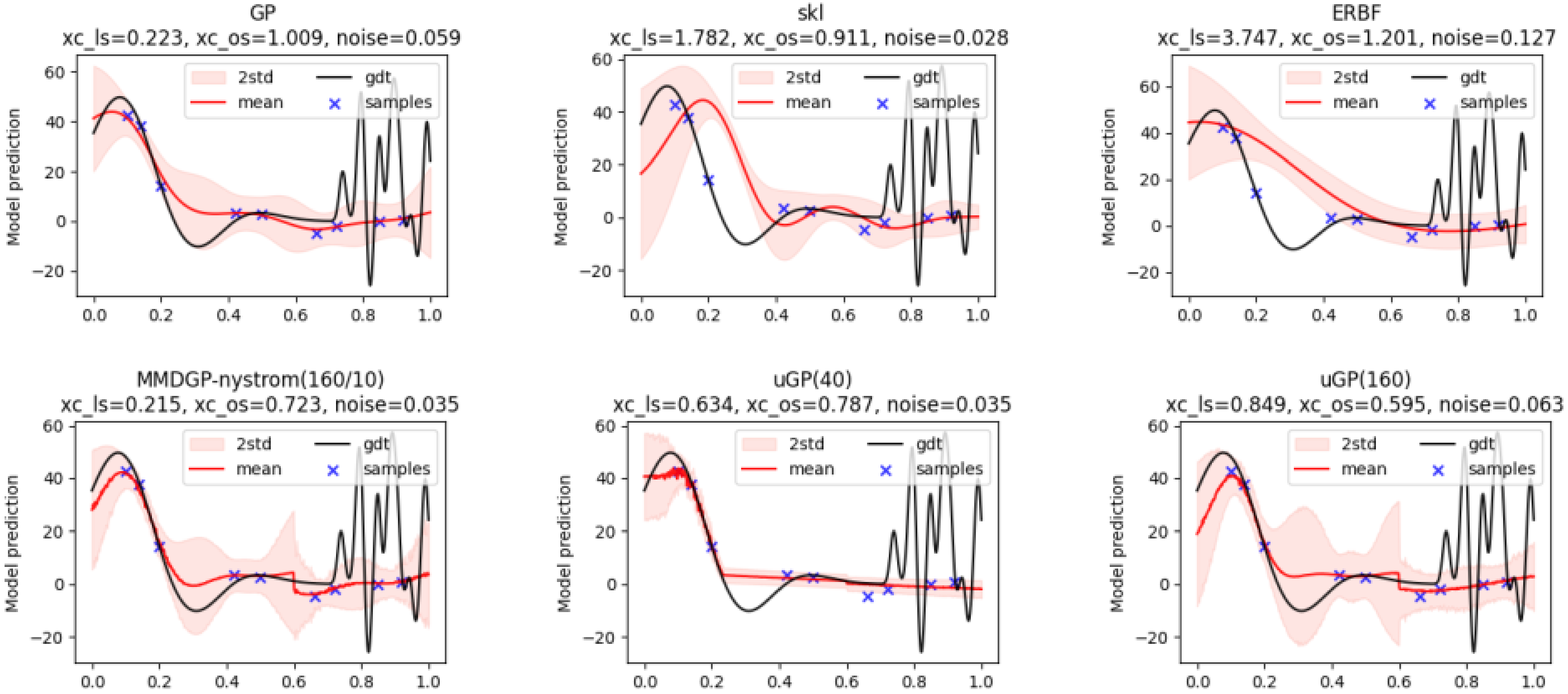
M: #training samples
N: #testing samples
m: #sampling size
h : #sub-sampling size

Evaluation: Modeling Complex Input Uncertainty

➢ Step-changing χ^2 distribution:



- $P_x = \chi^2(k = g(x), \sigma = 0.01), g(x) = \begin{cases} 0.5, & x \in [0.0, 0.6) \\ 7.0, & x \in [0.6, 1.0] \end{cases}$



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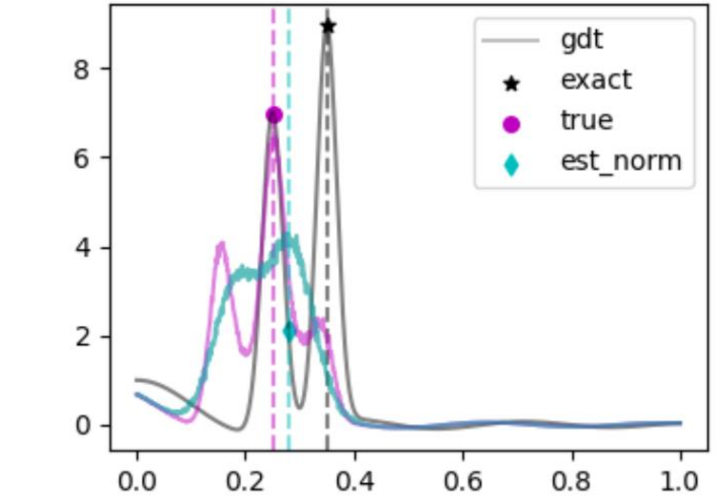
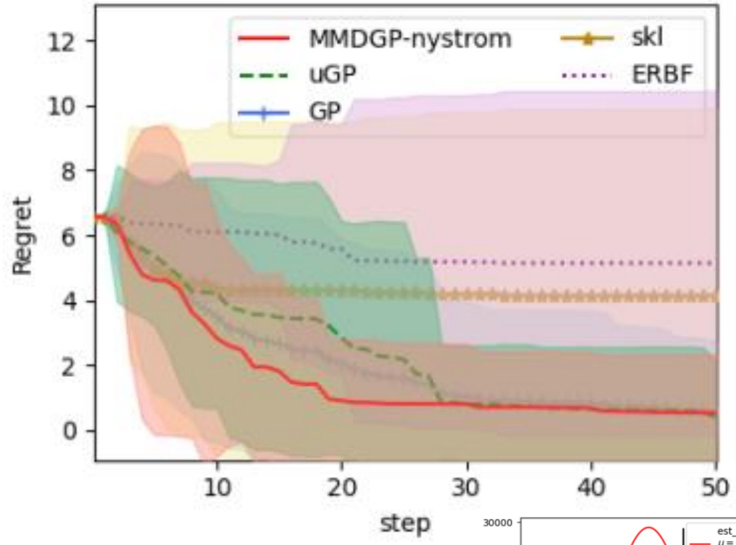
Evaluation: Posterior Inference

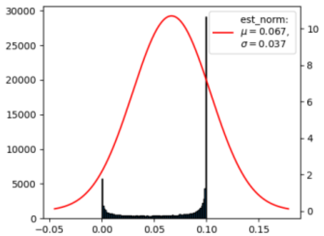
Table 1: Performance of Posterior inference for 512 samples.

Method	Sampling Size	Sub-sampling Size	**Inference Time (seconds)**	**Batch Size (samples)**
Empirical	20	-	1.143 ± 0.083	512
Empirical	100	-	8.117 ± 0.040	128
Empirical	1000	-	840.715 ± 2.182	1
Nystrom	100	10	0.780 ± 0.001	512
Nystrom	1000	100	21.473 ± 0.984	128

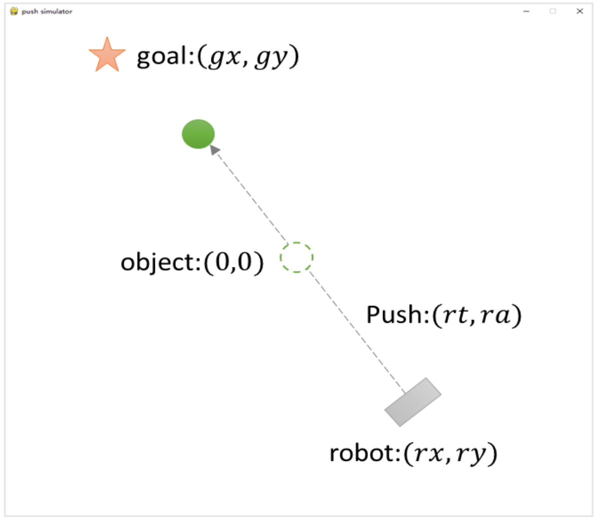
Evaluation: Robust Optimization with Non-Gaussian Inputs

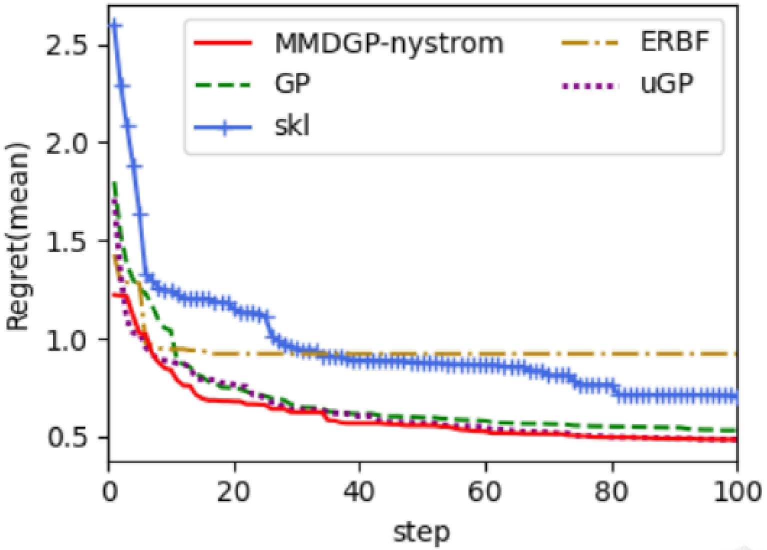




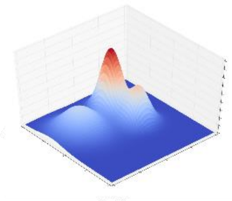


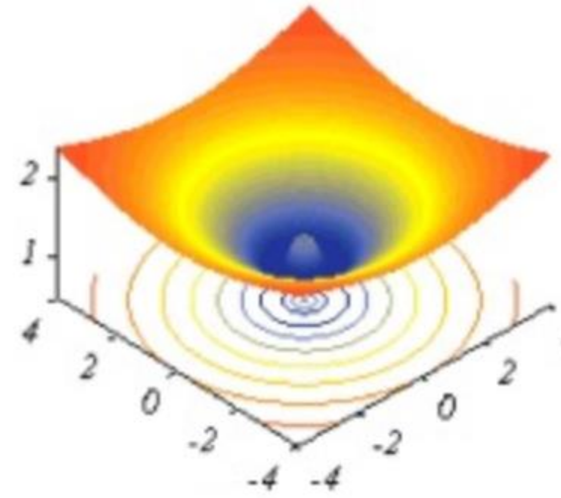
1D double-peak function
w/ ***Beta*** input distribution

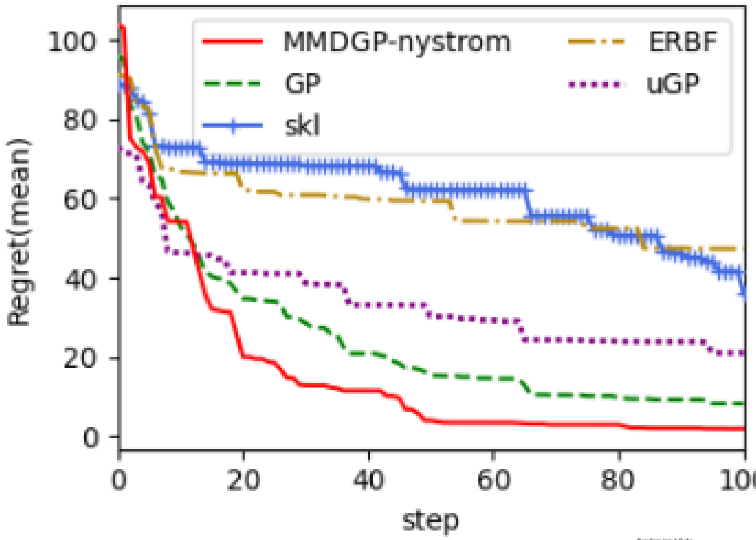




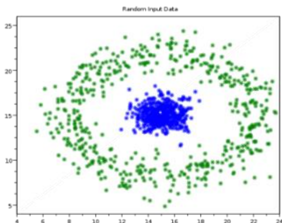
3D Robot pushing
w/ ***Gaussian Mixture*** distribution







10D bumped-bowl
with ***circular*** distribution



Thank you for listening!

Poster session: Great Hall & Hall B1+B2 #1225

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