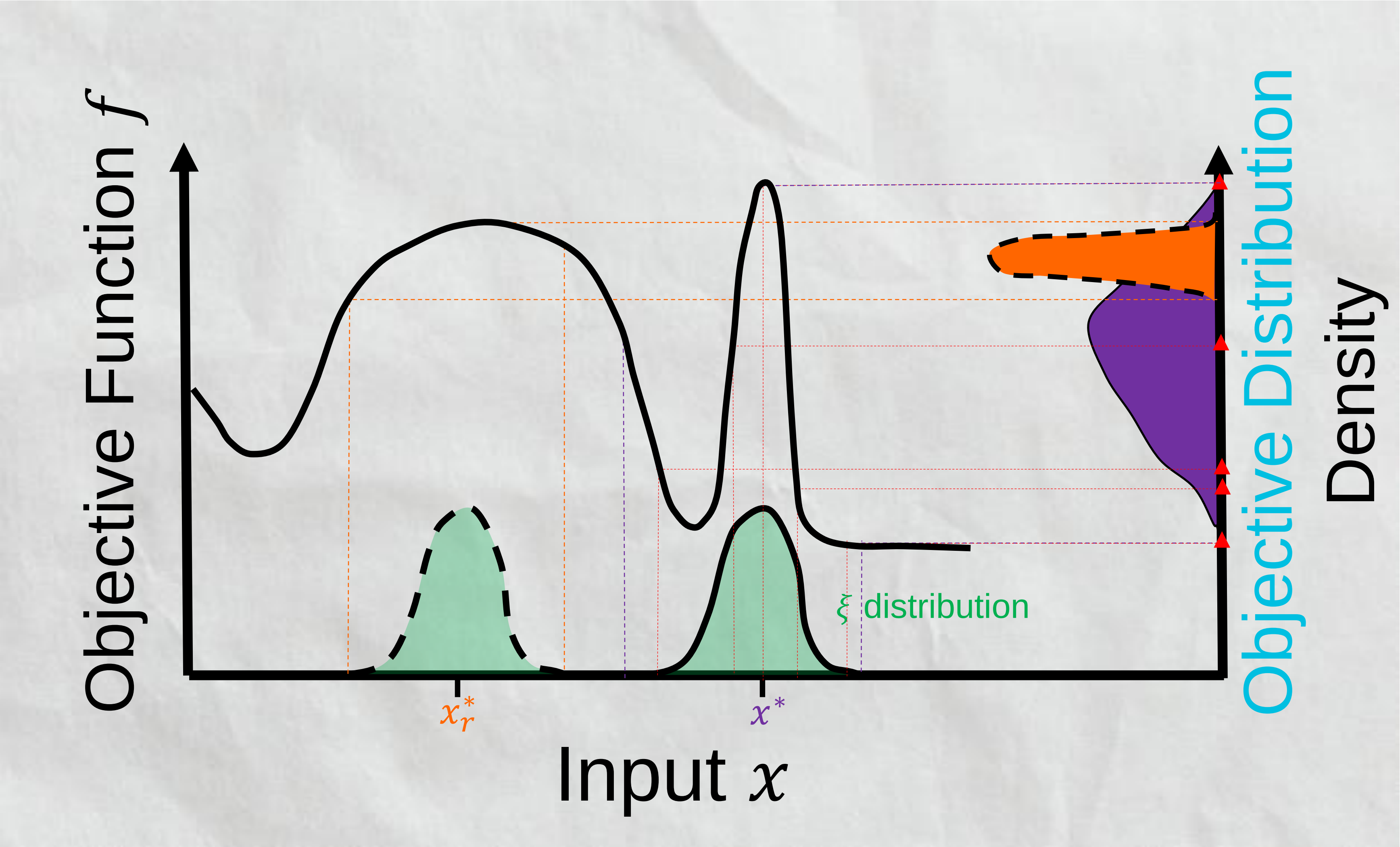
SPECTRAL REPRESENTATION OF ROBUSTNESS MEASURES FOR OPTIMIZATION UNDER INPUT UNCERTAINTY

Jixiang Qing, Tom Dhaene, Ivo Couckuyt

PROBLEM FORMULATION

- Robust optimization
  - Optimize black box function f
  - Consider **Input Uncertainty**
- What is a robust solution?
  - First moment: $\mathbb{J}_{\xi}(f) = \mathbb{E}_{\xi}[f(x+\xi)]$
  - Second moment: $\mathbb{V}_{\xi}(f) = \mathbb{V}_{\xi}[f(x+\xi)]$



"Solution x_r^* is more robust than x^*"

Mean: $\mathbb{E}_{\xi}[f(x_r^* + \xi)] \geq \mathbb{E}_{\xi}[f(x^* + \xi)]$

Variance: $\mathbb{V}_{\xi}[f(x_r^* + \xi)] \leq \mathbb{V}_{\xi}[f(x^* + \xi)]$

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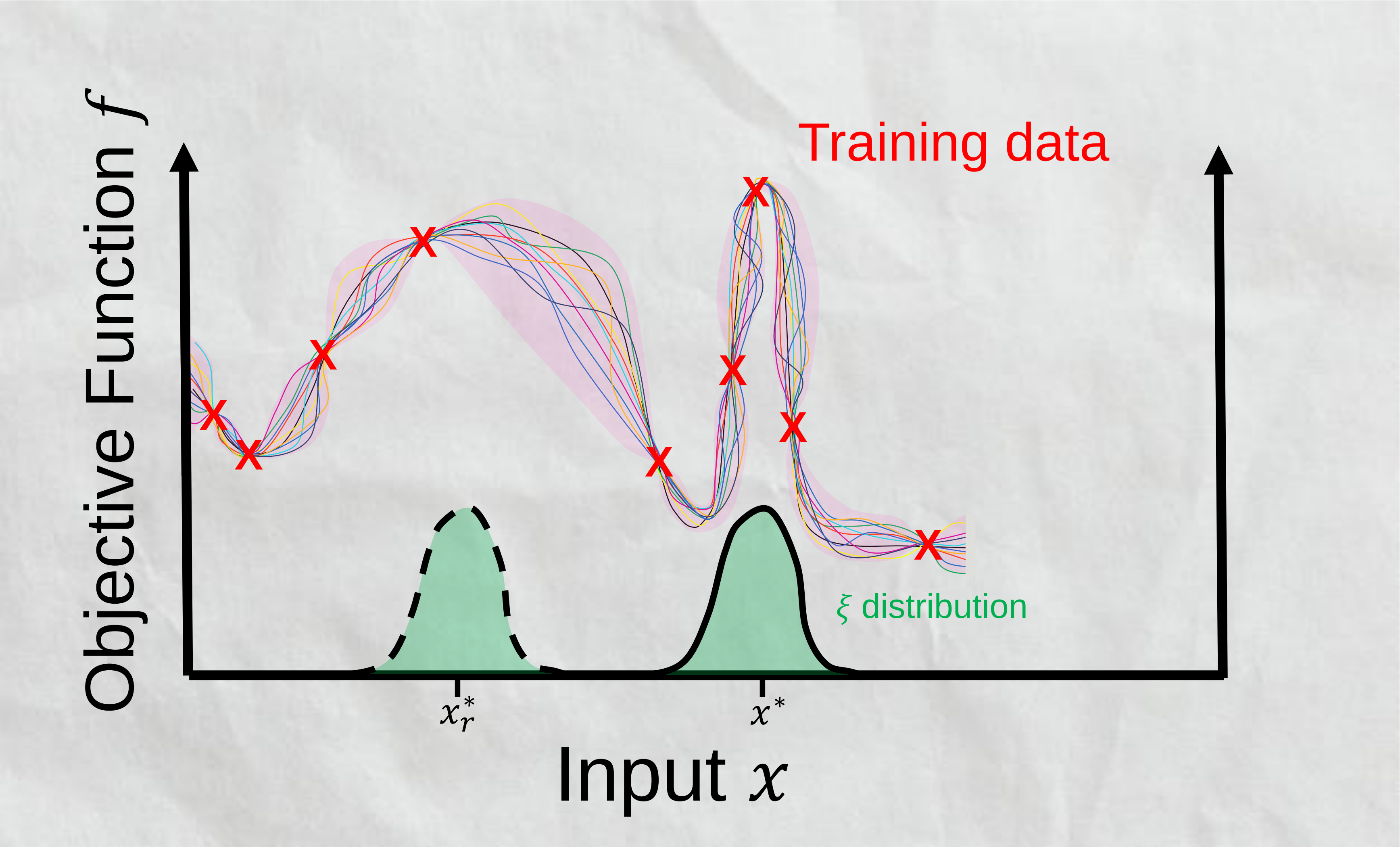
- **Bayesian** approach:
  - Gaussian Process $f \sim \mathcal{GP}$
  - Bayesian Treatment of the above moments
    - $\mathbb{J}_{\xi}[\mathcal{GP}(f)] = \mathbb{E}_{\xi}[\mathcal{GP}\ (x+\xi)]$
    - $\mathbb{V}_{\xi}[\mathcal{GP}(f)] = \mathbb{V}_{\xi}[\mathcal{GP}\ (x+\xi)]$



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APPROACH

Bochner's Theorem

$k(x,x')$
$= \sigma^2 \int p(\omega) \cos(\omega^T L(x-x'))\, d\omega$

$\approx$

Inner Product Form

$\phi^T(x)\phi(x')$

Feature mapping function

Bayesian Linear Model

$\mathcal{GP} \simeq \phi(x)^T \Theta$

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APPROACH

Bochner's Theorem

$k(x, x') = \sigma^2 \int p(\omega) \cos\left(\omega^T L(x - x')\right) d\omega \approx$

Random Fourier Features

Inner Product Form

$\phi^T(x)\phi(x')$

Feature mapping function

Monte Carlo

Bayesian Linear Model

$\mathcal{GP} \simeq \phi(x)^T \Theta$

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APPROACH

Bochner's Theorem

Inner Product Form

Bayesian Linear Model

$$k(x,x') = \sigma^2 \int p(\omega)\cos\left(\omega^T L(x-x')\right) d\omega \approx \phi^T(x)\phi(x')$$

Feature mapping function

$$\mathcal{GP} \simeq \phi(x)^T \Theta$$

Quadrature Fourier Features

Numerical Quadrature

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- $\mathbb{J}_{\xi}[\mathcal{GP}(f)] \simeq \mathbb{E}_{\xi}[\phi(x+\xi)^T]\Theta$
- $\mathbb{V}_{\xi}[\mathcal{GP}(f)] \simeq \Theta^T \mathbb{E}_{\xi}[\phi(x+\xi)^T]\Theta - \left[\mathbb{E}_{\xi}[\phi(x+\xi)^T]\Theta\right]^2$

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We derive expressions for

- ξ ~ (multivariate) Normal distribution
- ξ ~ Uniform distribution

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Fourier feature base robustness measures

A spectral representation (i.e., a parametric representation) of robustness measures that supports **sampling** continuous posterior trajectories

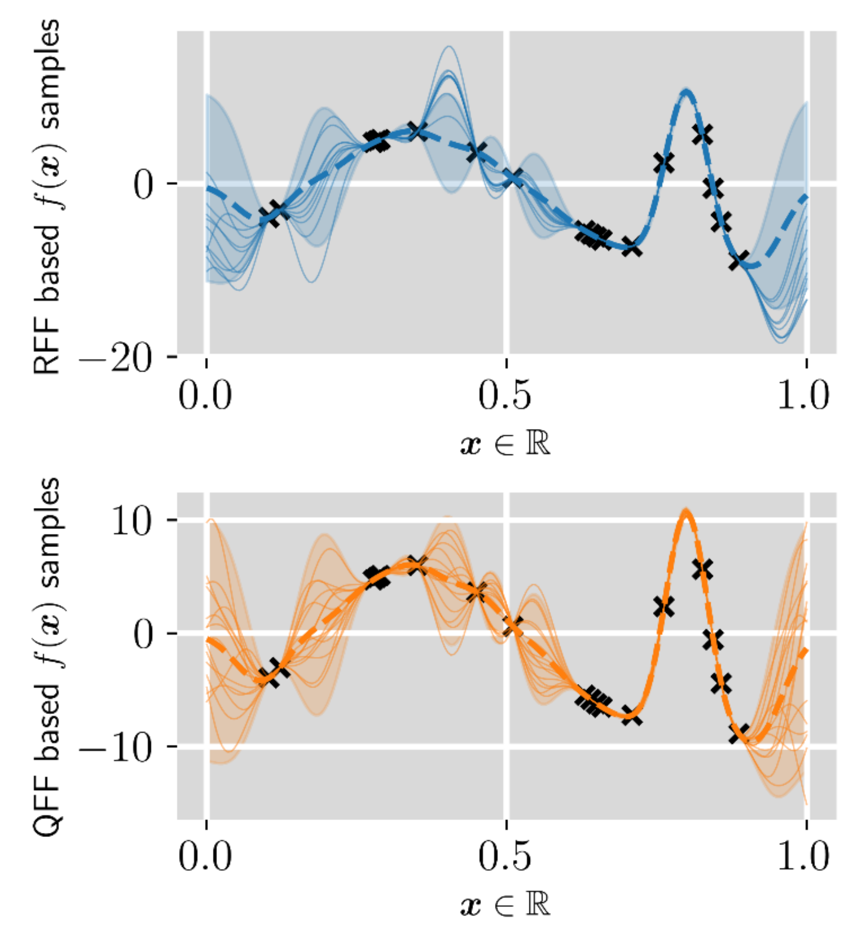
MAIN CONTRIBUTION

Fourier feature-based robustness measures

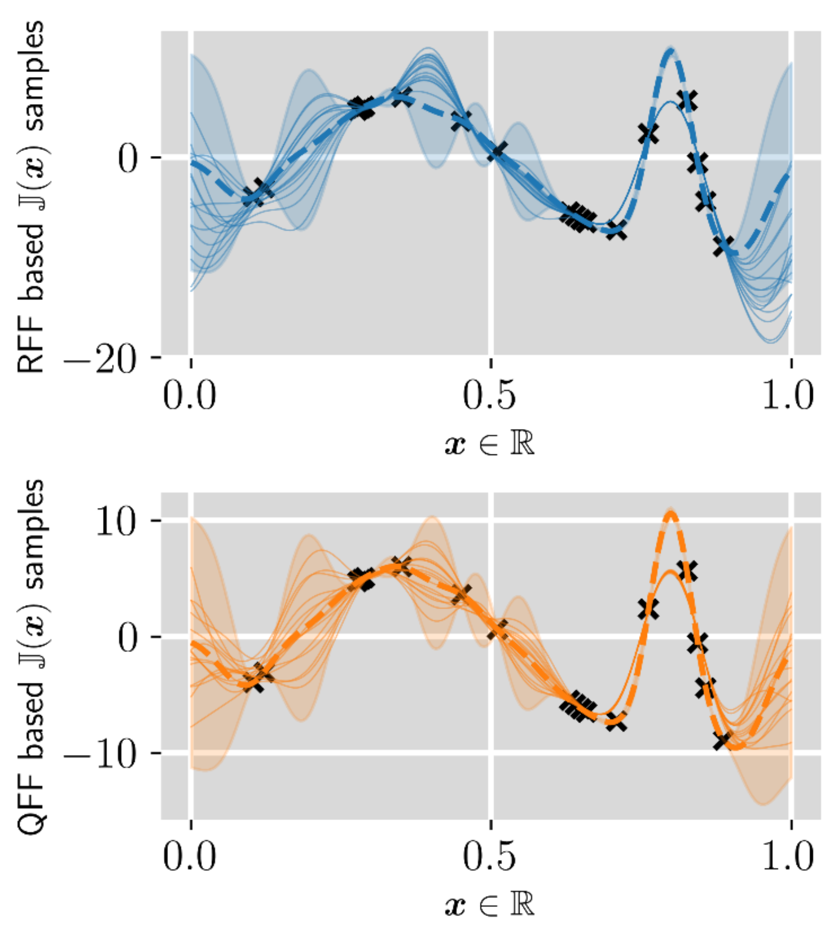
A spectral representation (i.e., a parametric representation) of robustness measures that supports sampling continuous posterior trajectories

Application in **Robust Bayesian Optimization**

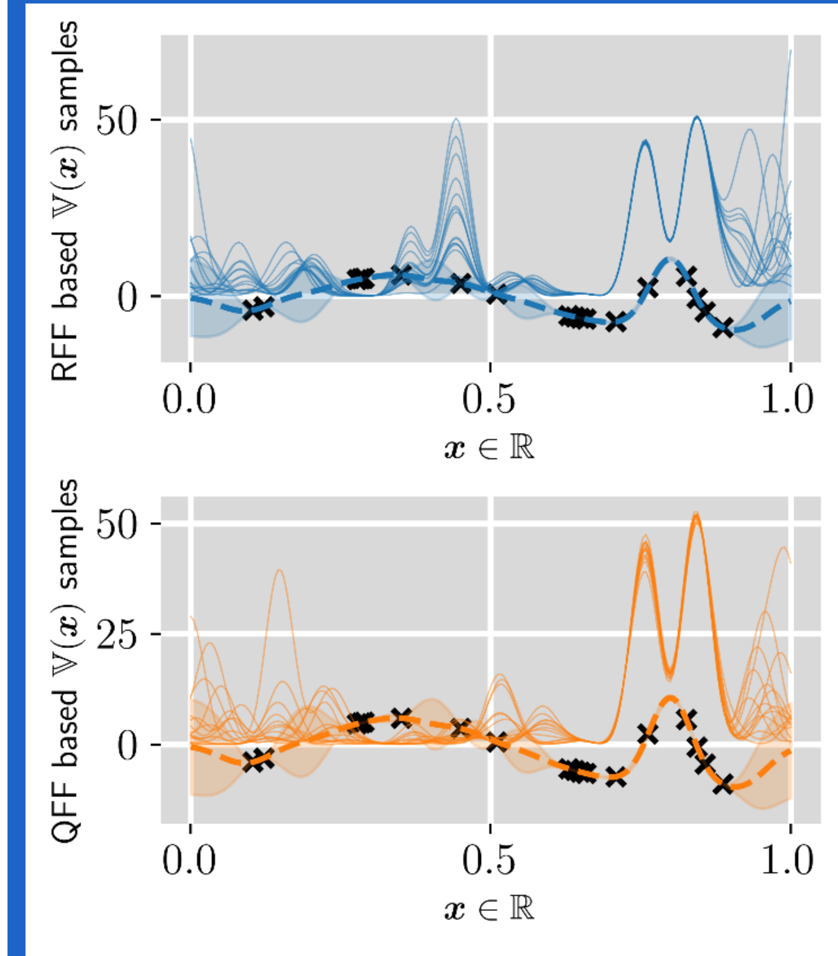
- Supports **various problem formulations**
- Supports **various acquisition functions**



Sample f posterior



Sample $\mathbb{J}$ posterior



Sample $\mathbb{V}$ posterior

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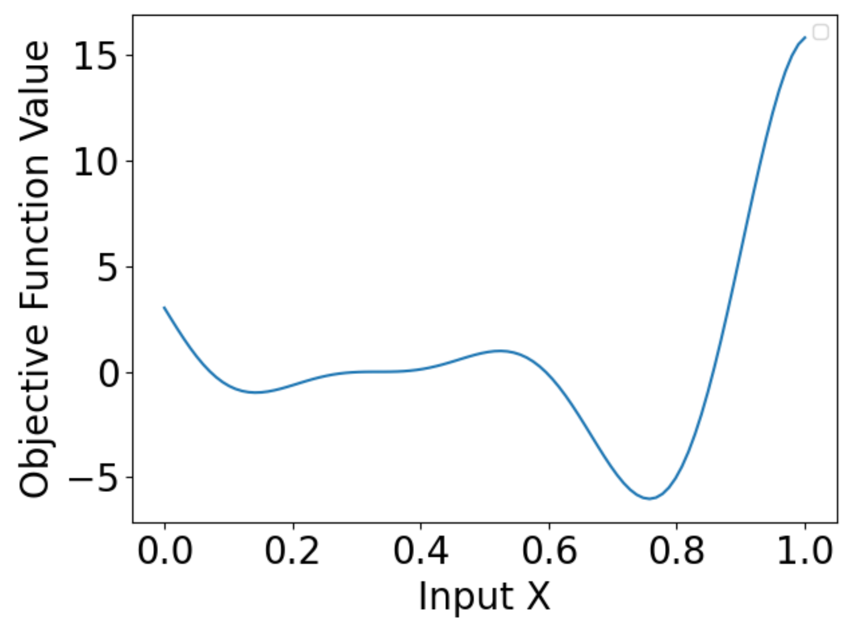
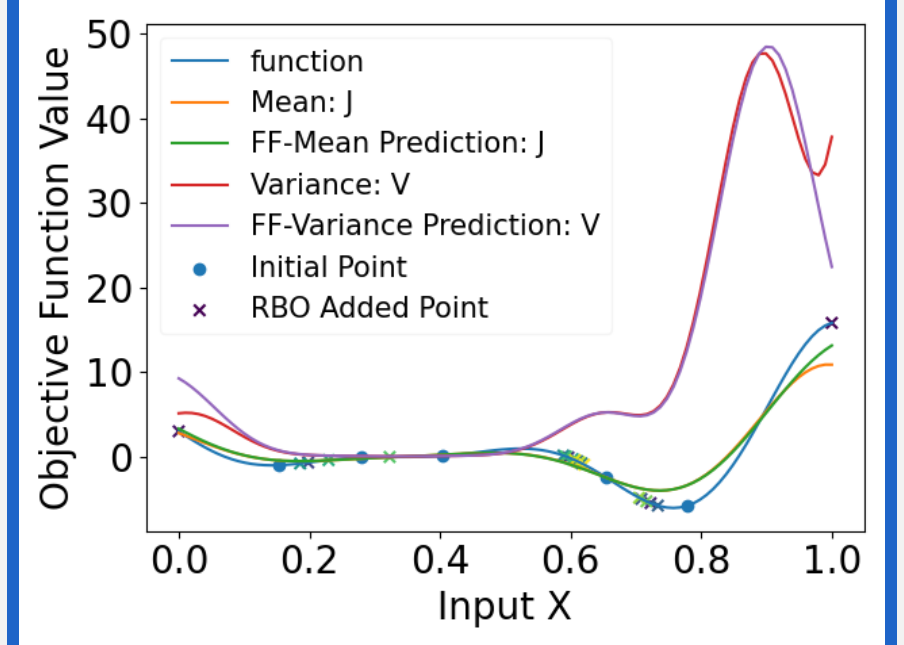
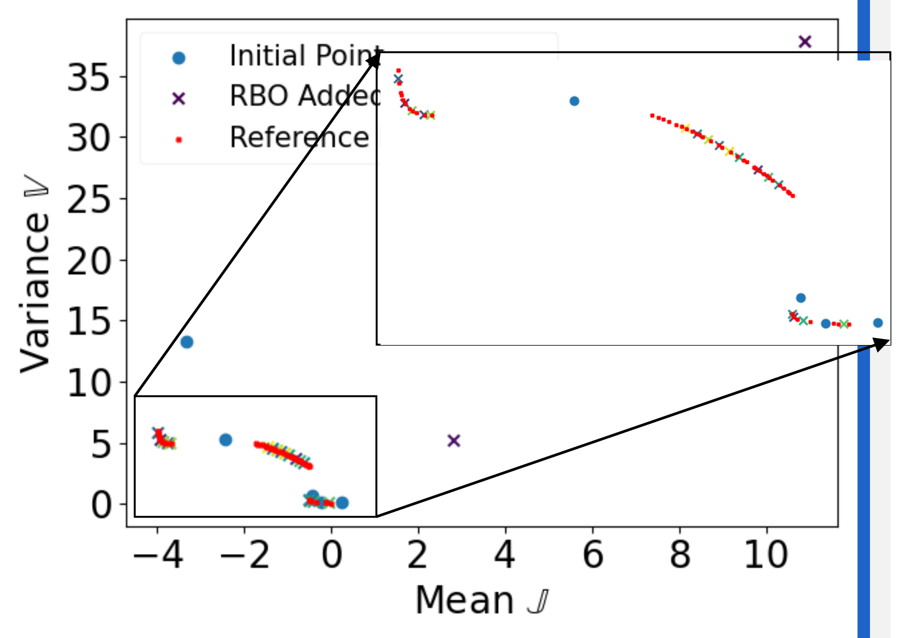
Proof of Concept



Benchmark Function



RBO Added Points



Pareto frontier

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Code is available at:

https://github.com/TsingQAQ/gp_mean_var_rbo

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