

Regret bounds for meta Bayesian optimization with an **unknown** Gaussian process prior

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Leslie Pack Kaelbling



Dec 5 @ NeurIPS 18



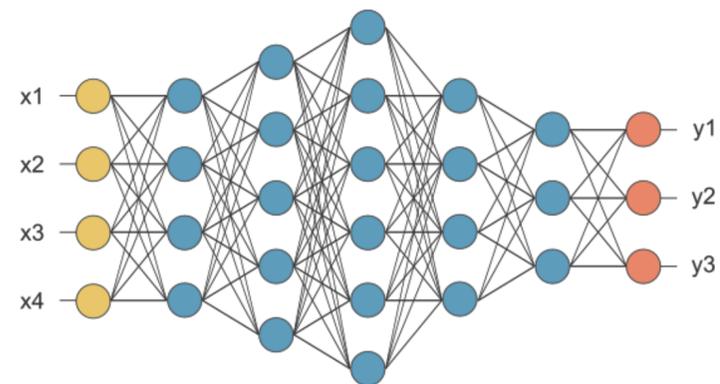
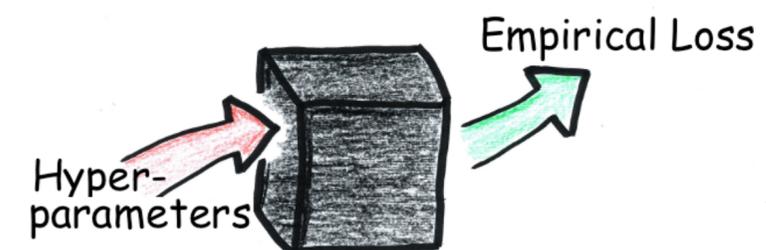
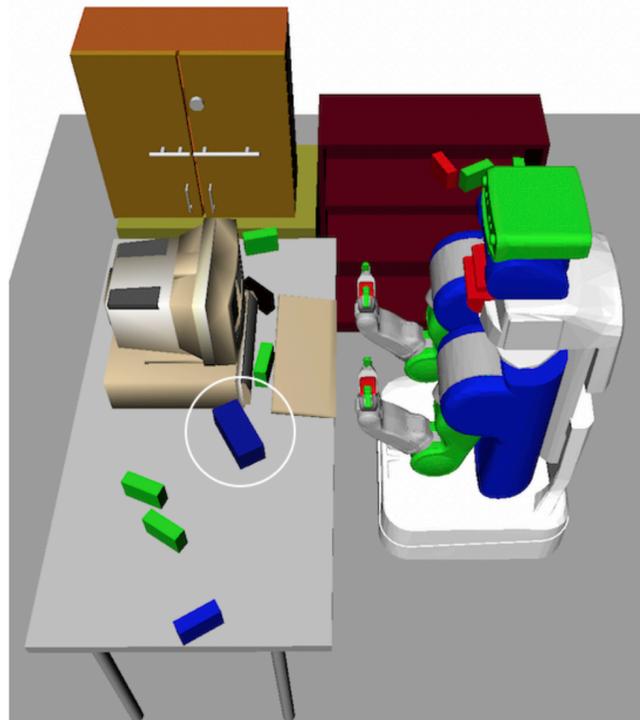
Poster #22

Bayesian optimization

Goal: $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Challenges:

- f is expensive to evaluate
- f is multi-peak
- no gradient information
- evaluations can be noisy

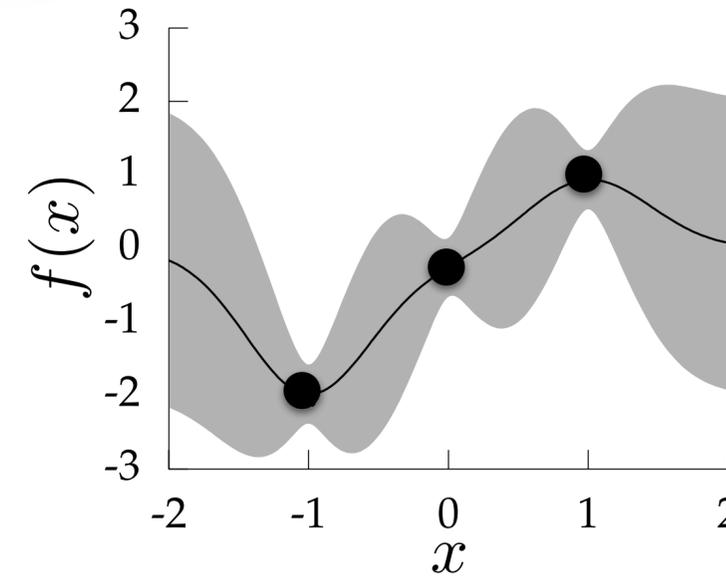


Bayesian optimization

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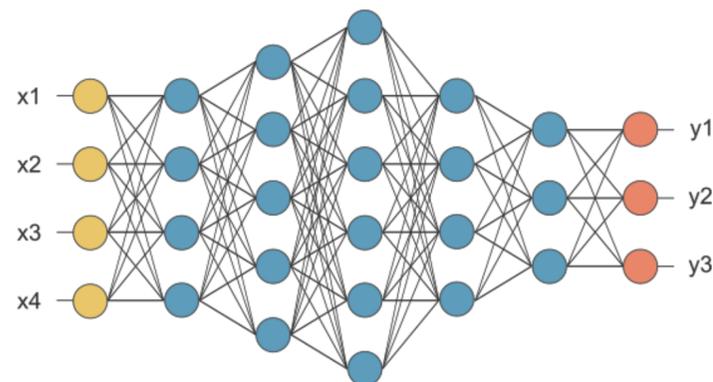
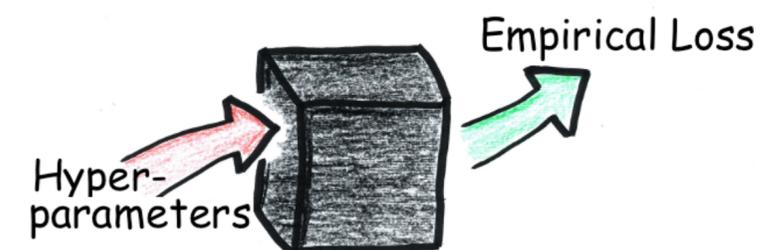
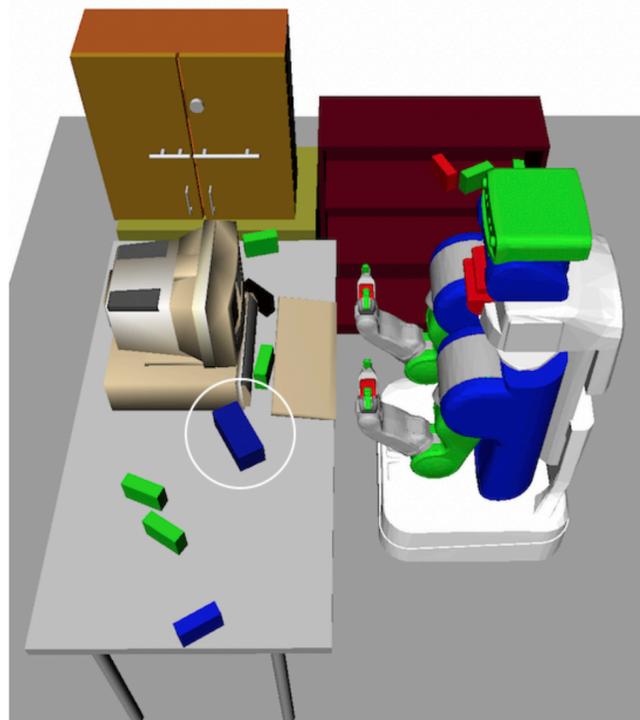
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Assume a GP prior $f \sim GP(\mu, k)$

LOOP

- choose new query point(s) to evaluate
- compute the posterior GP model

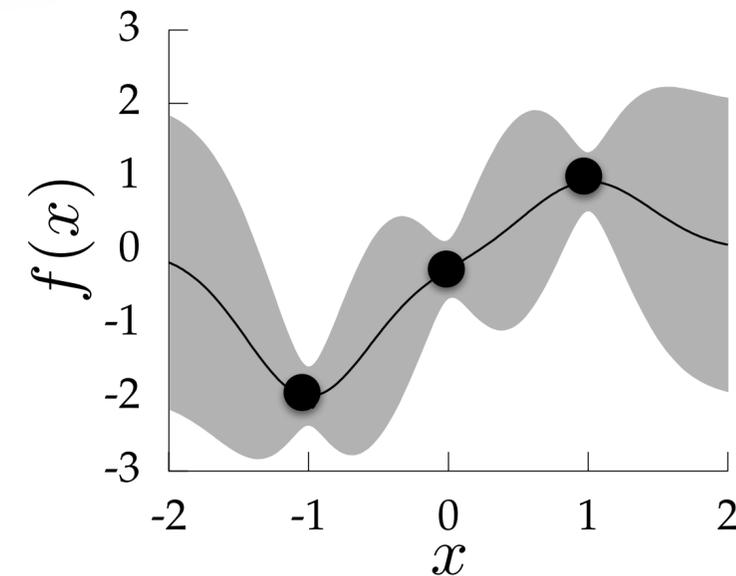
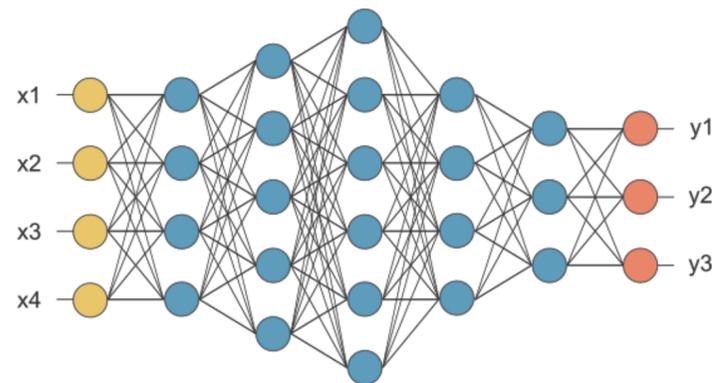
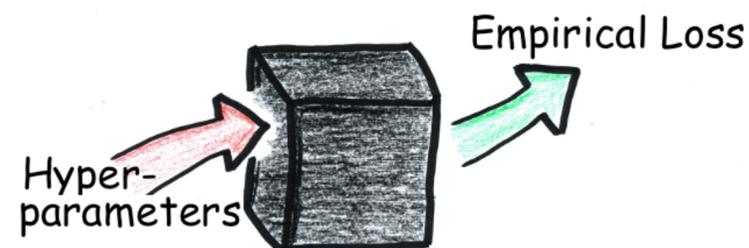
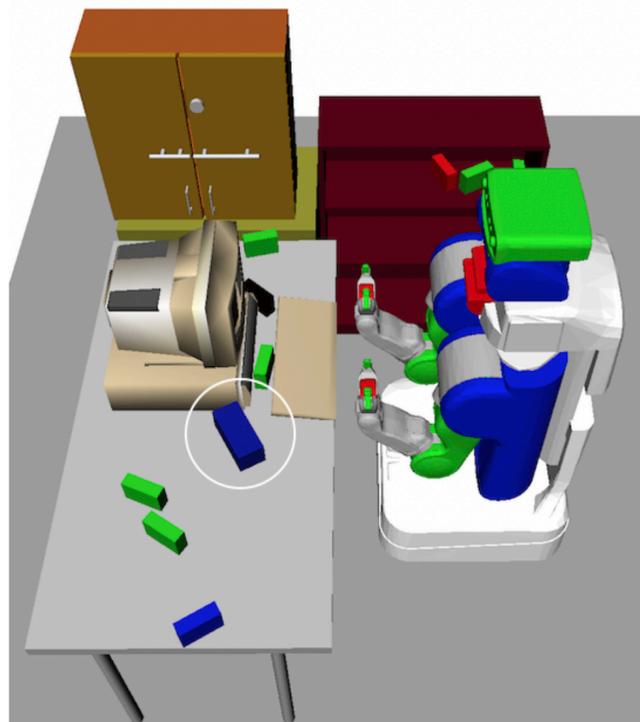


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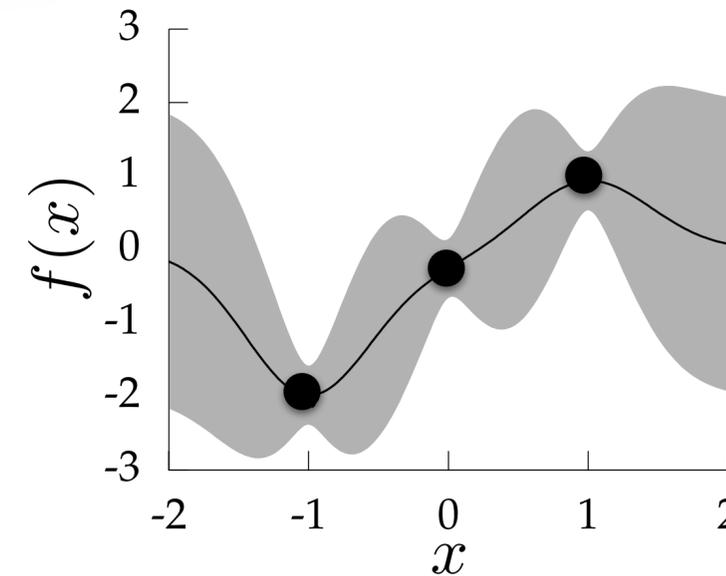
How to choose the prior?

Bayesian optimization

Goal: $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Challenges:

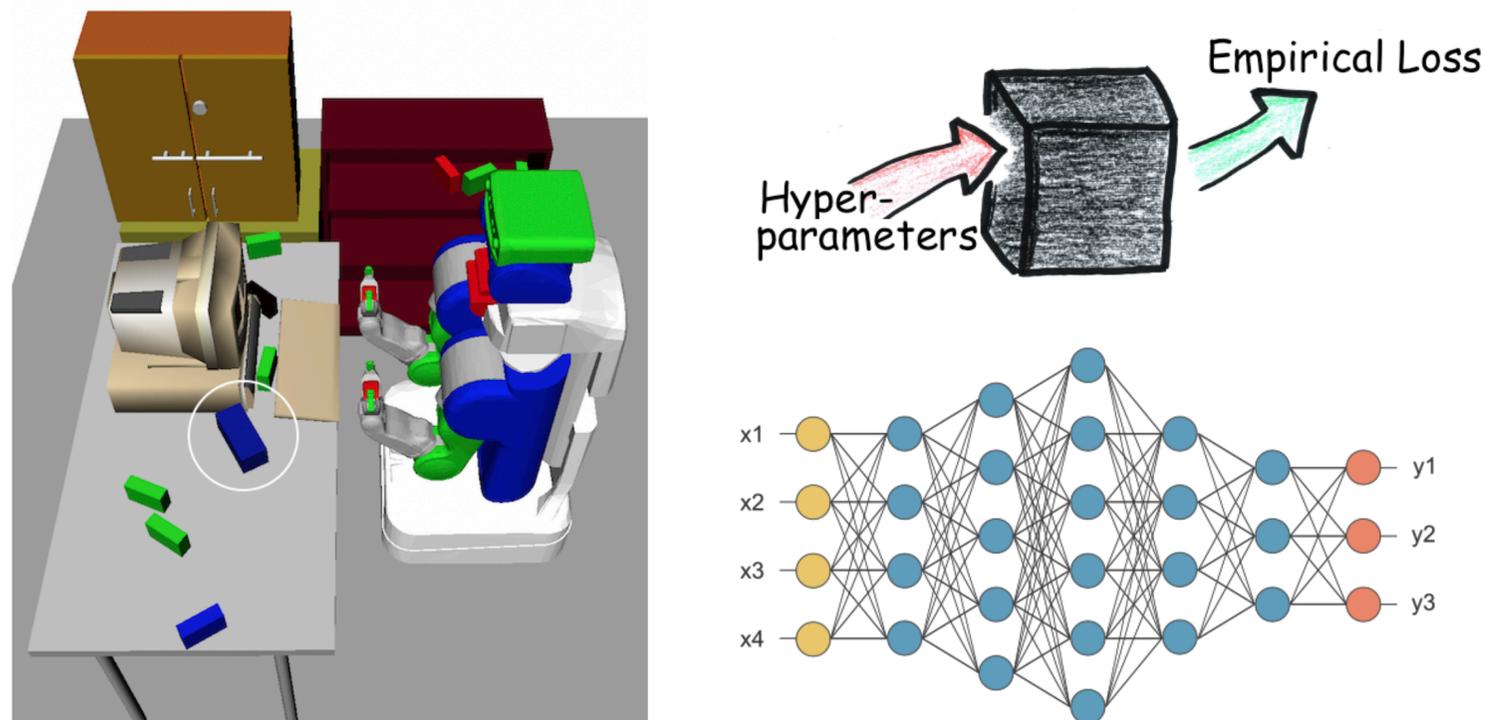
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- *re-estimate the prior parameters*
e.g. by maximizing marginal data likelihood every few iterations

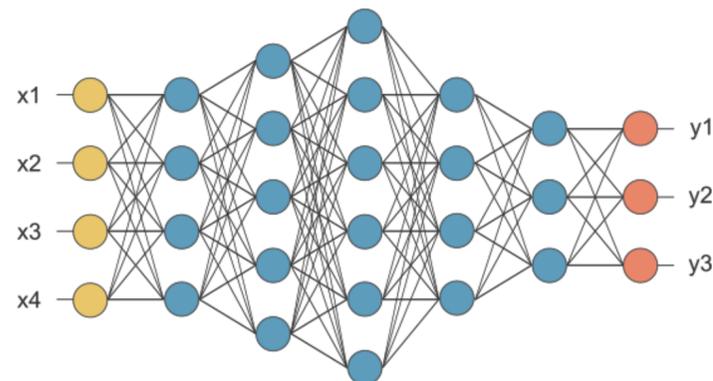
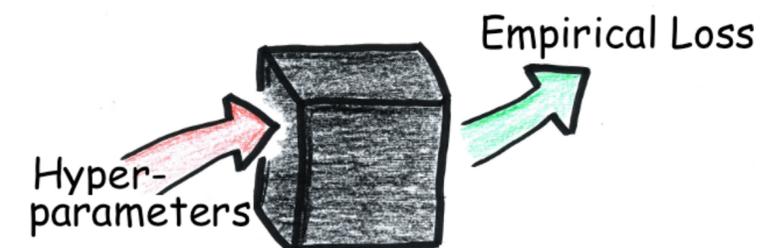
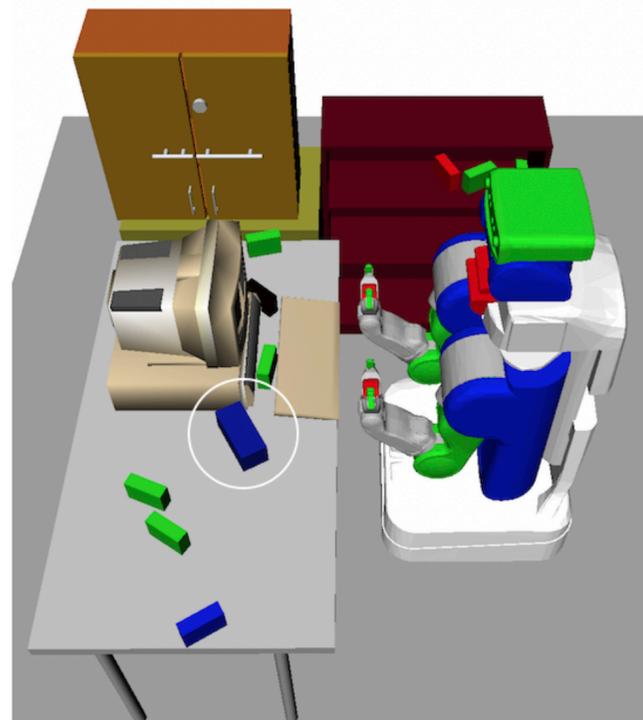


Bayesian optimization

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Which comes first?
Data or prior?



Assume a GP prior $f \sim GP(\mu, k)$

LOOP

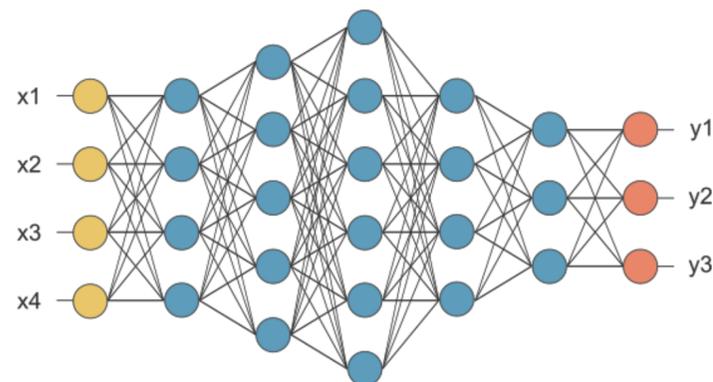
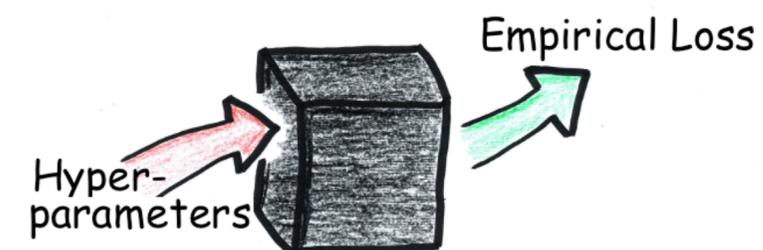
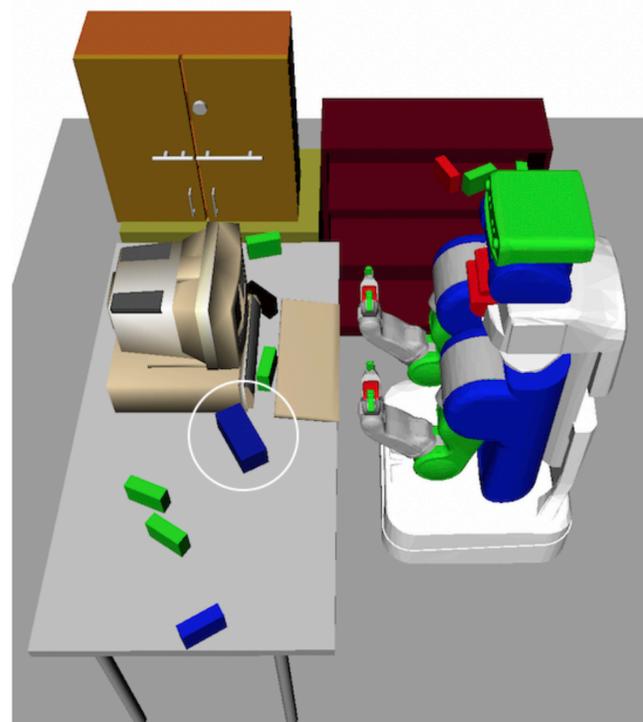
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Bayesian optimization

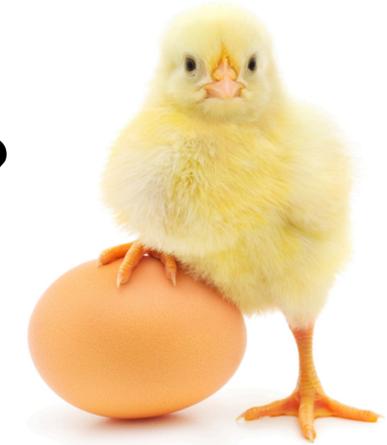
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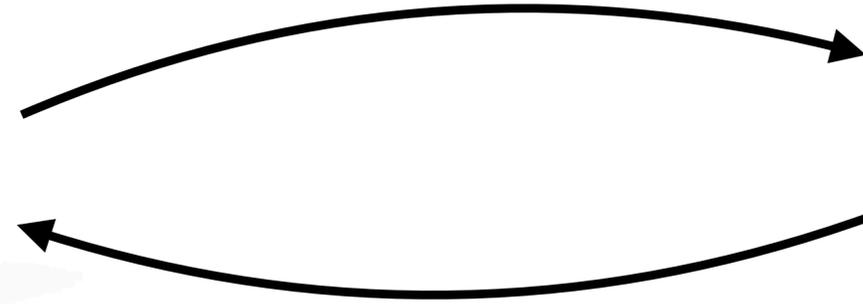
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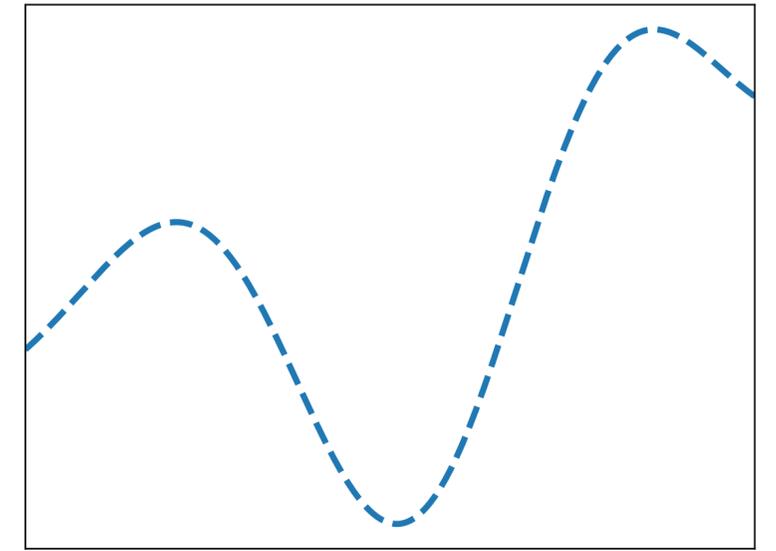
Hard to analyze.

Bayesian optimization with an unknown GP prior

prior model

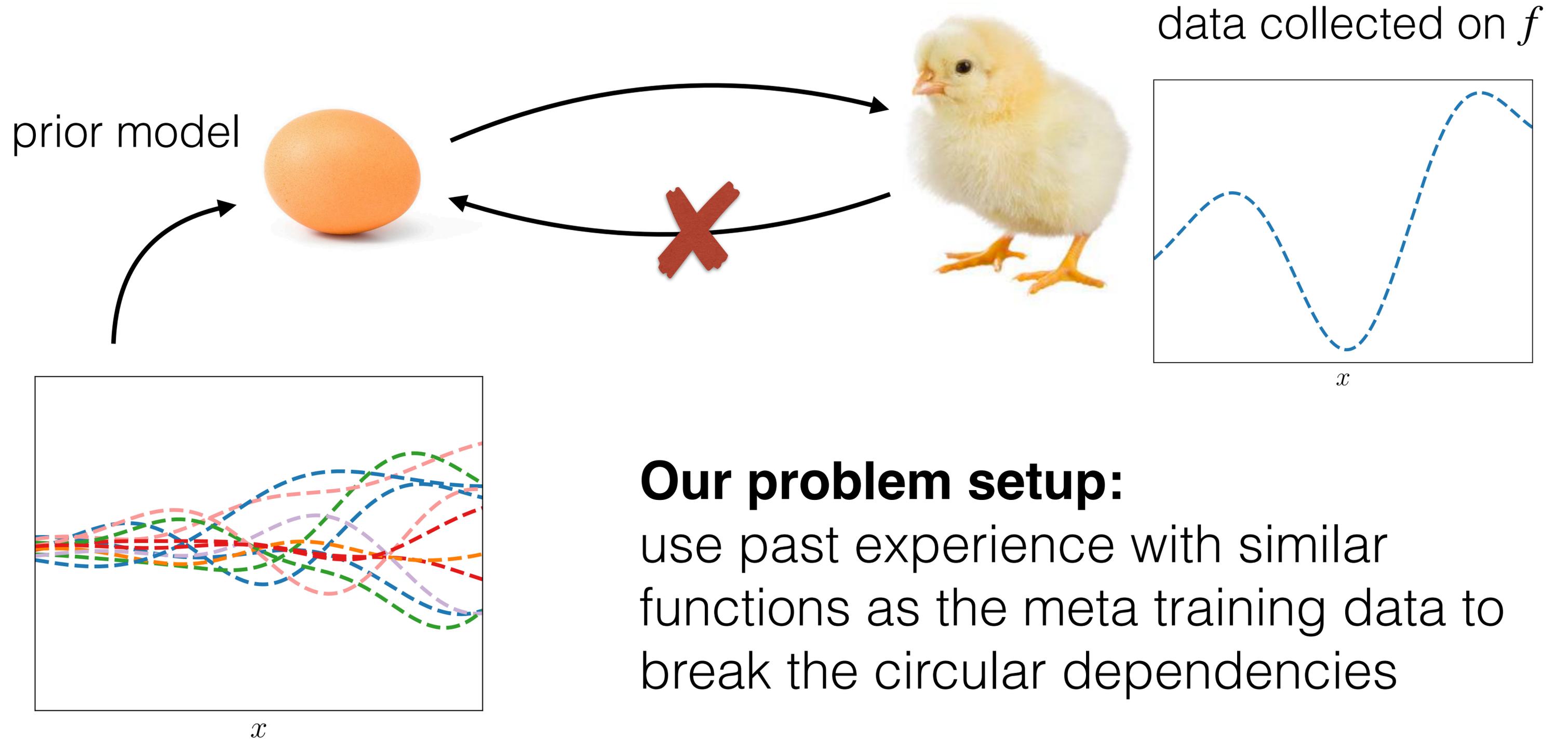


data collected on f



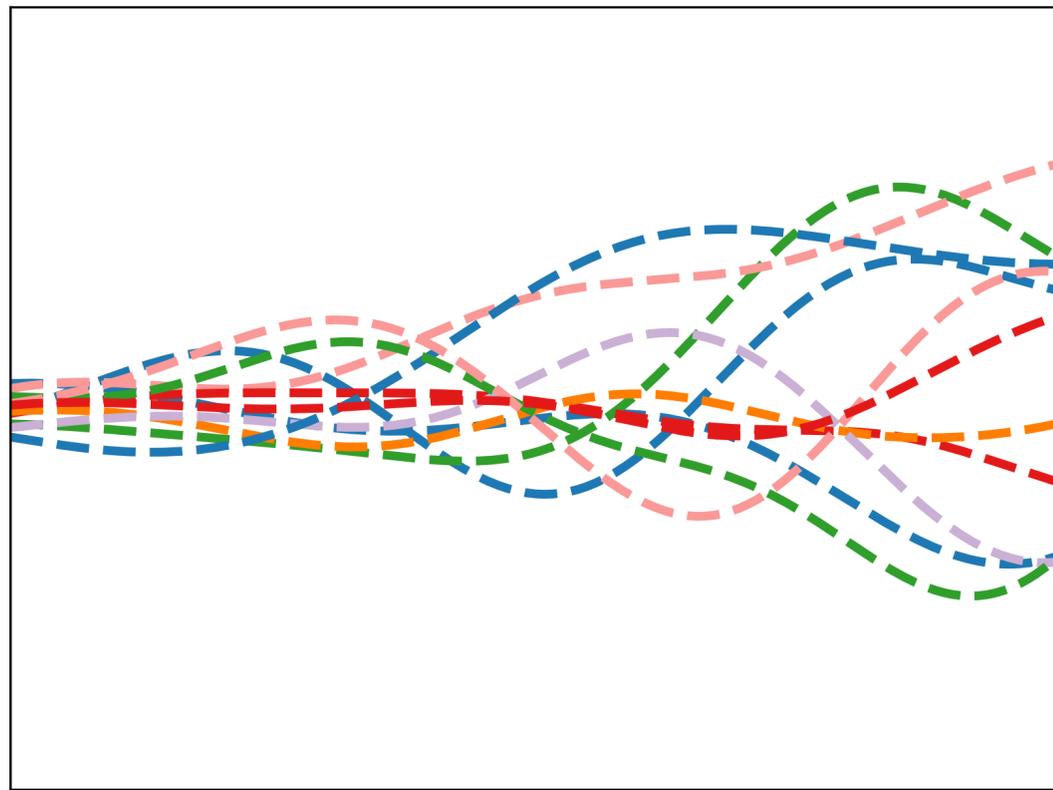
x

Bayesian optimization with an unknown GP prior



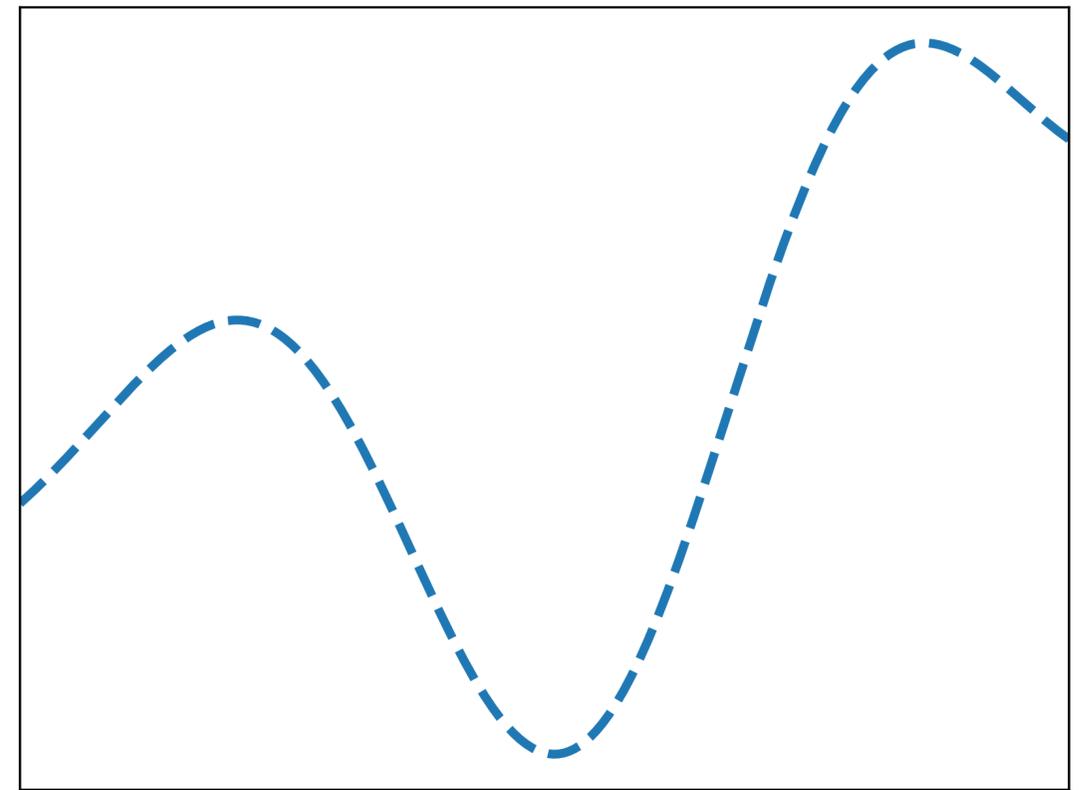
Meta Bayesian optimization with an unknown GP prior

Offline phase



x

Online phase



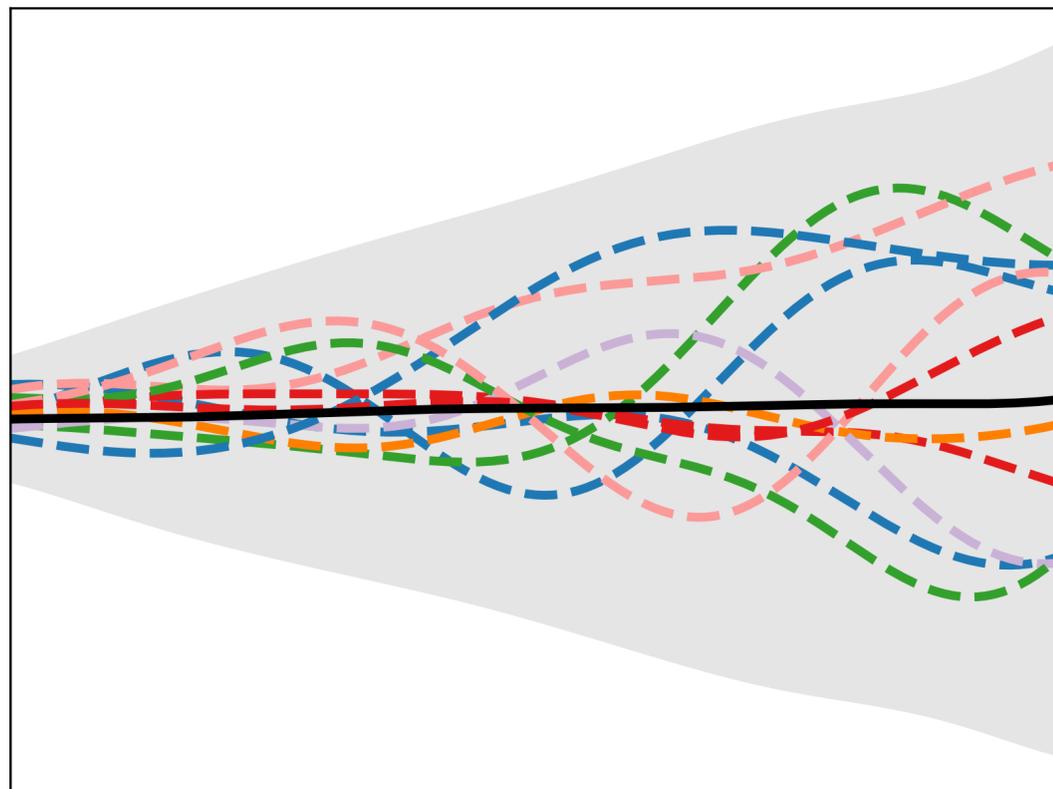
x

Meta Bayesian optimization with an unknown GP prior

Estimate the GP prior from offline data sampled from the same prior

Offline phase

— $\hat{\mu}(x)$ $\hat{\mu}(x) \pm 3\sqrt{\hat{k}(x)}$

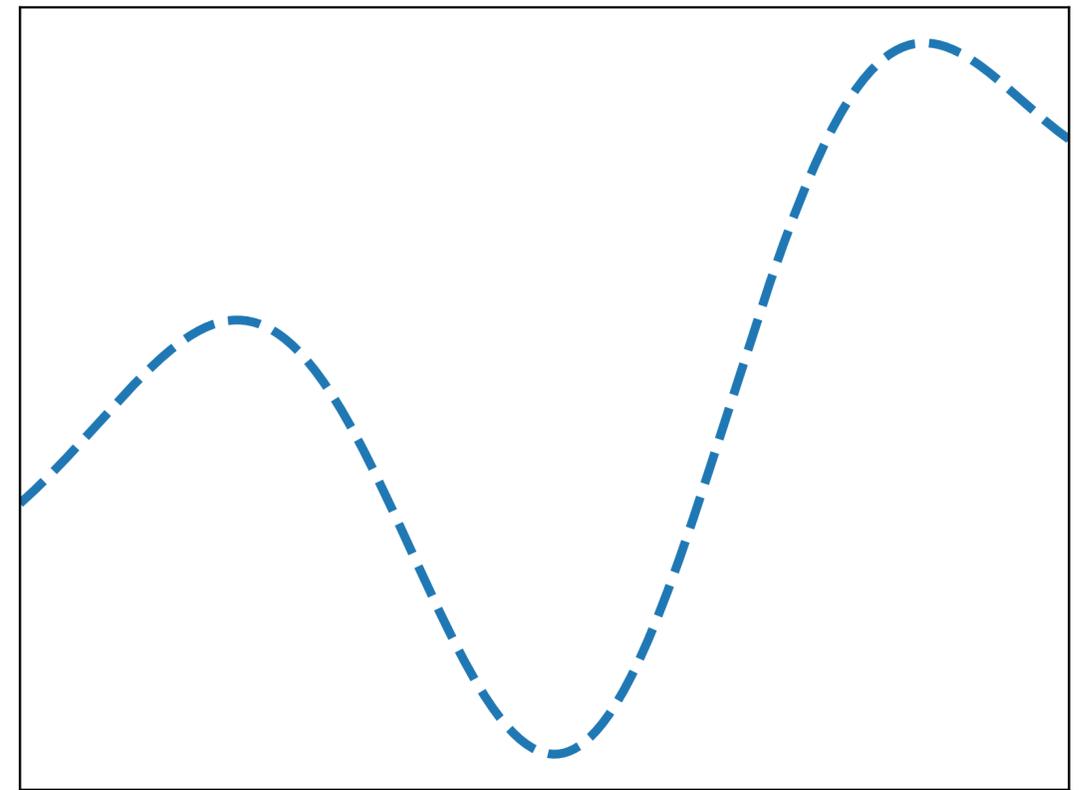


x

Estimated prior

$\hat{\mu}, \hat{k}$

Online phase



x

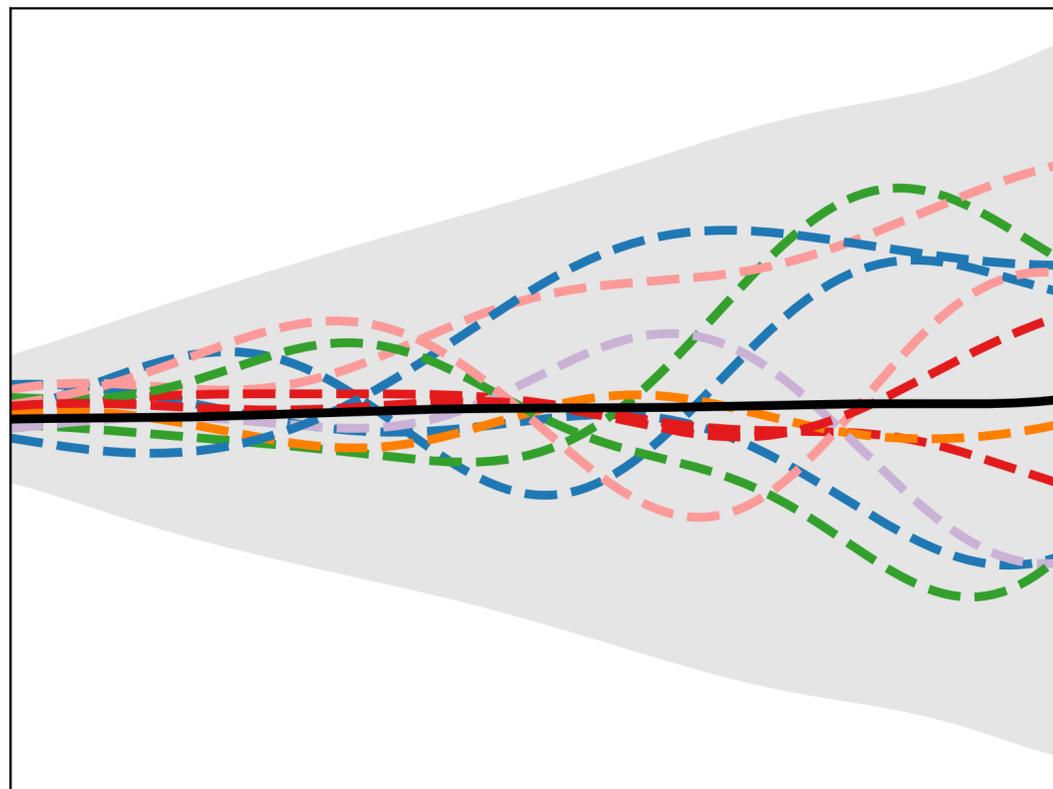
Meta Bayesian optimization with an unknown GP prior

Estimate the GP prior from offline data sampled from the same prior

Construct unbiased estimators of the posterior and use a variant of GP-UCB

Offline phase

— $\hat{\mu}(x)$ $\hat{\mu}(x) \pm 3\sqrt{\hat{k}(x)}$



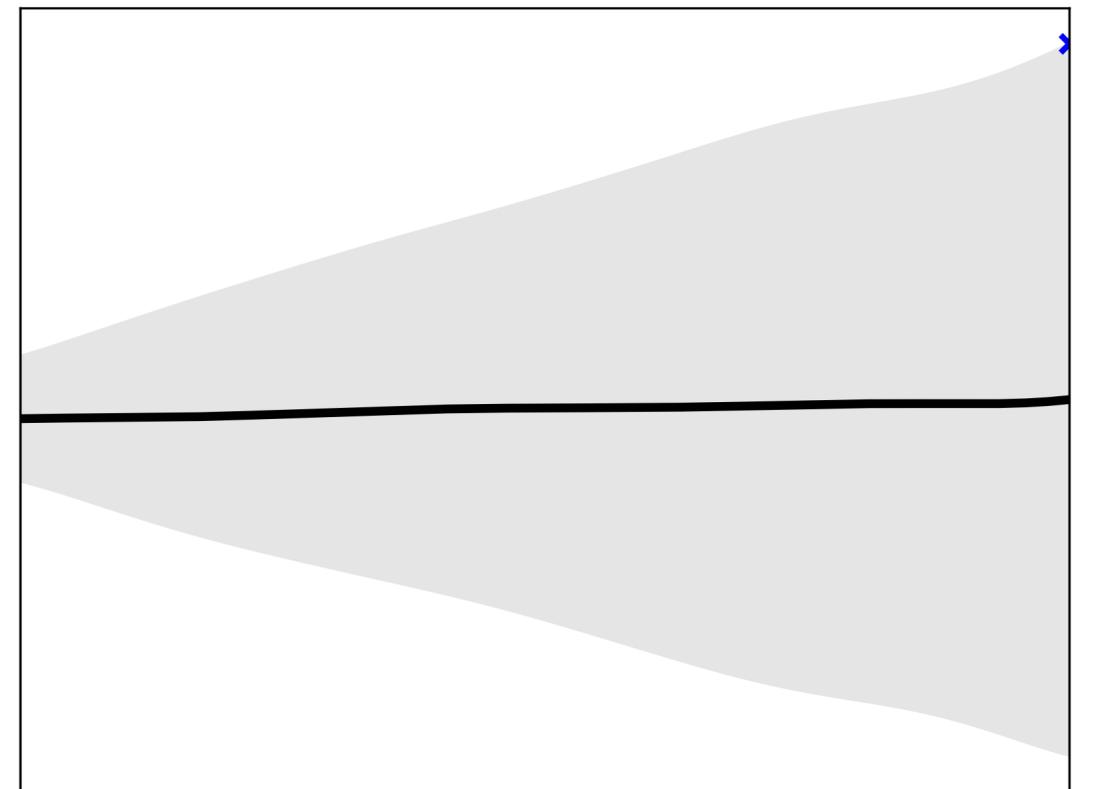
x

Estimated prior

$\hat{\mu}, \hat{k}$

Online phase

— $\hat{\mu}_0(x)$ $\hat{\mu}_0(x) \pm \zeta_1\sqrt{\hat{k}_0(x)}$



x

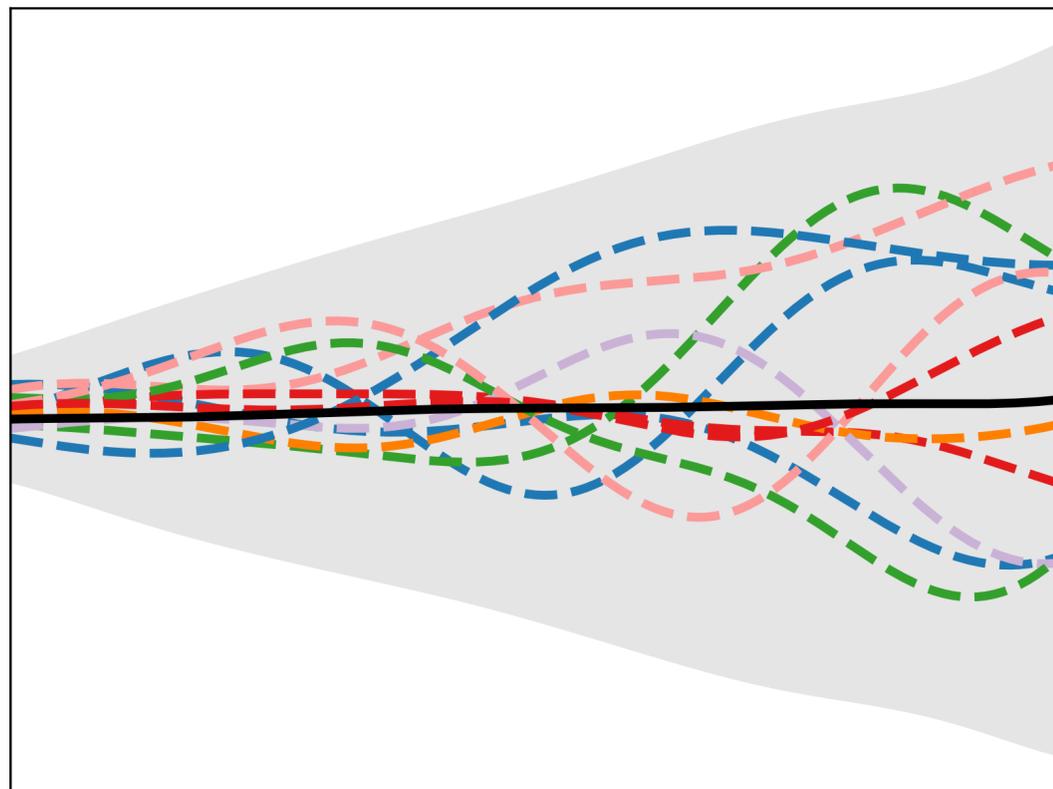
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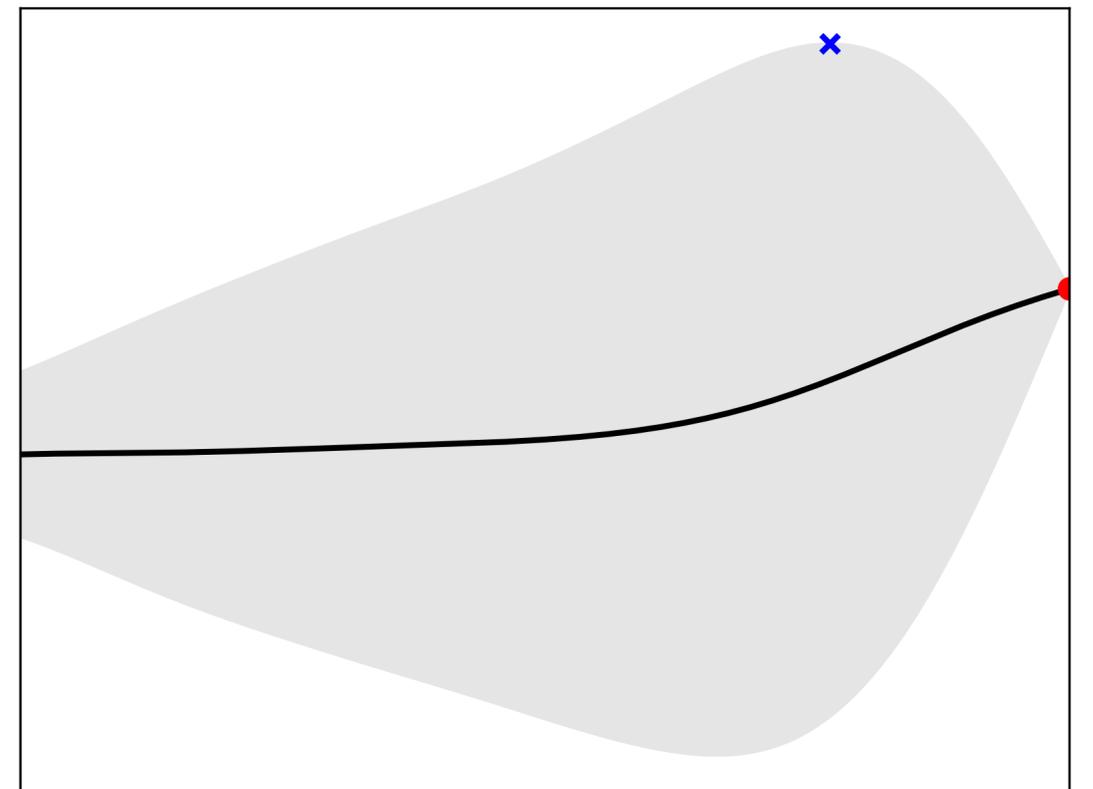


Estimated prior

$\hat{\mu}, \hat{k}$

Online phase

— $\hat{\mu}_1(x)$ $\hat{\mu}_1(x) \pm \zeta_2\sqrt{\hat{k}_1(x)}$



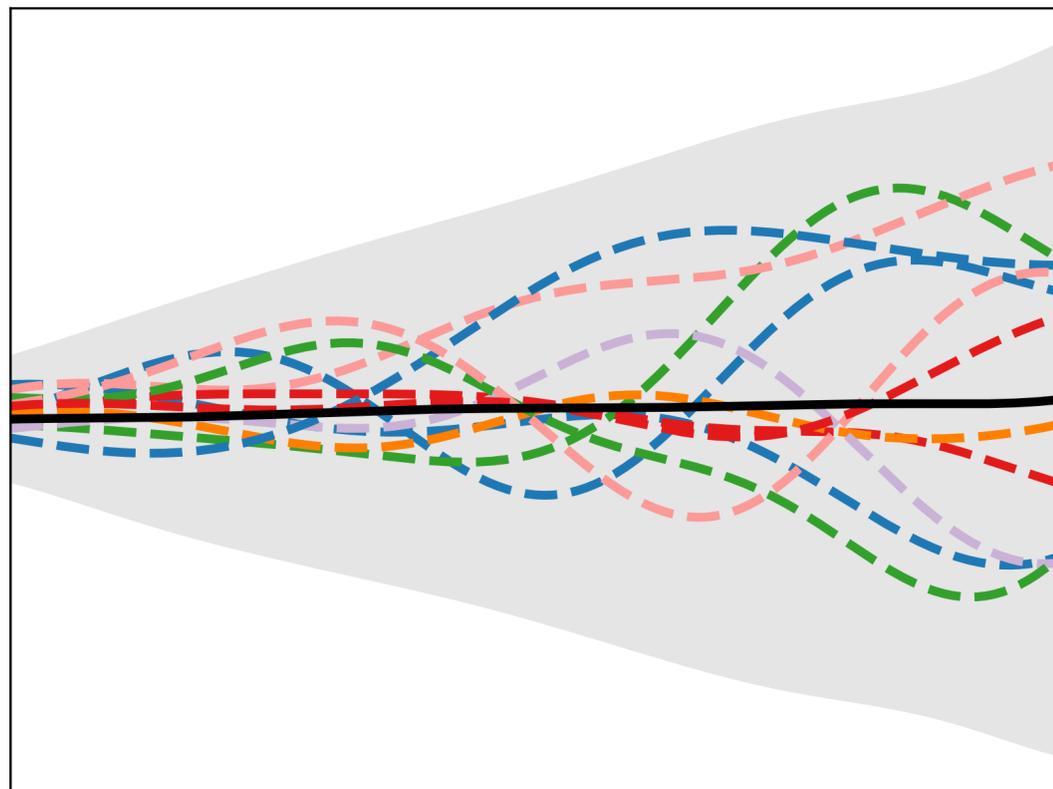
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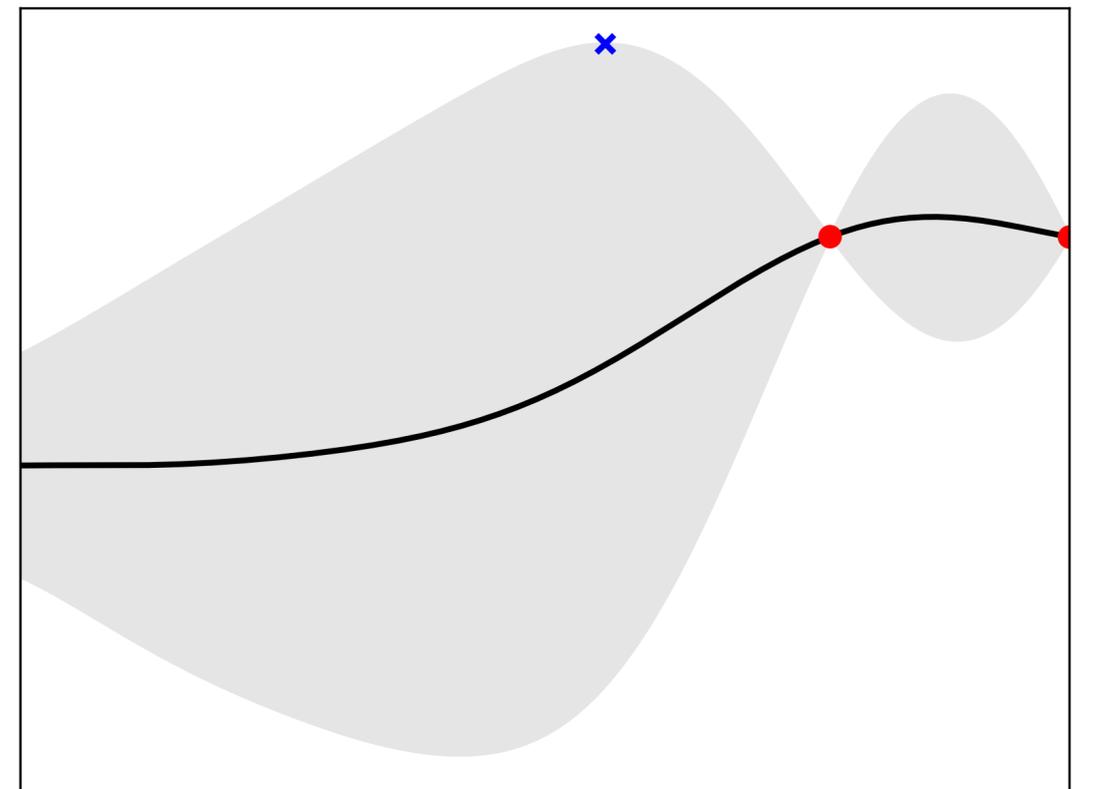
x

Estimated prior

$\hat{\mu}, \hat{k}$

Online phase

— $\hat{\mu}_2(x)$ $\hat{\mu}_2(x) \pm \zeta_3\sqrt{\hat{k}_2(x)}$



x

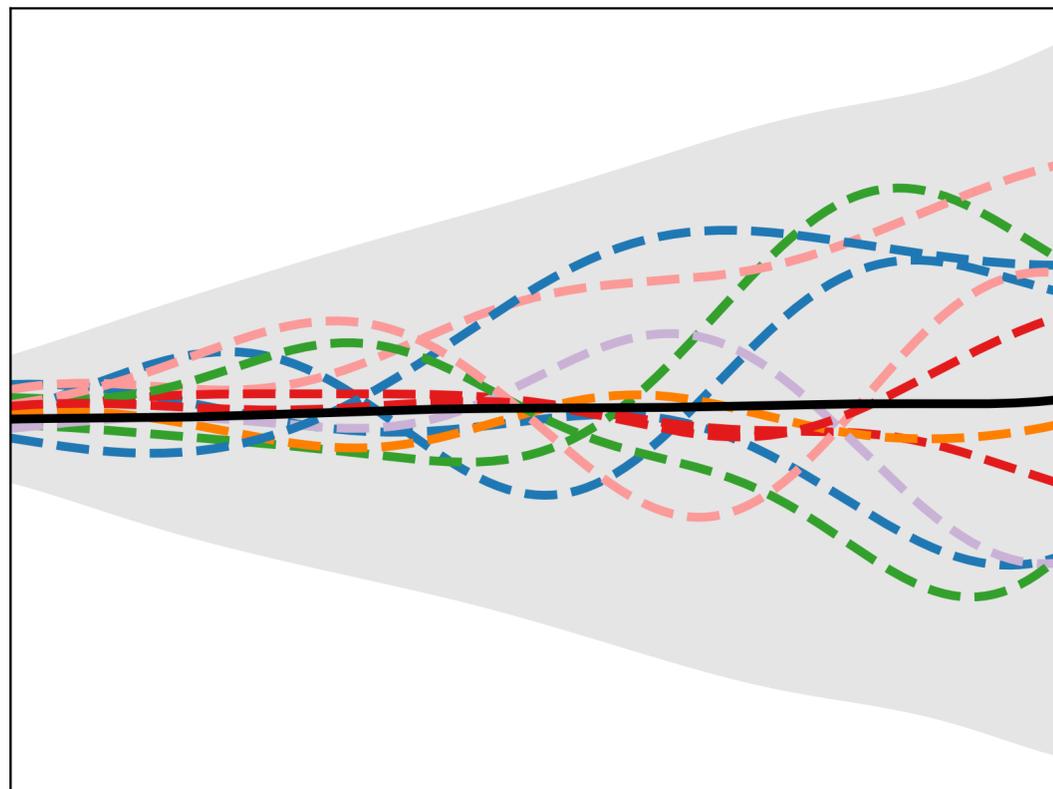
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Offline phase

— $\hat{\mu}(x)$ $\hat{\mu}(x) \pm 3\sqrt{\hat{k}(x)}$



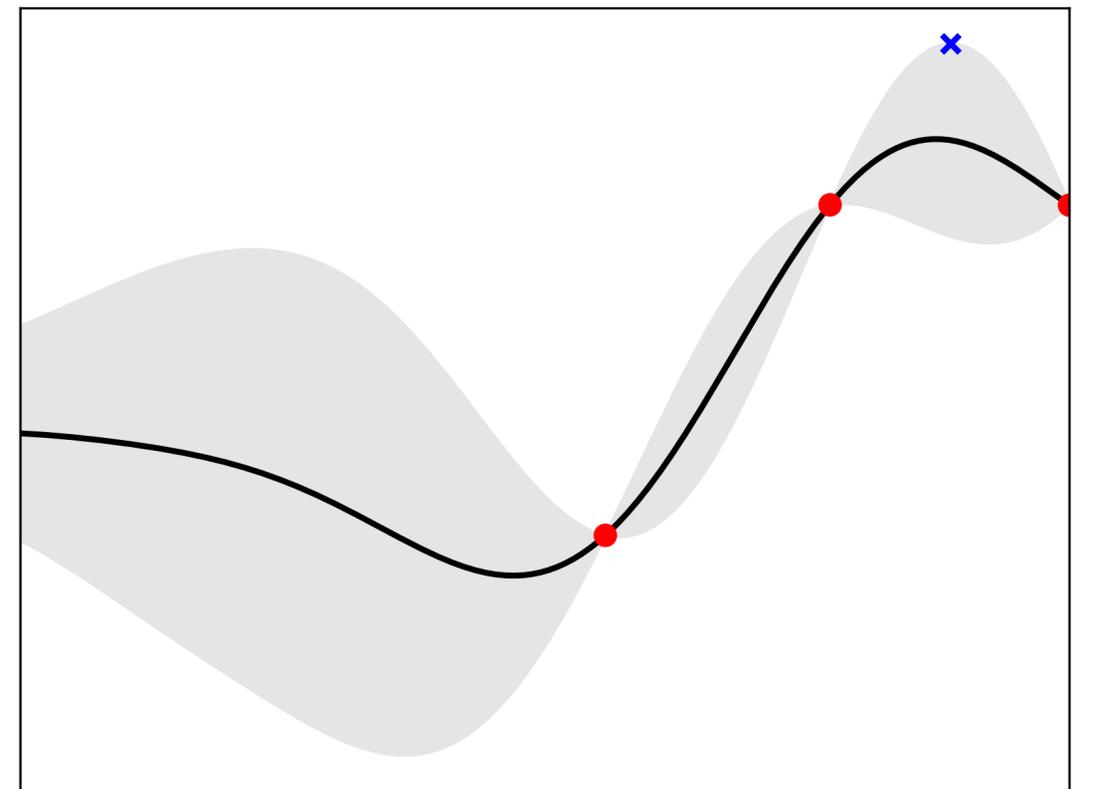
x

Estimated prior

$\hat{\mu}, \hat{k}$

Online phase

— $\hat{\mu}_3(x)$ $\hat{\mu}_3(x) \pm \zeta_4\sqrt{\hat{k}_3(x)}$



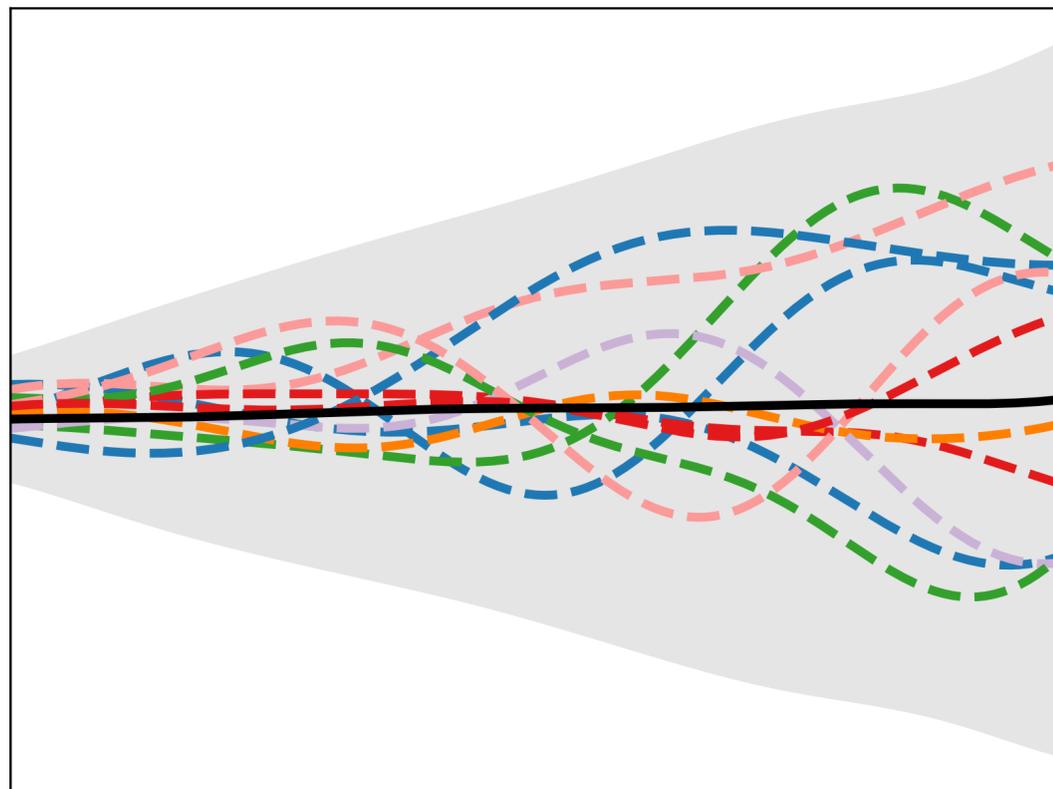
x

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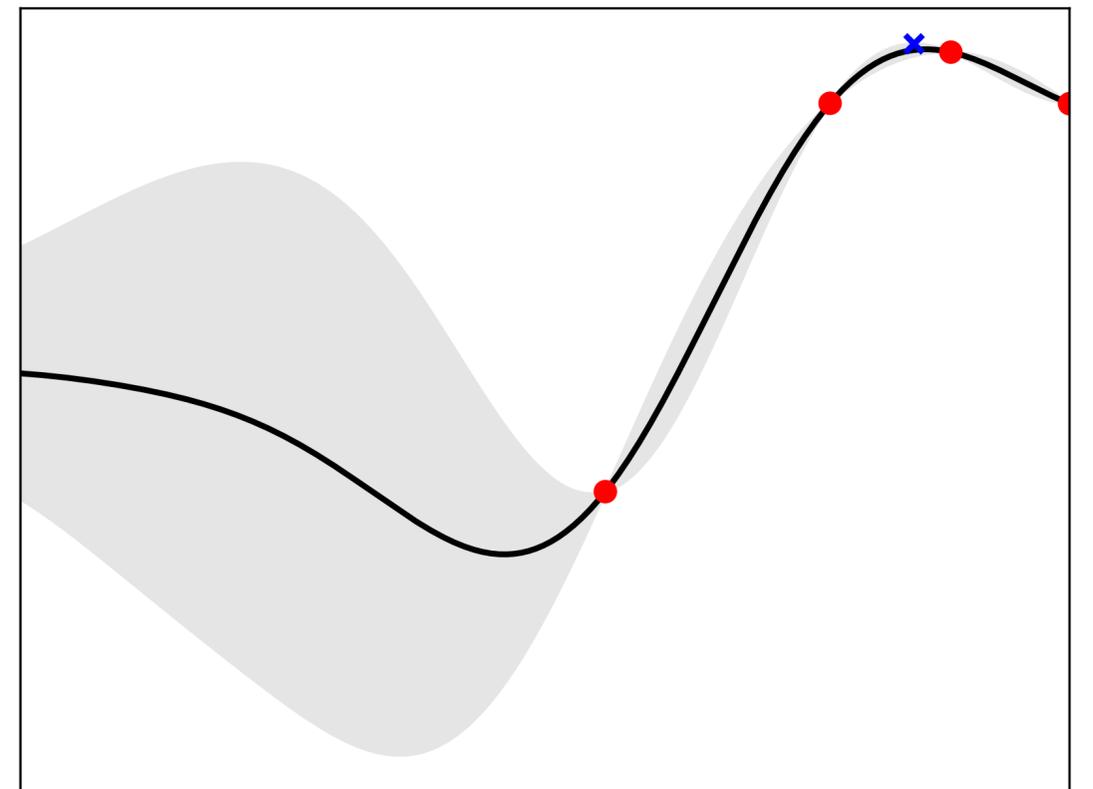
Estimated prior

$\hat{\mu}, \hat{k}$

Construct unbiased estimators of the posterior and use a variant of GP-UCB

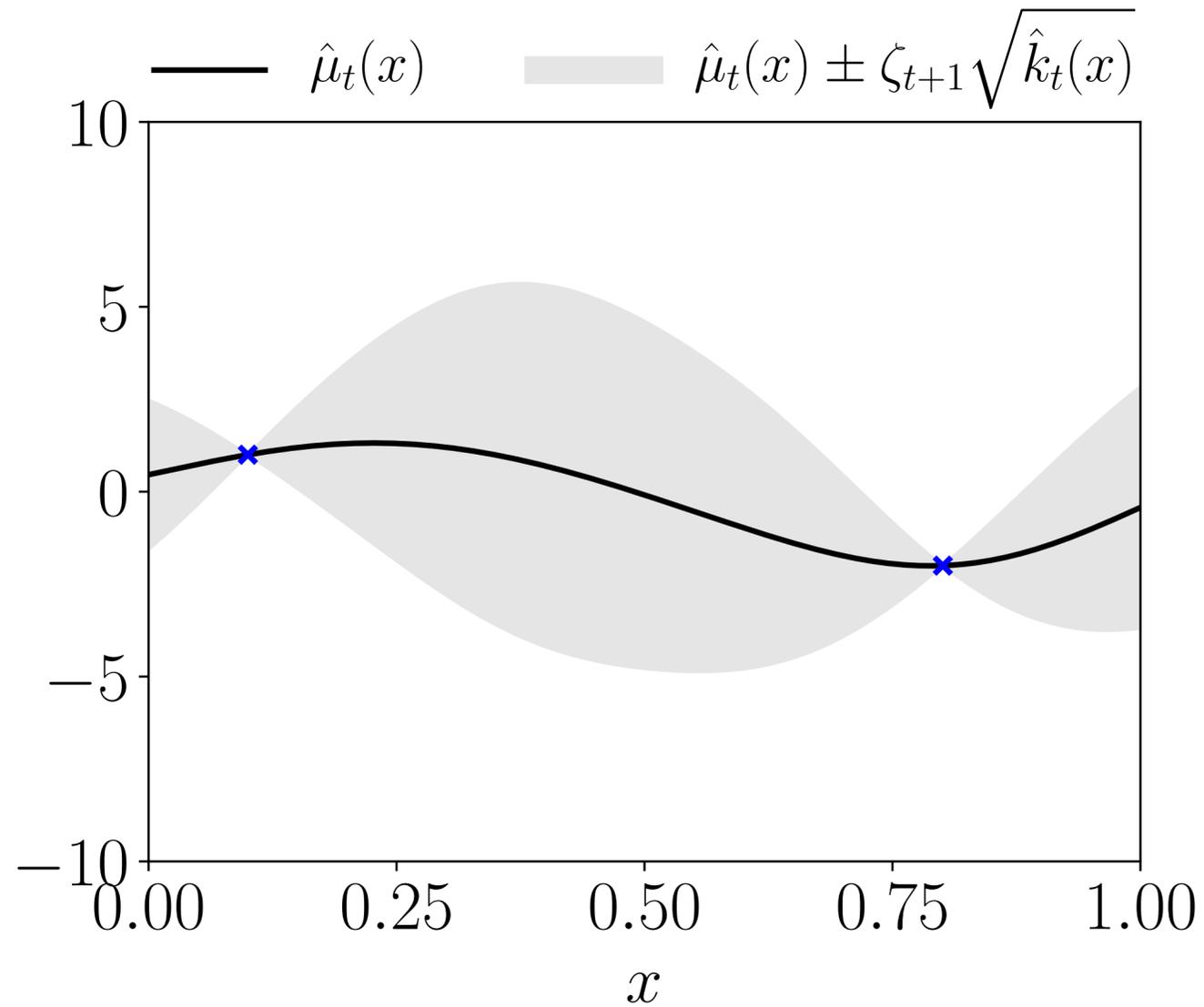
Online phase

— $\hat{\mu}_4(x)$ $\hat{\mu}_4(x) \pm \zeta_5\sqrt{\hat{k}_4(x)}$

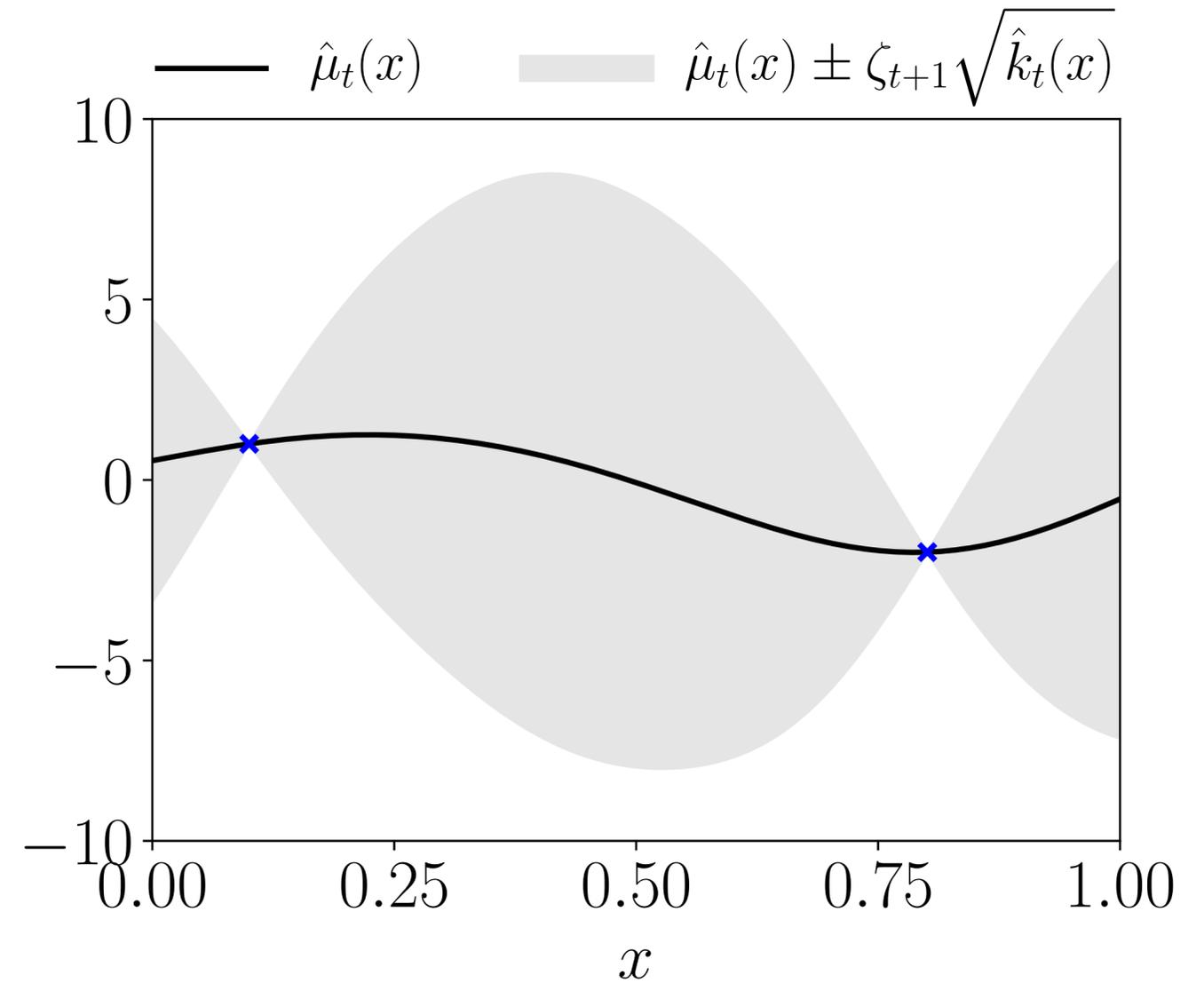


Effect of N , the number of meta training functions

$N = 1000$



$N = 100$



Bounding the regret of meta BO with an unknown GP prior

Theorem (finite input space)

Results for continuous input space @ poster #22

Important assumptions:

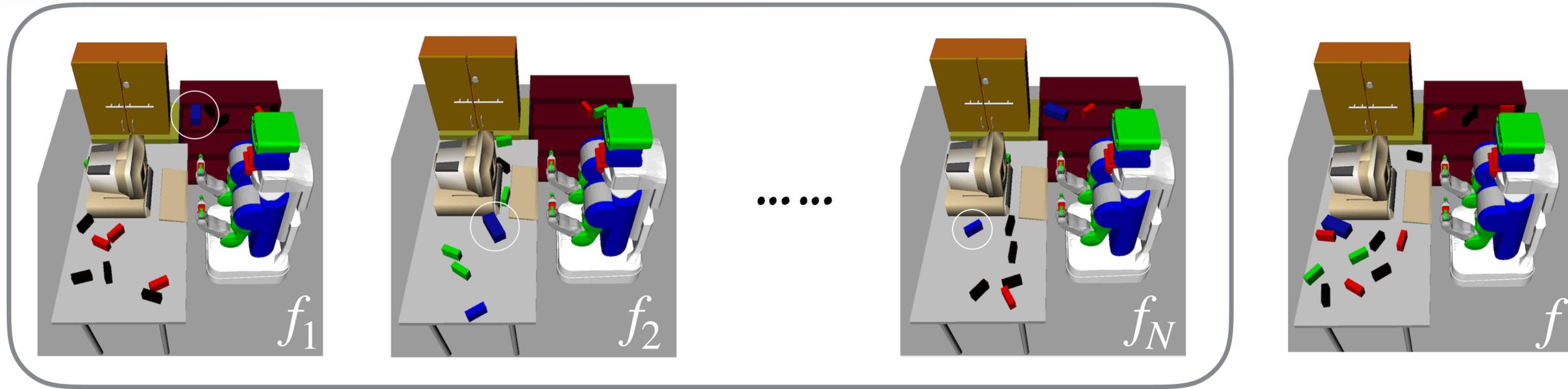
- meta-training functions come from the same prior
- enough number of meta-training functions $N \gtrsim T + 20$

Given T observations on the test function f , with high probability,

$$\text{simple regret } R_T \lesssim \left(o\left(\sqrt{\frac{1}{N-T}}\right) + C \right) \left(\sqrt{o\left(\frac{\log T}{T}\right) + \sigma^2} \right) \rightarrow C\sigma$$

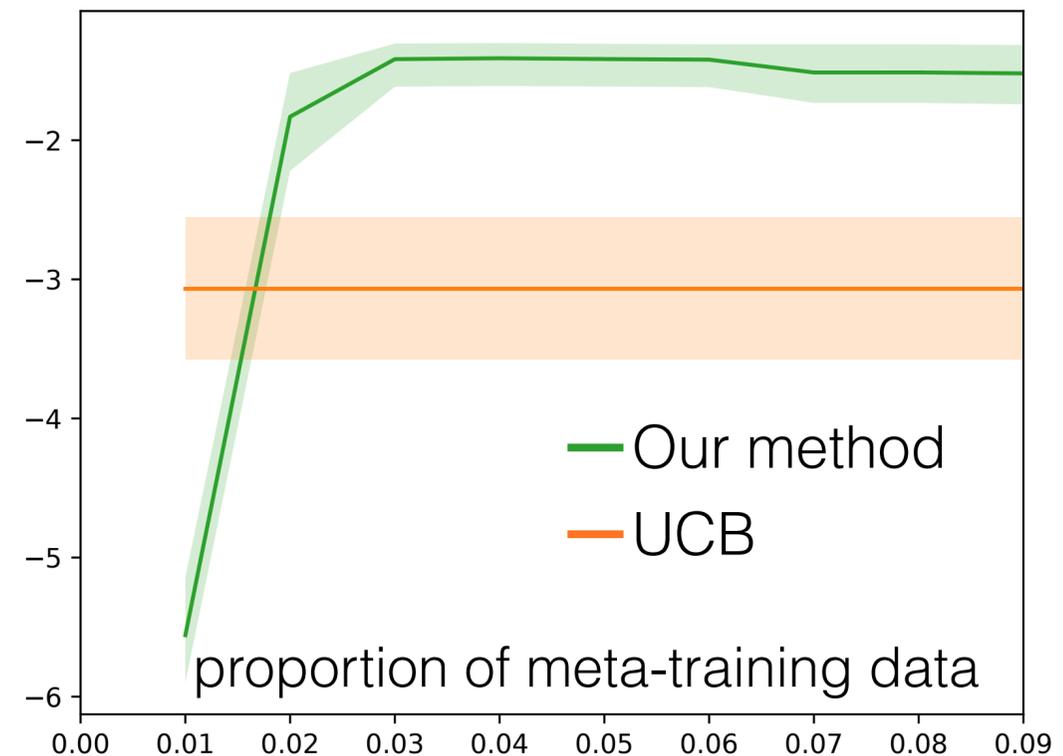
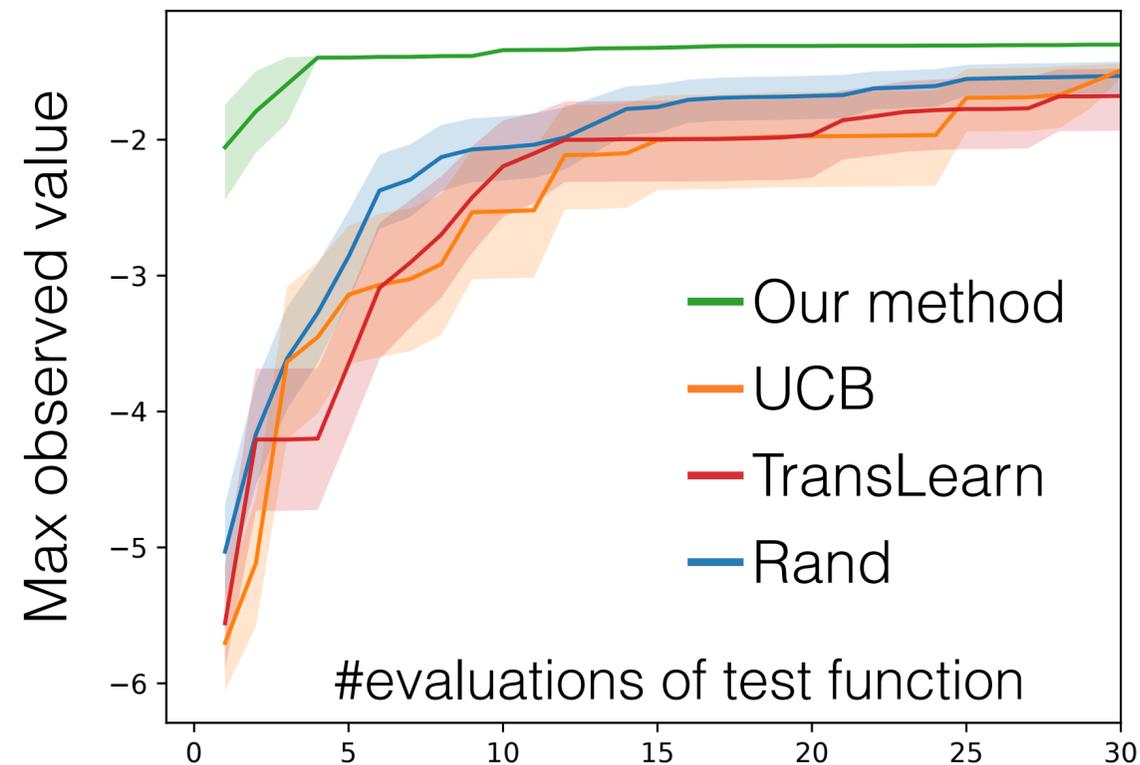
constant ≈ 10 linear kernel observation noise

Empirical results on block picking and placing



meta-training data $N = 1500$

test function



Regret bounds for meta Bayesian optimization with an **unknown** Gaussian process prior

Poster #22



More results on:

- estimation details for discrete and continuous input spaces
- regret bounds for compact input space in R^d
- regret bounds for *probability of improvement* in the meta learning setting
- empirical results on robotics tasks

https://ziw.mit.edu/meta_bo