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

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LEARNING & INTELLIGENT SYSTEMS

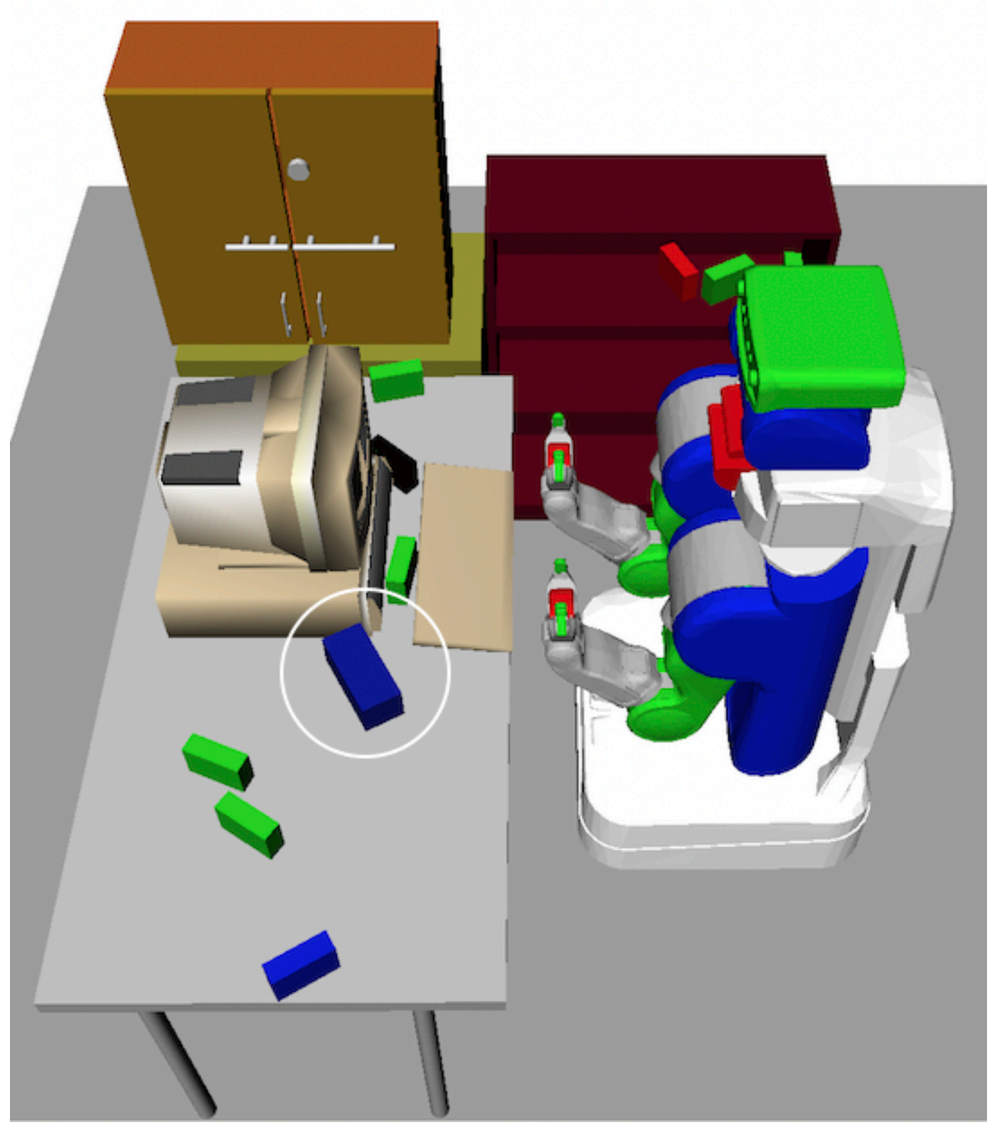
Poster #22

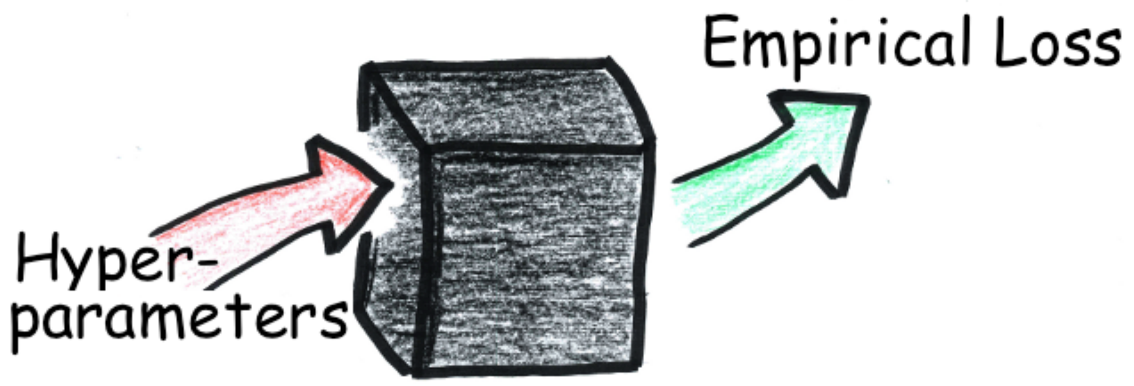
Bayesian optimization

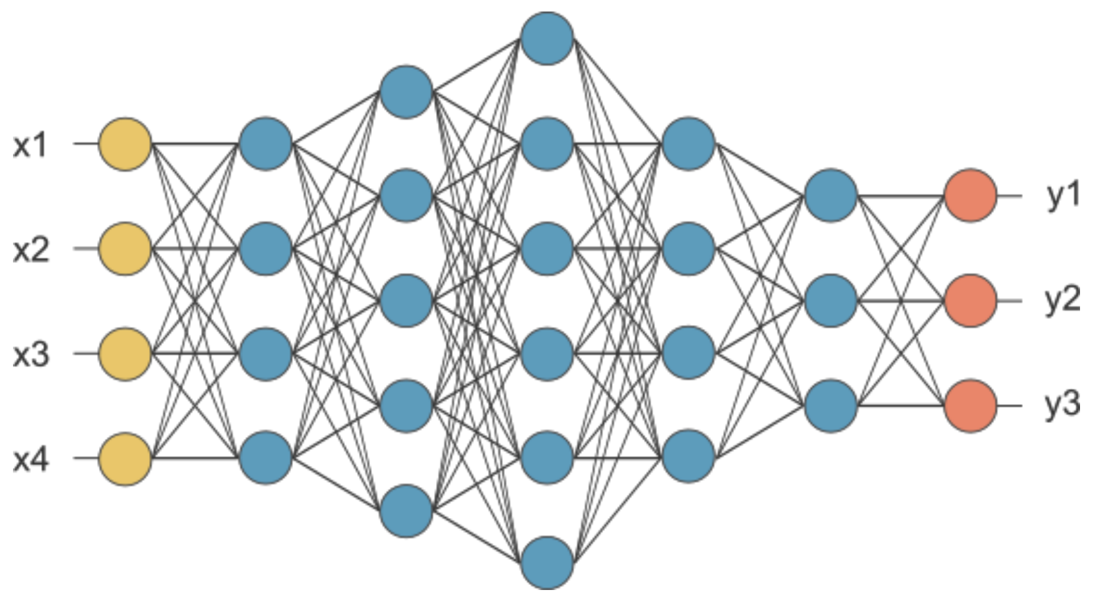
Goal: $$x^* = \underset{x \in \mathfrak{X}}{\operatorname{argmax}}\, f(x)$$

Challenges:

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







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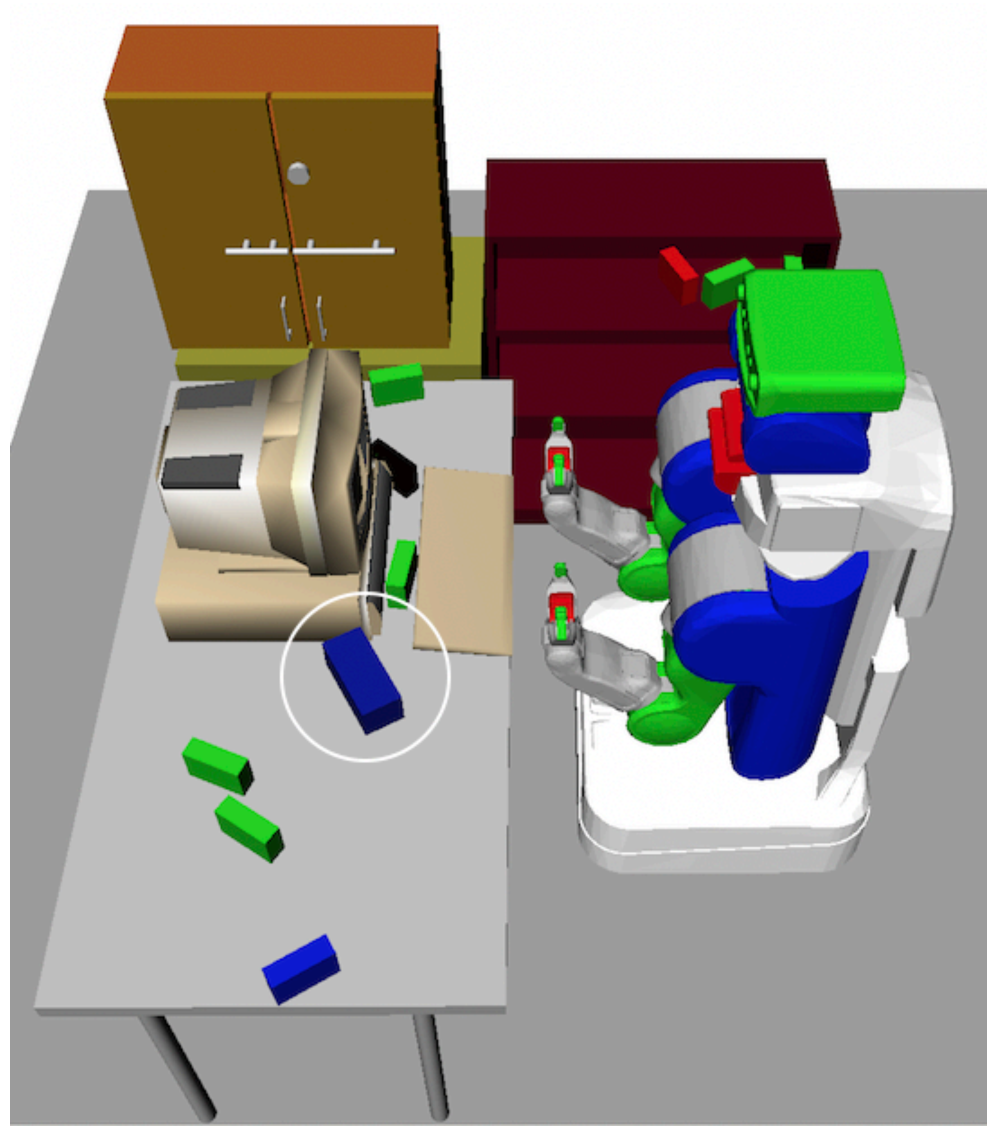

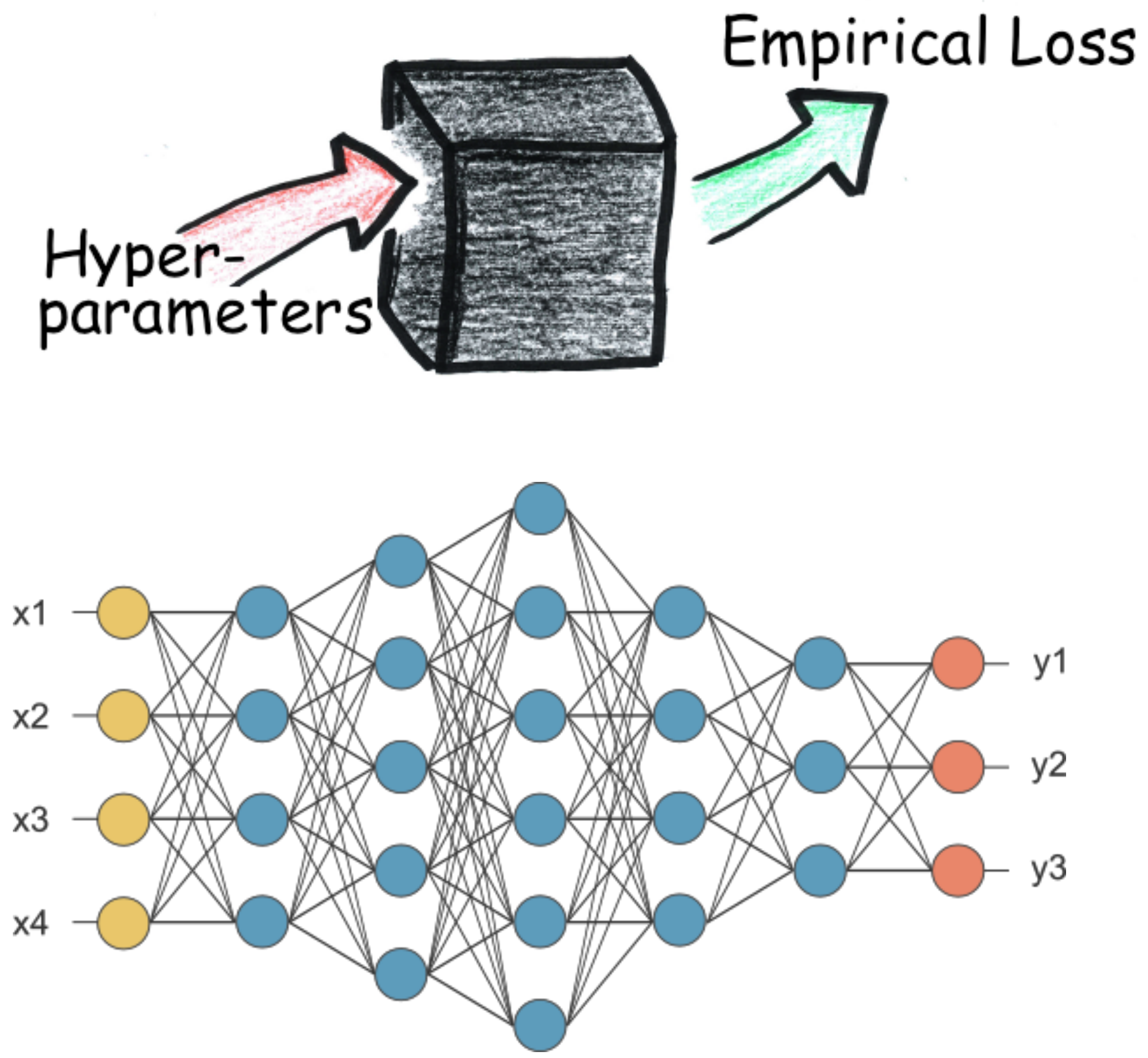

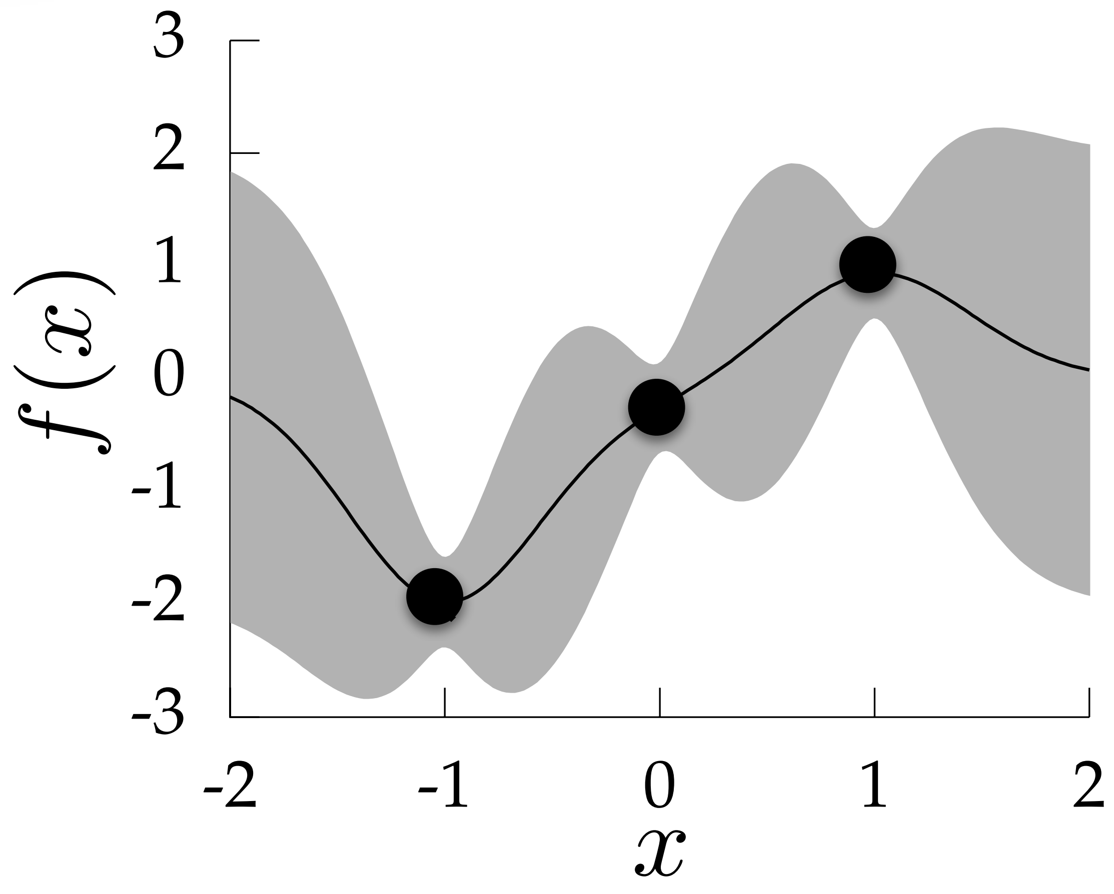

Assume a GP prior $f \sim GP(\mu, k)$

LOOP

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

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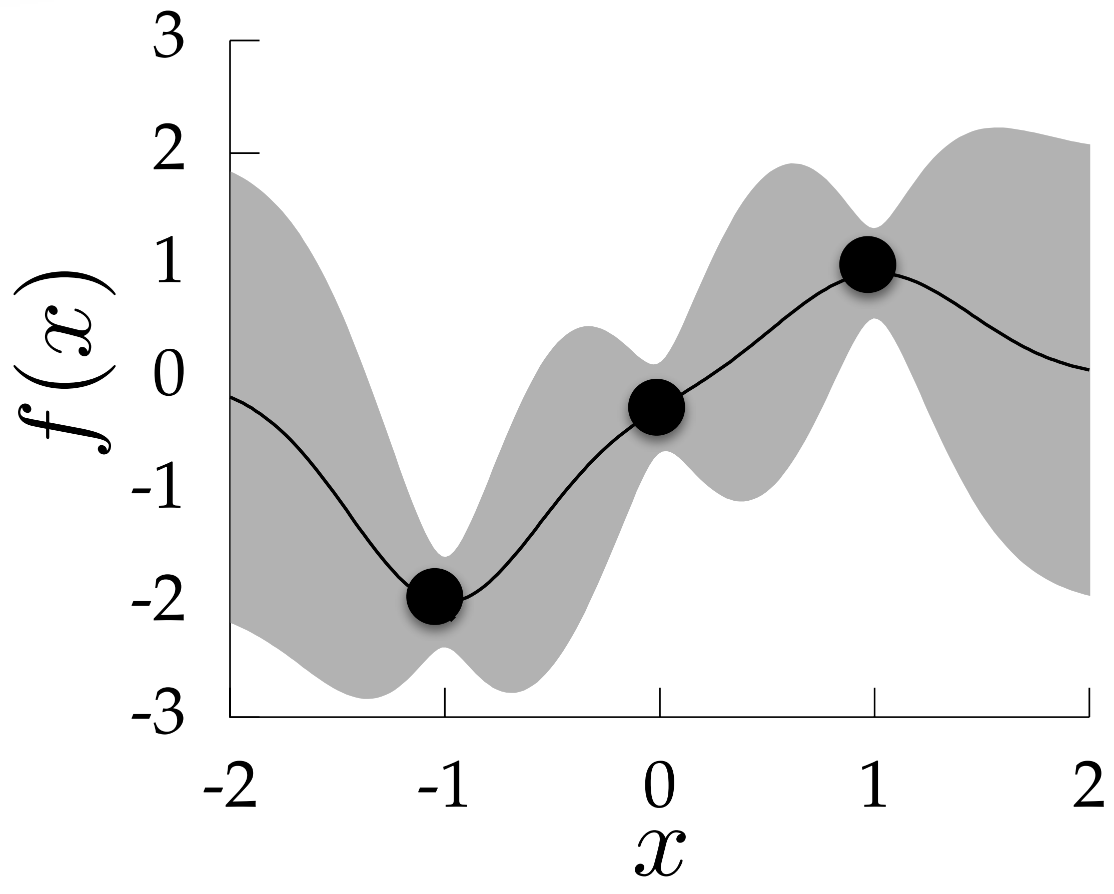

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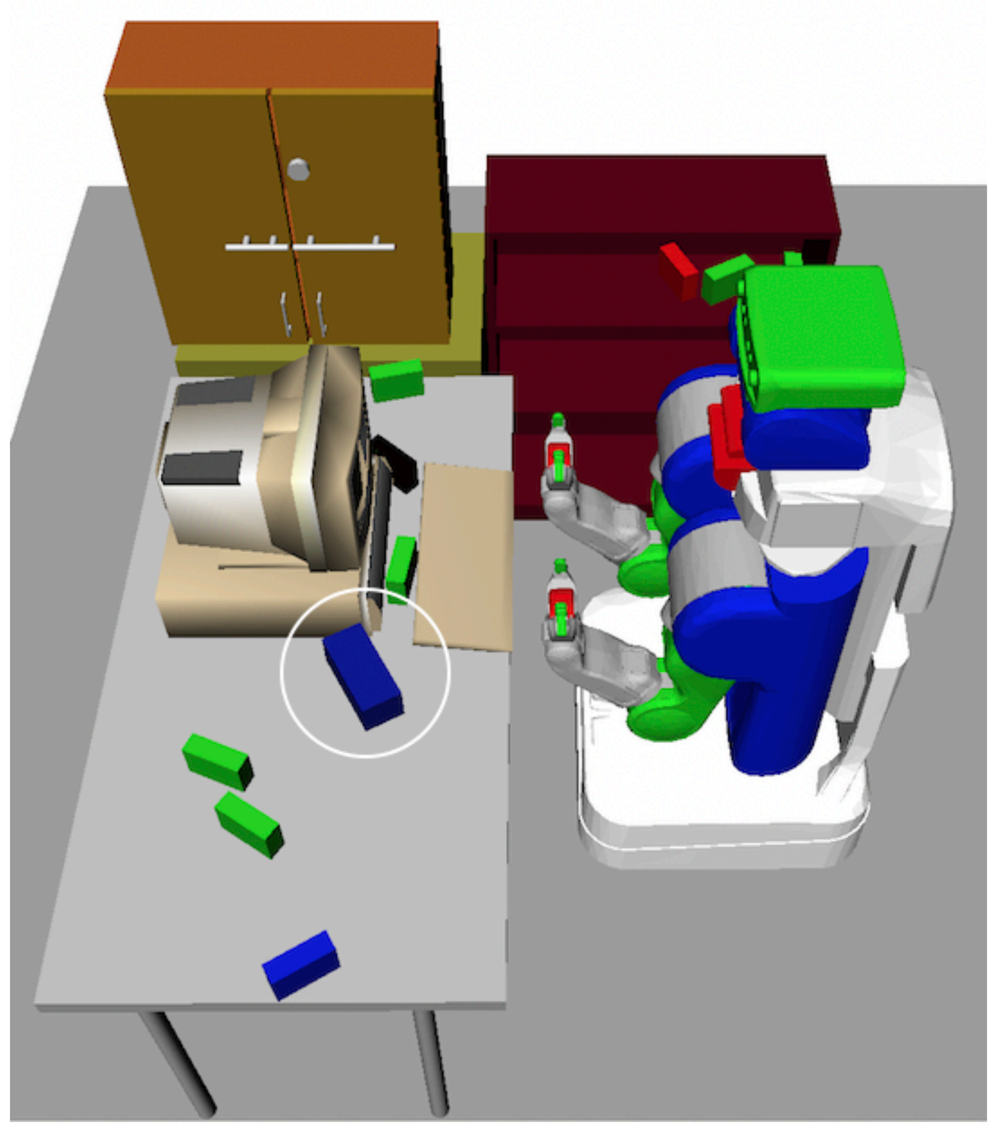

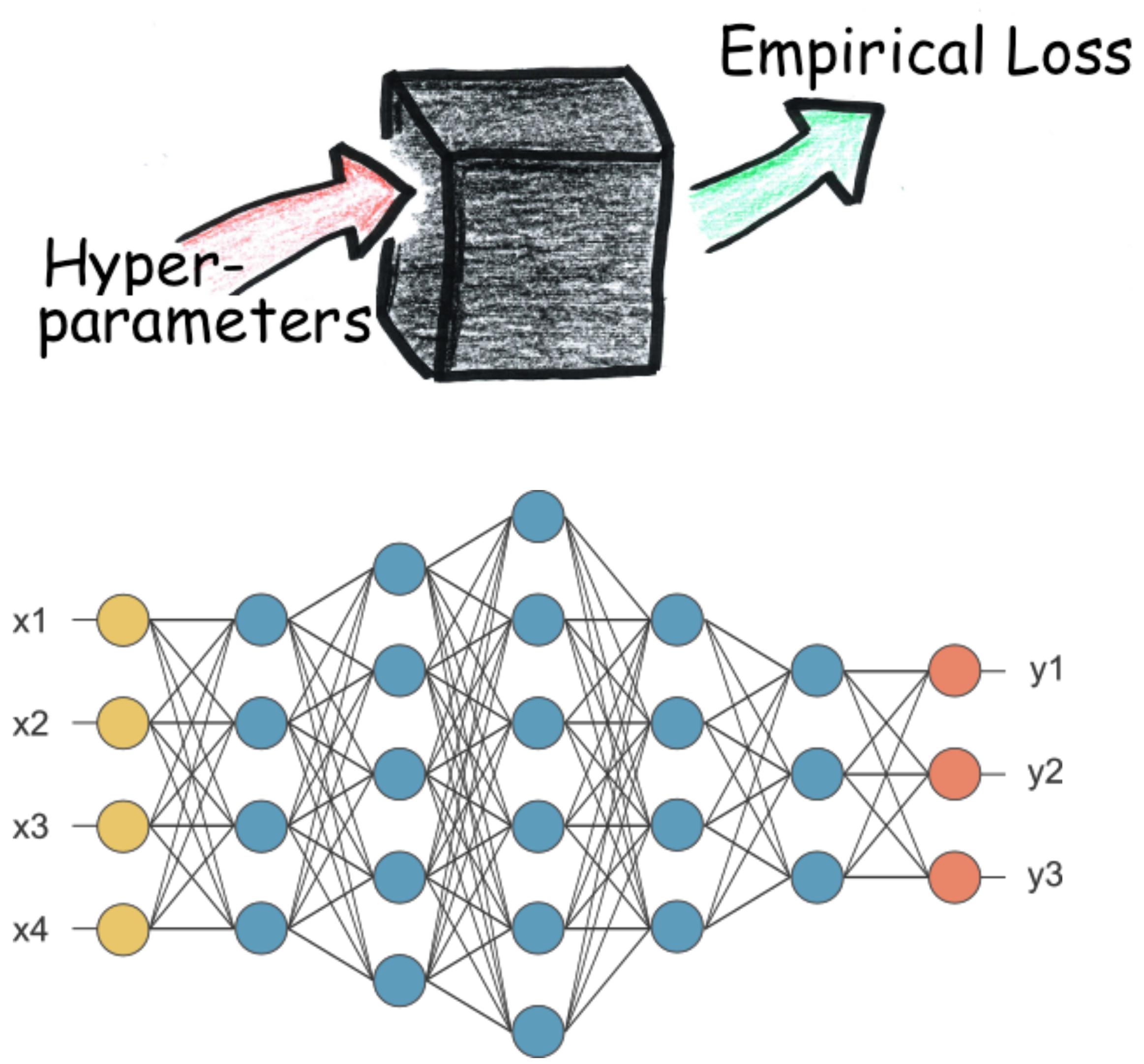

How to choose the prior?

Bayesian optimization

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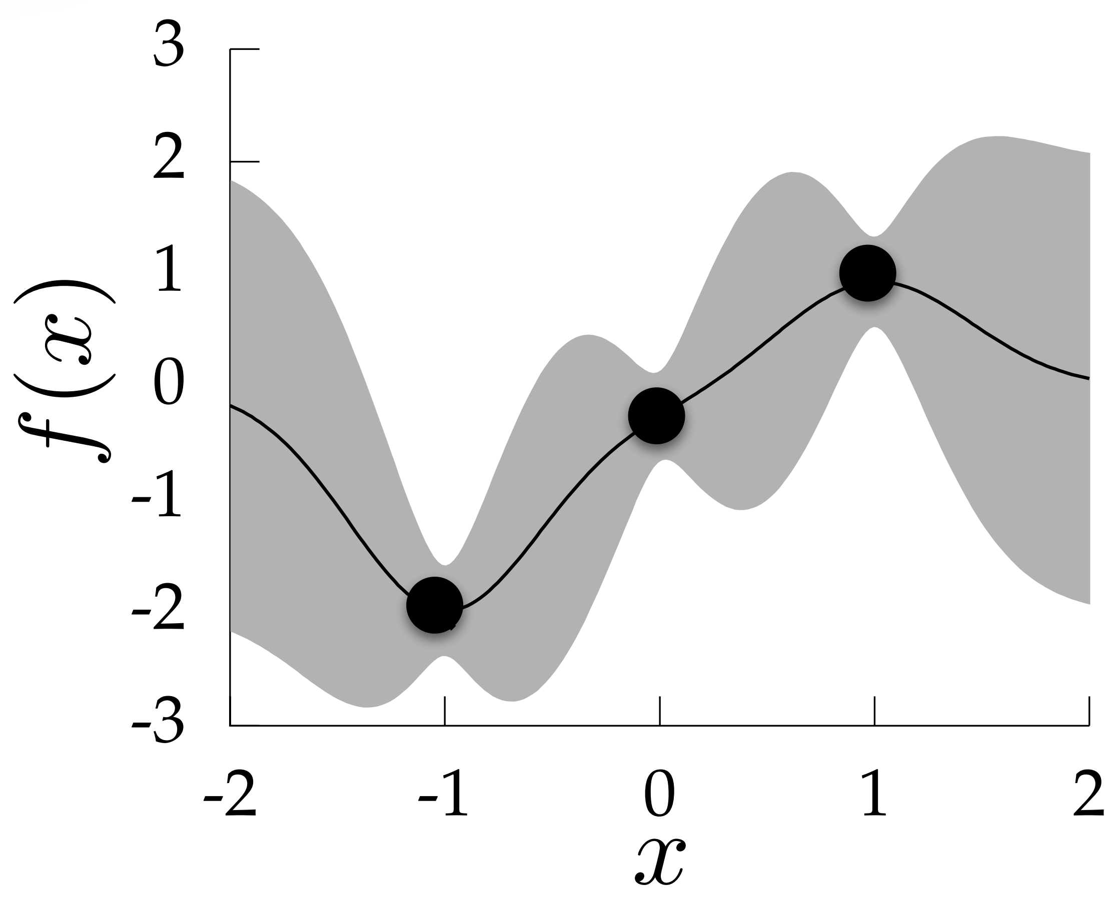

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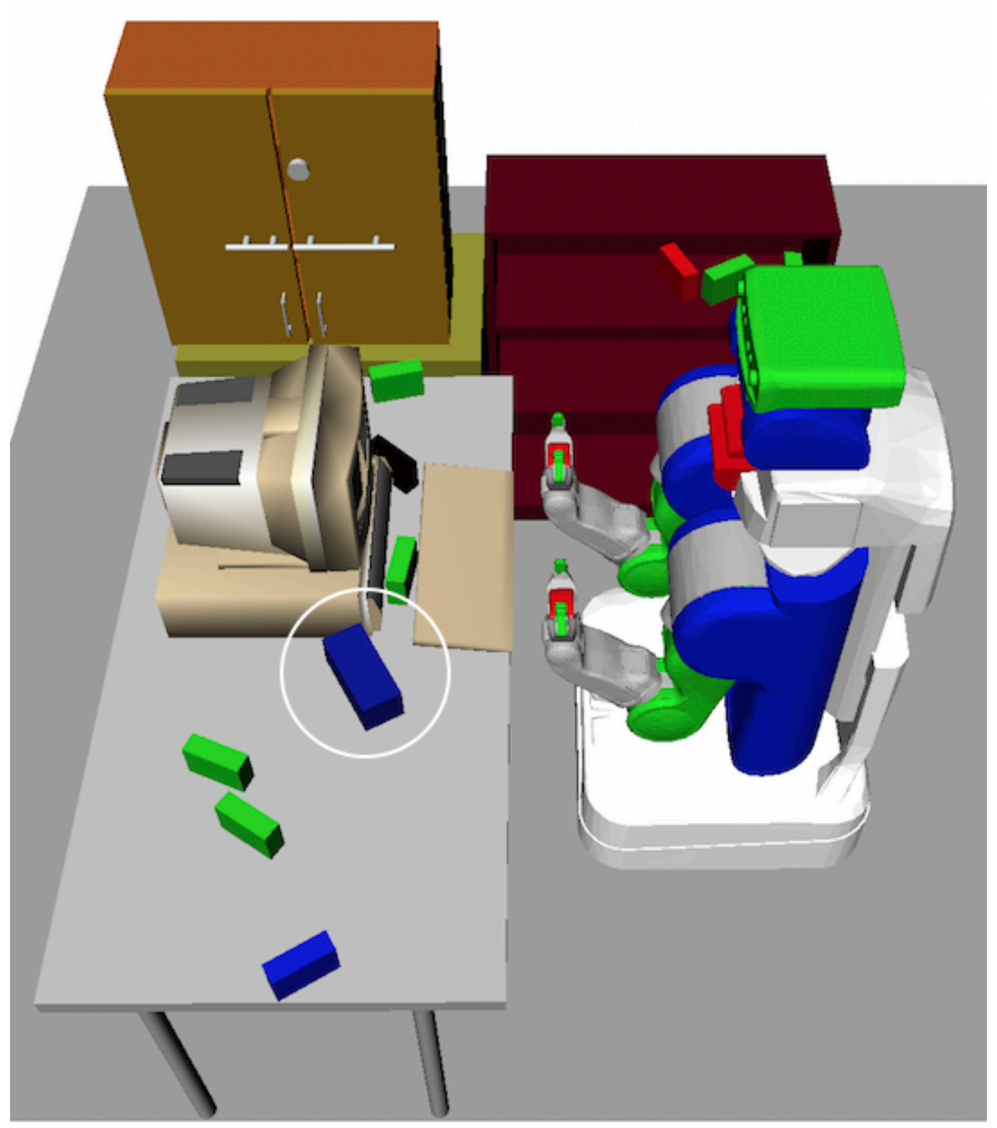
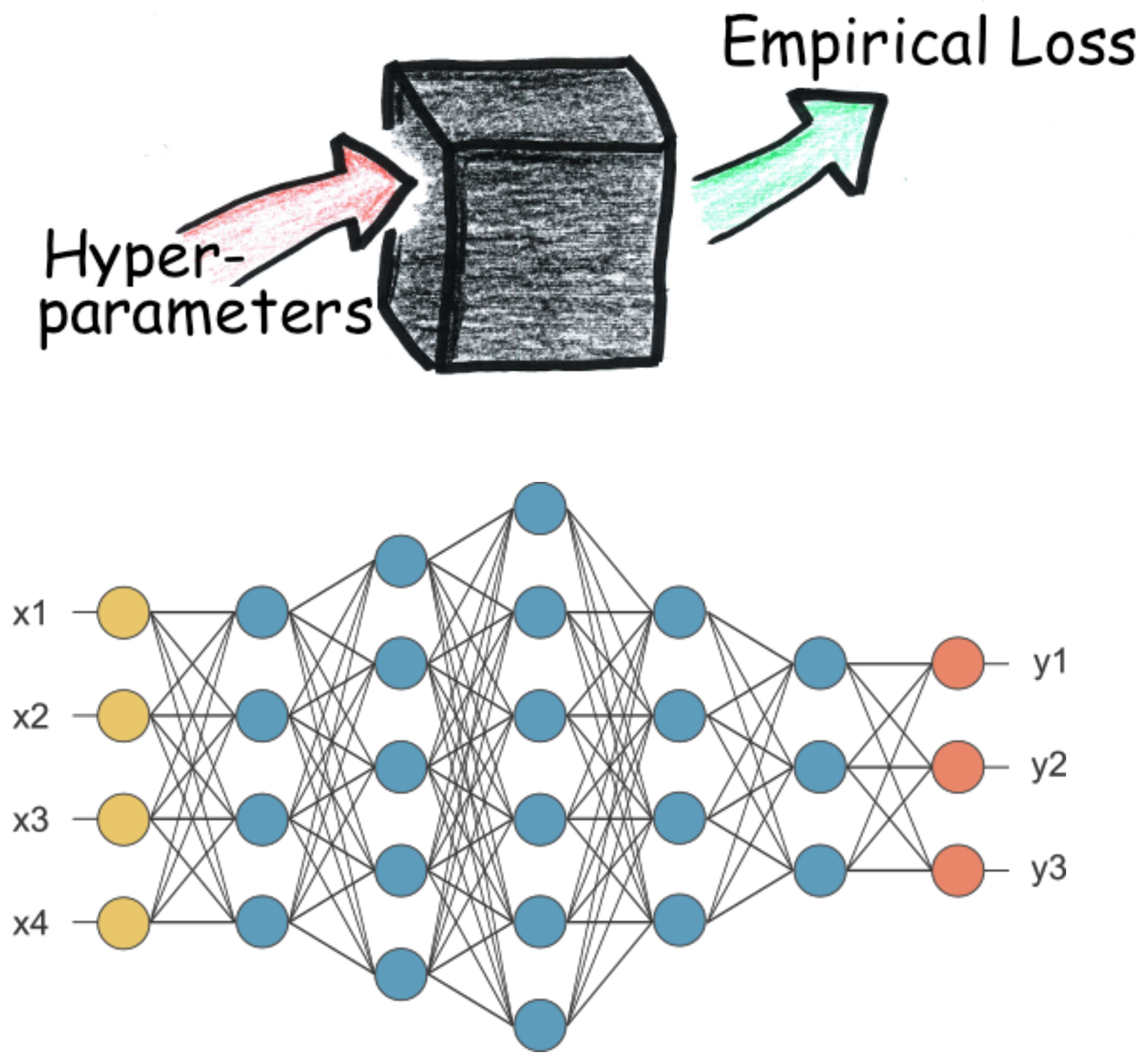
- *re-estimate the prior parameters*

  e.g. by maximizing marginal data likelihood every few iterations





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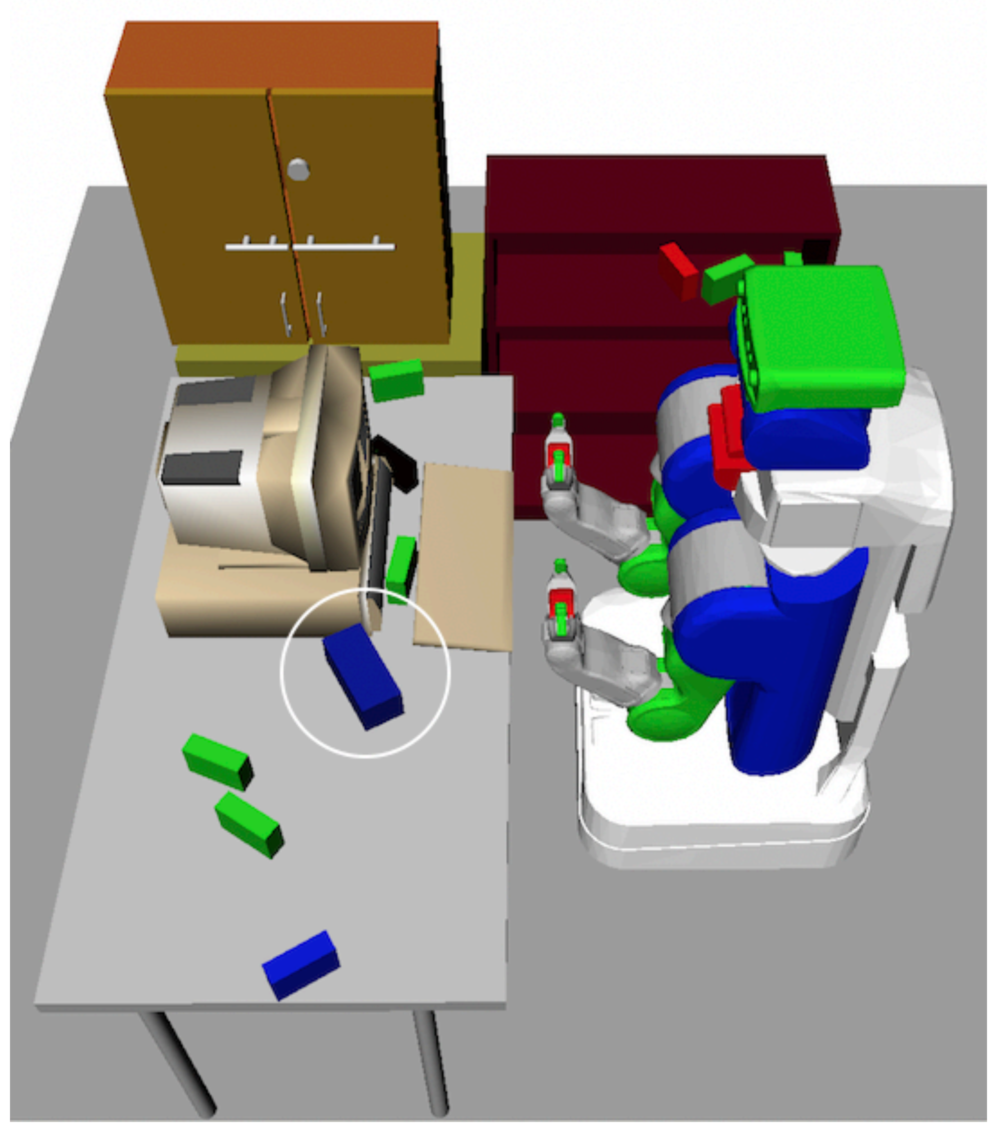

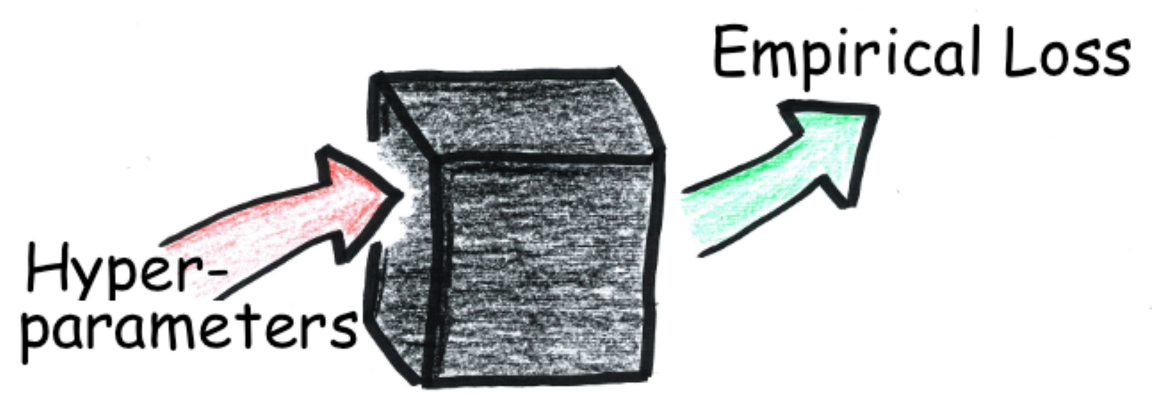

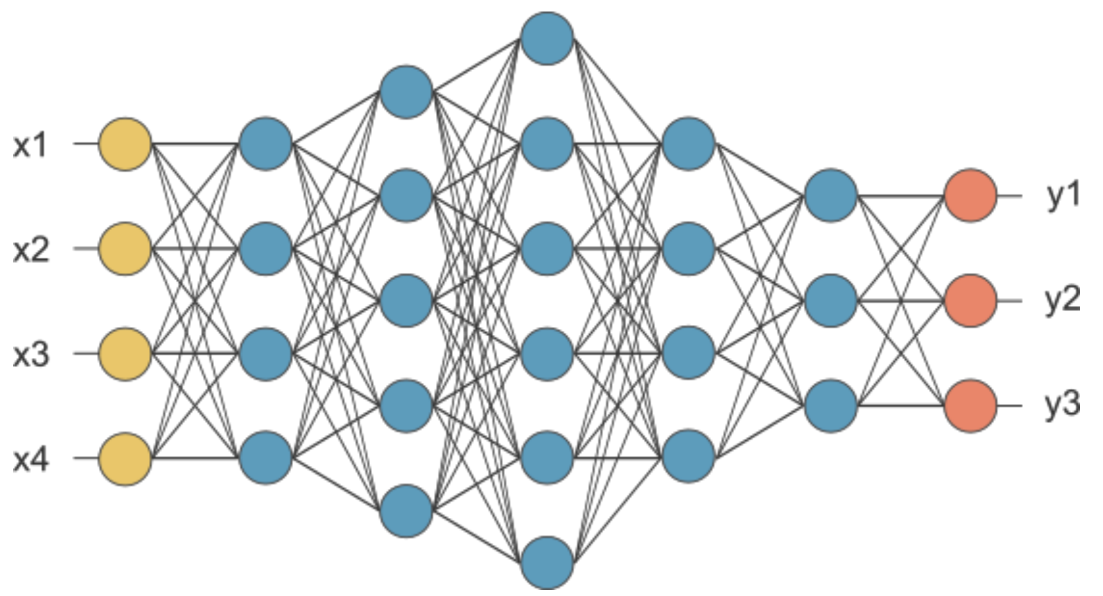

Which comes first?
Data or prior?

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Bayesian optimization

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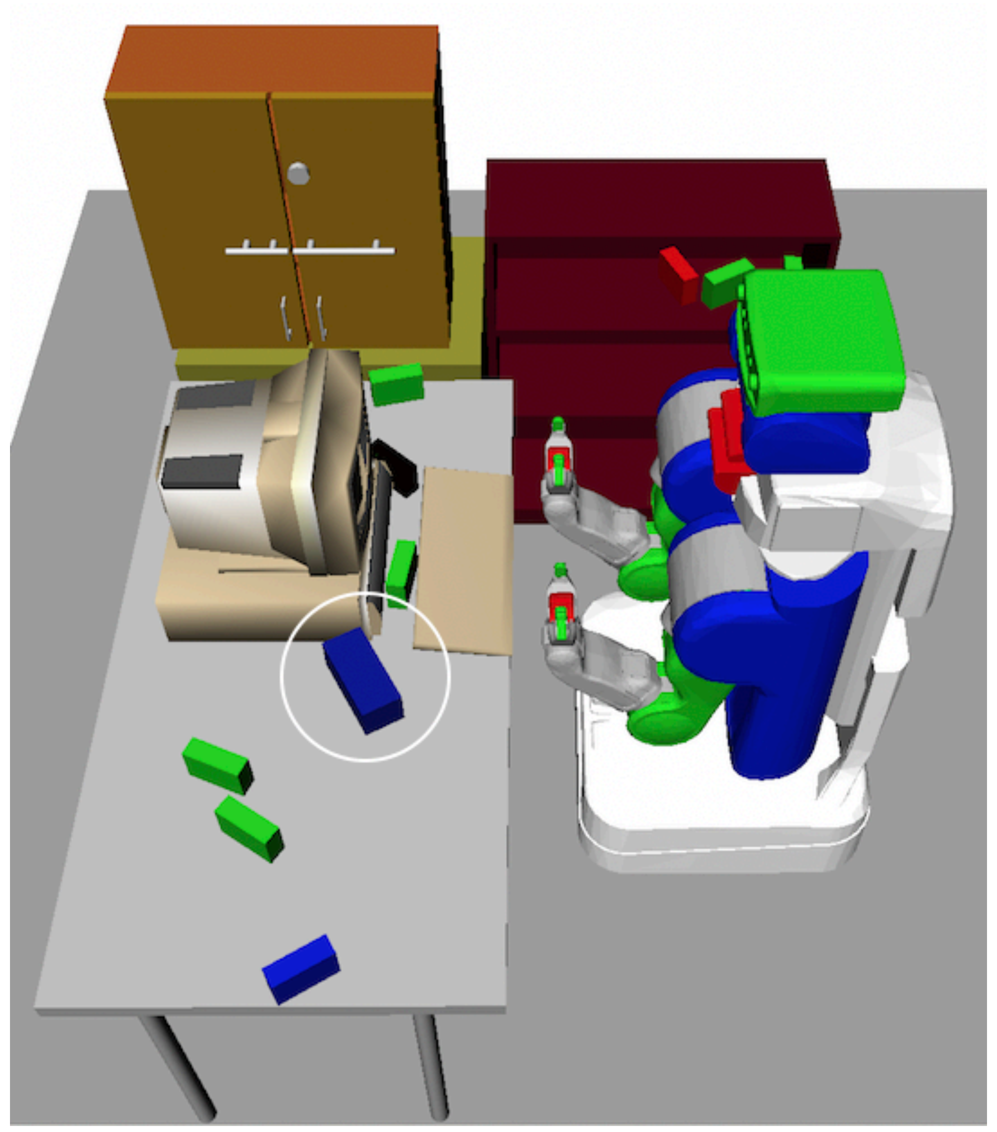

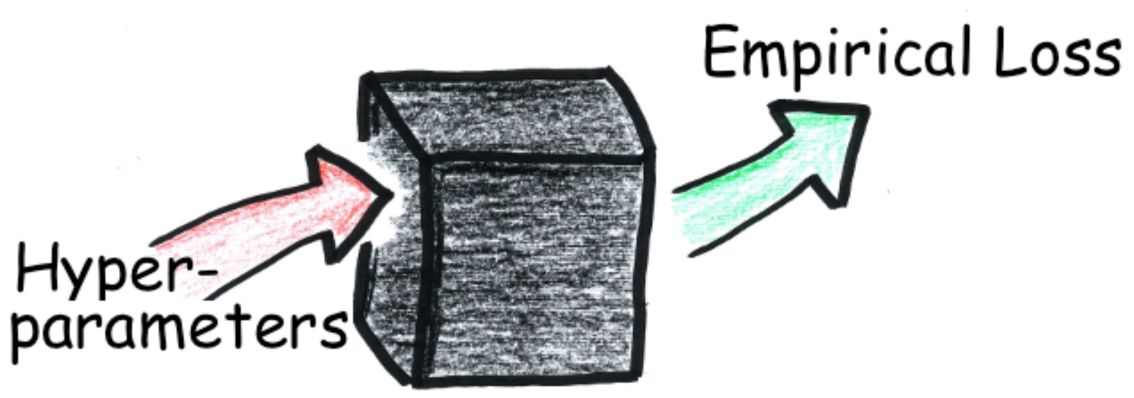

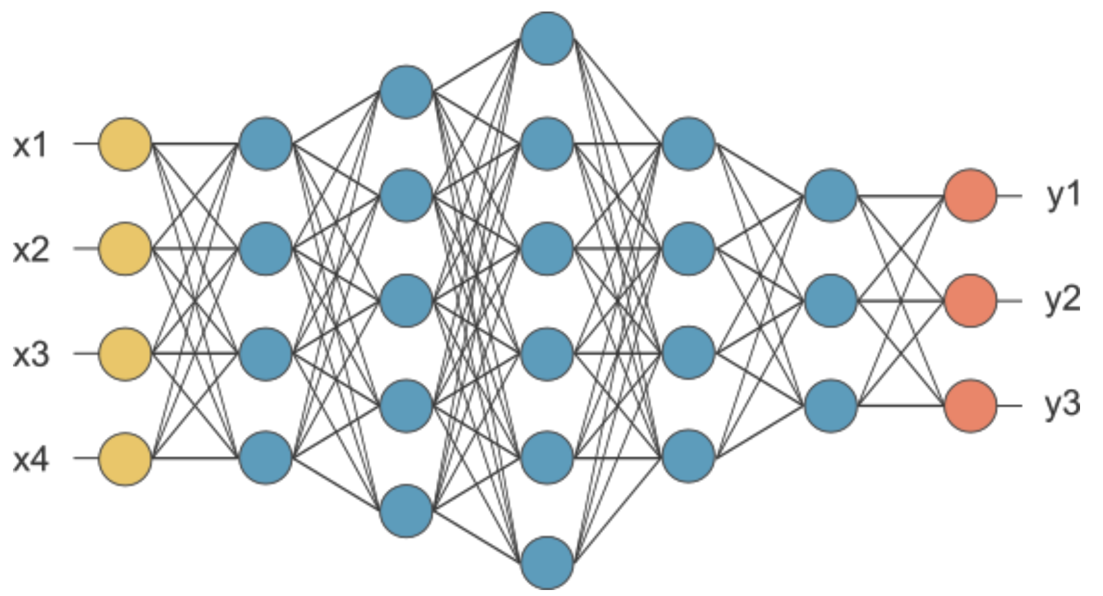

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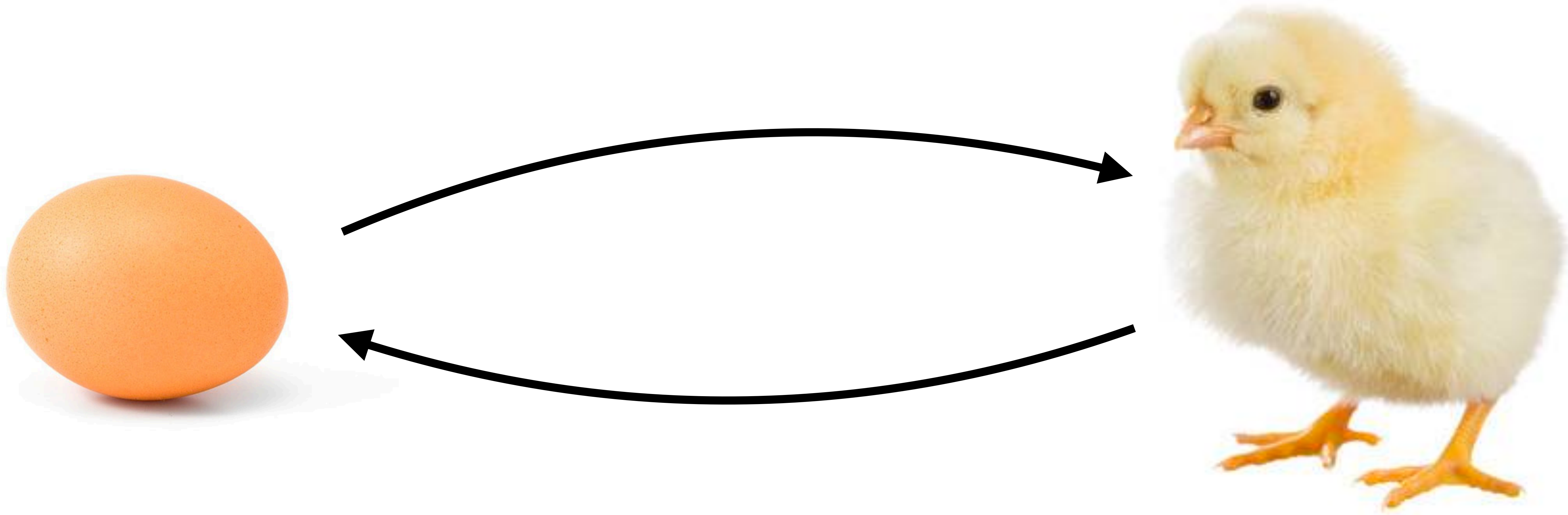
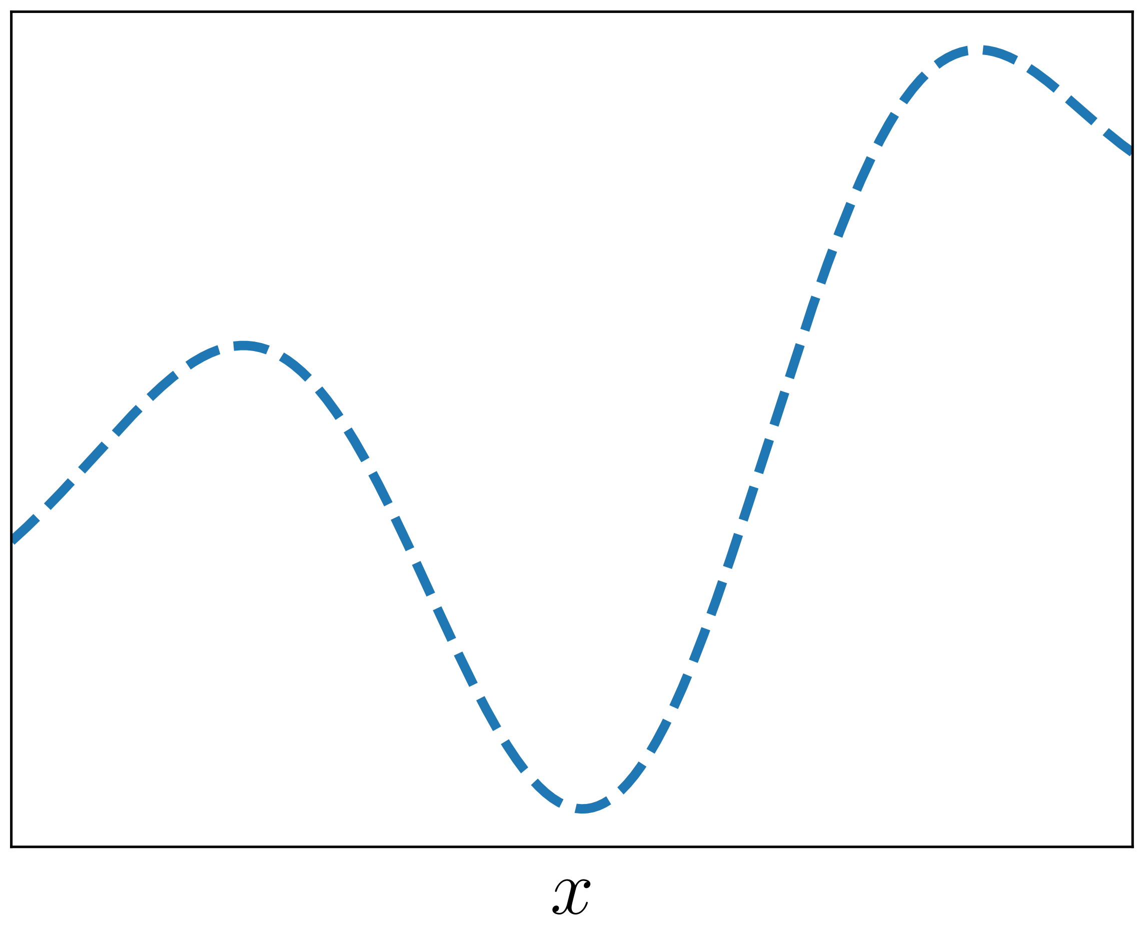
Hard to analyze.

Bayesian optimization with an unknown GP prior

prior model



data collected on f



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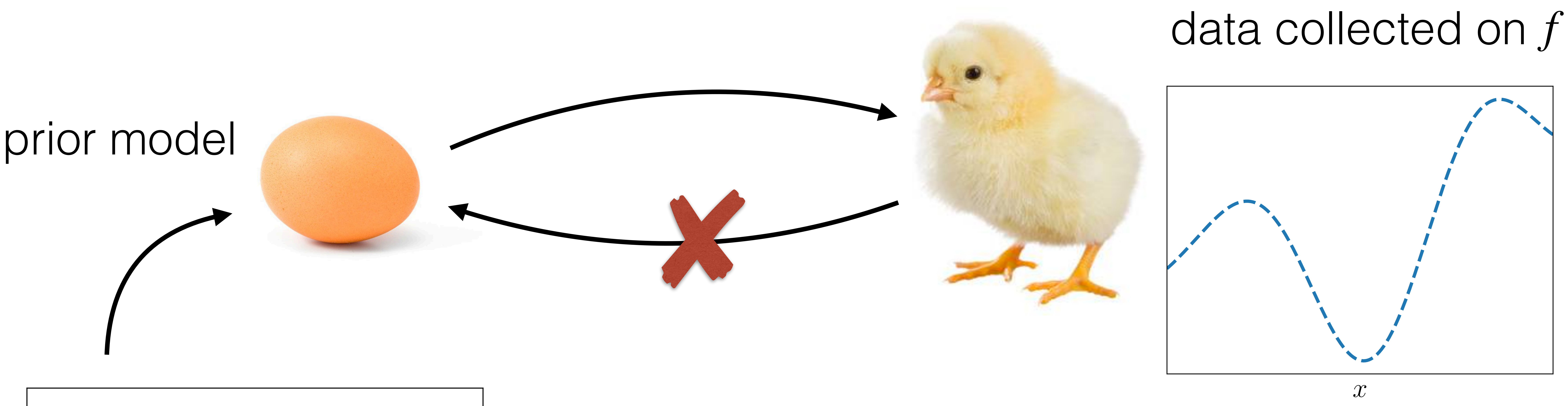
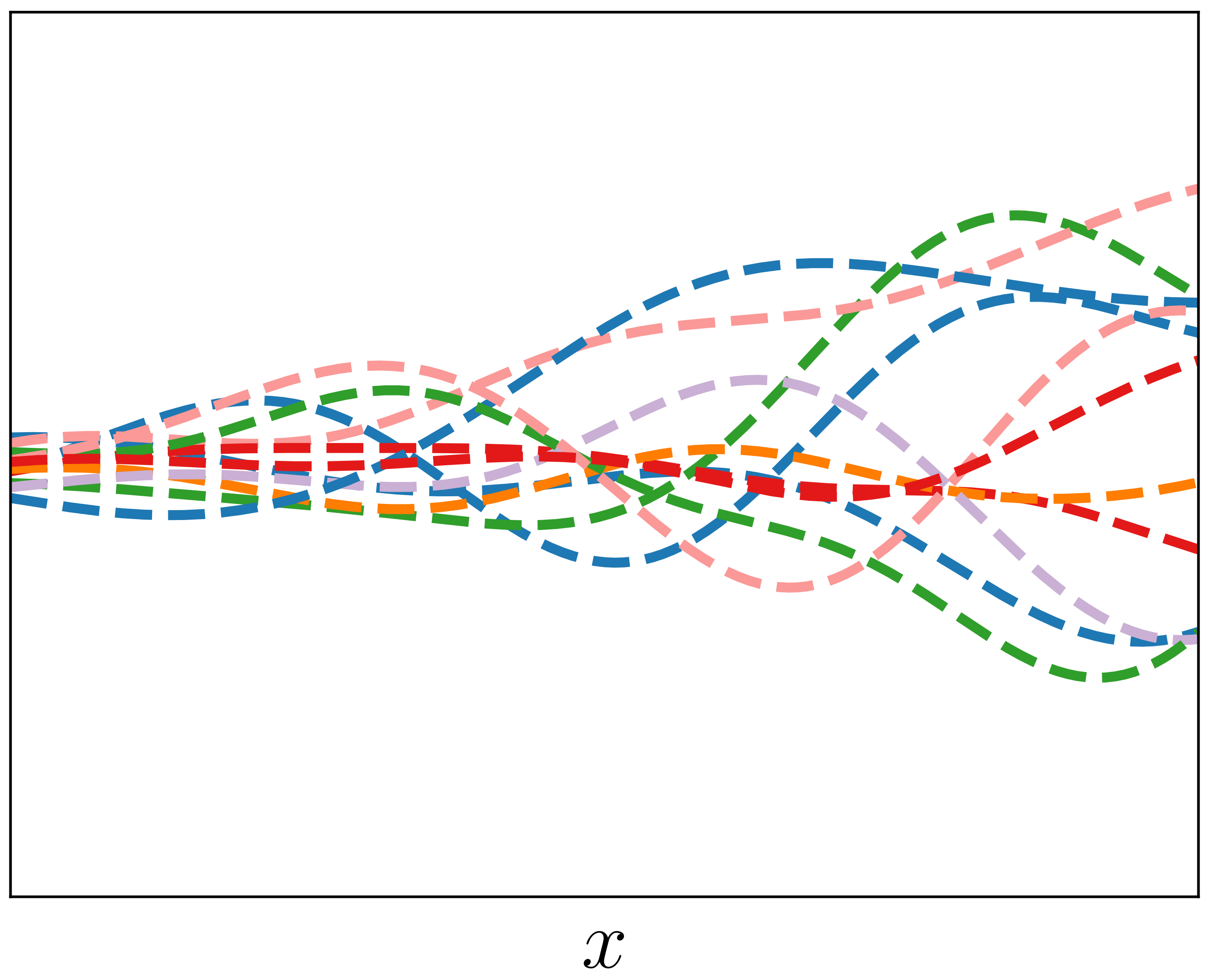


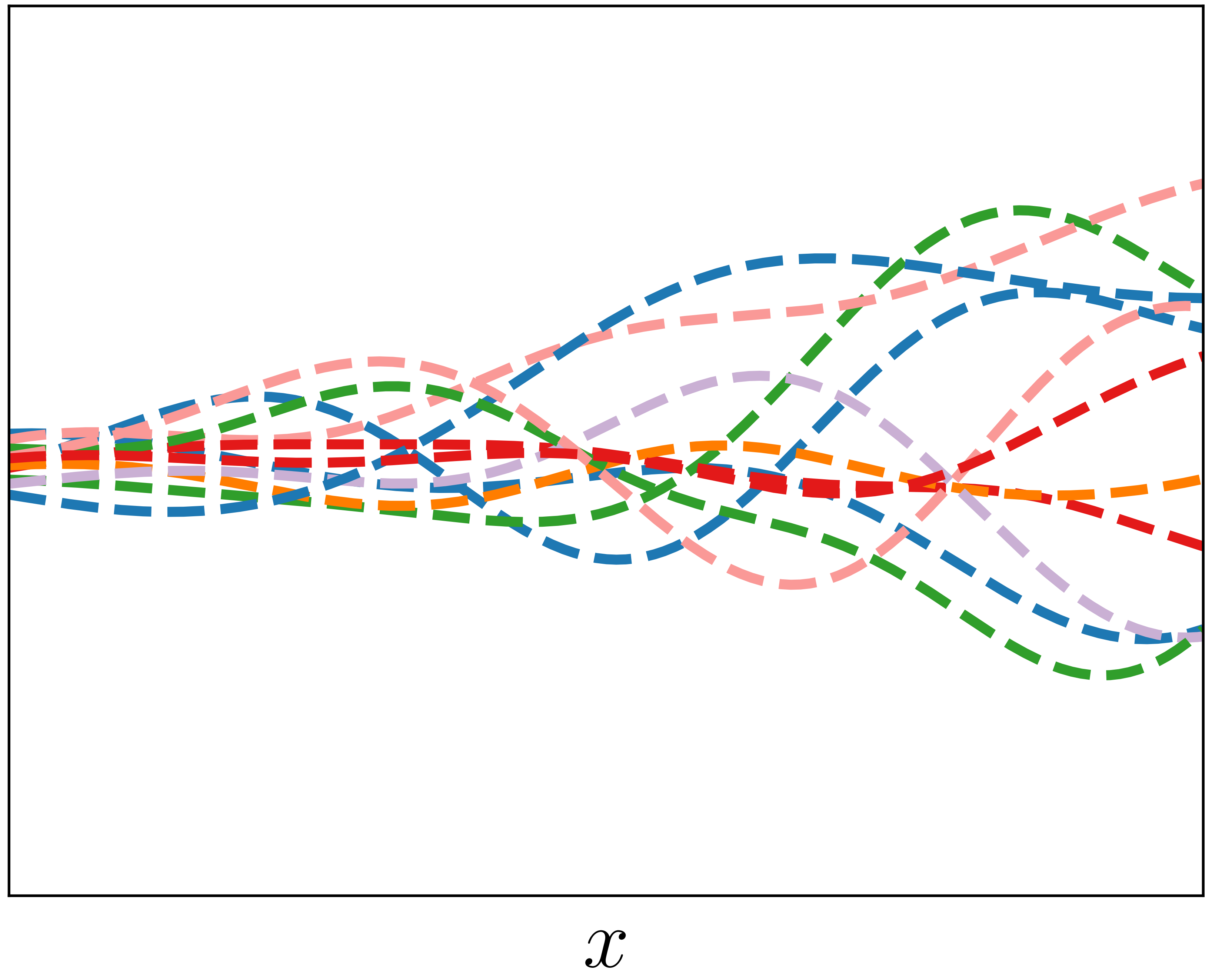


Our problem setup:

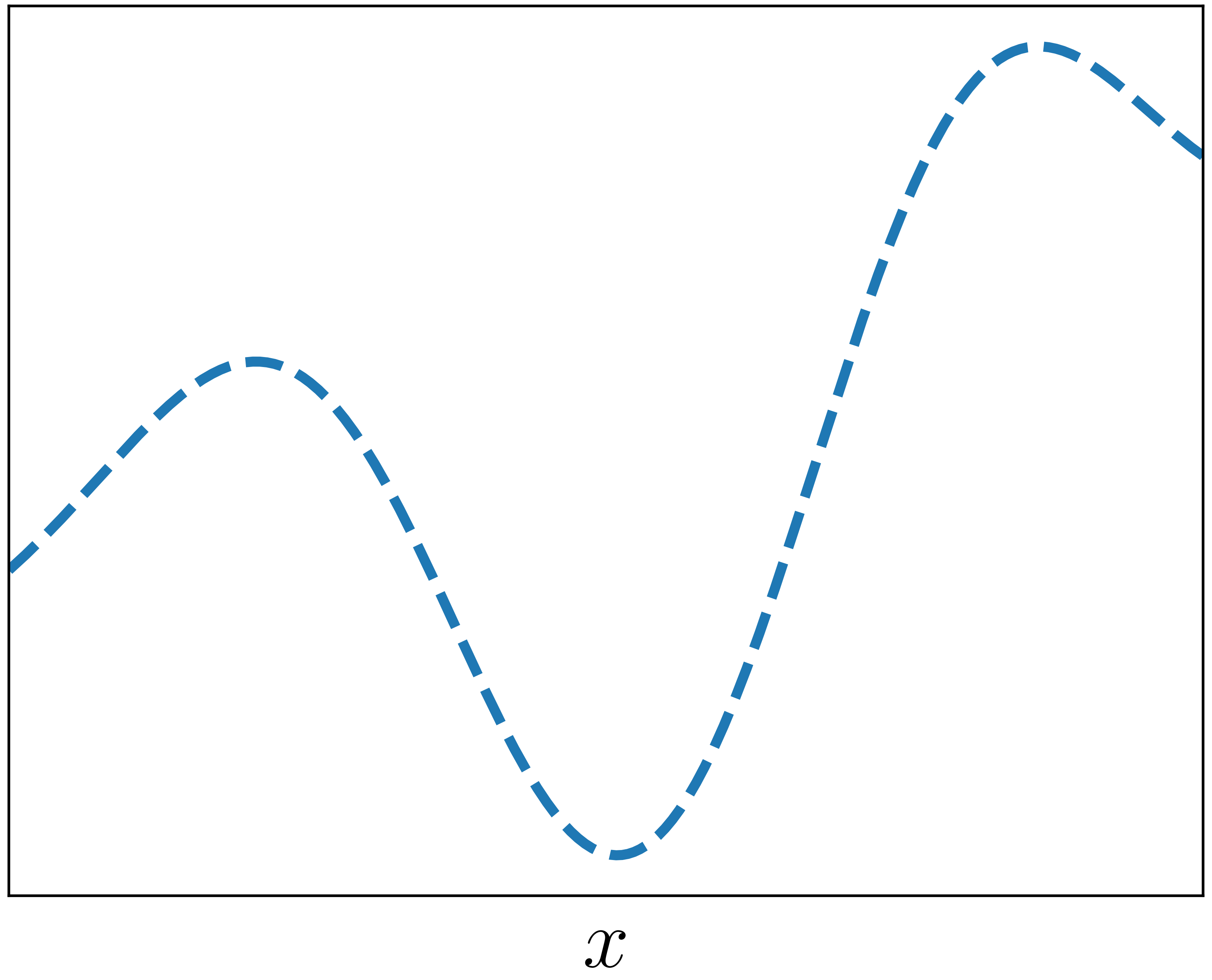
use meta training data to break the circular dependencies

Meta Bayesian optimization with an unknown GP prior

Offline phase

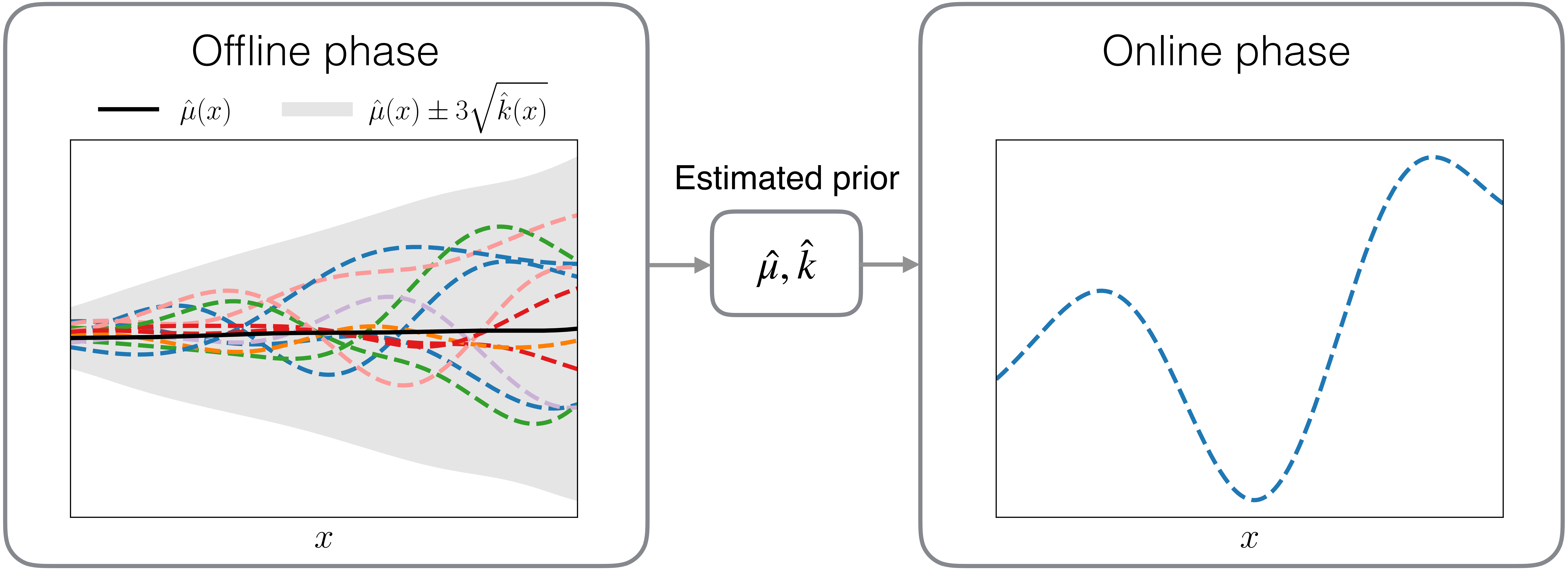


Online phase



Meta Bayesian optimization with an unknown GP prior

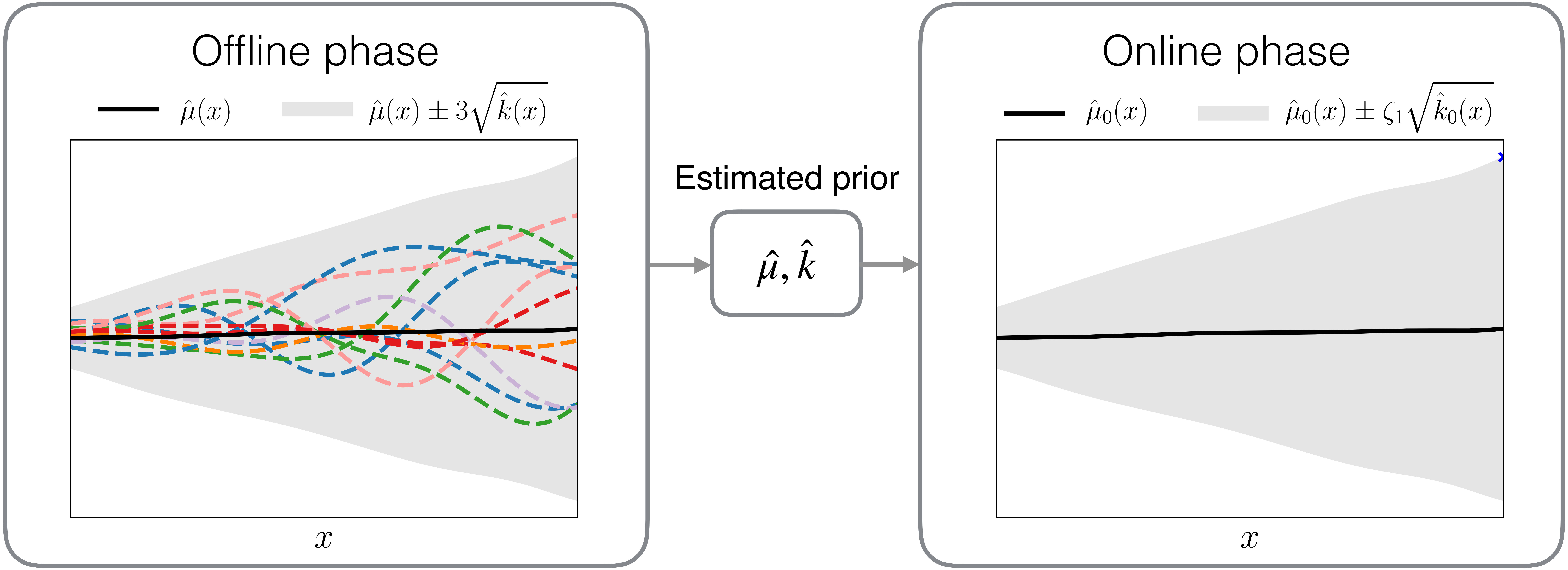
Estimate the GP prior from offline data
sampled from the same prior



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



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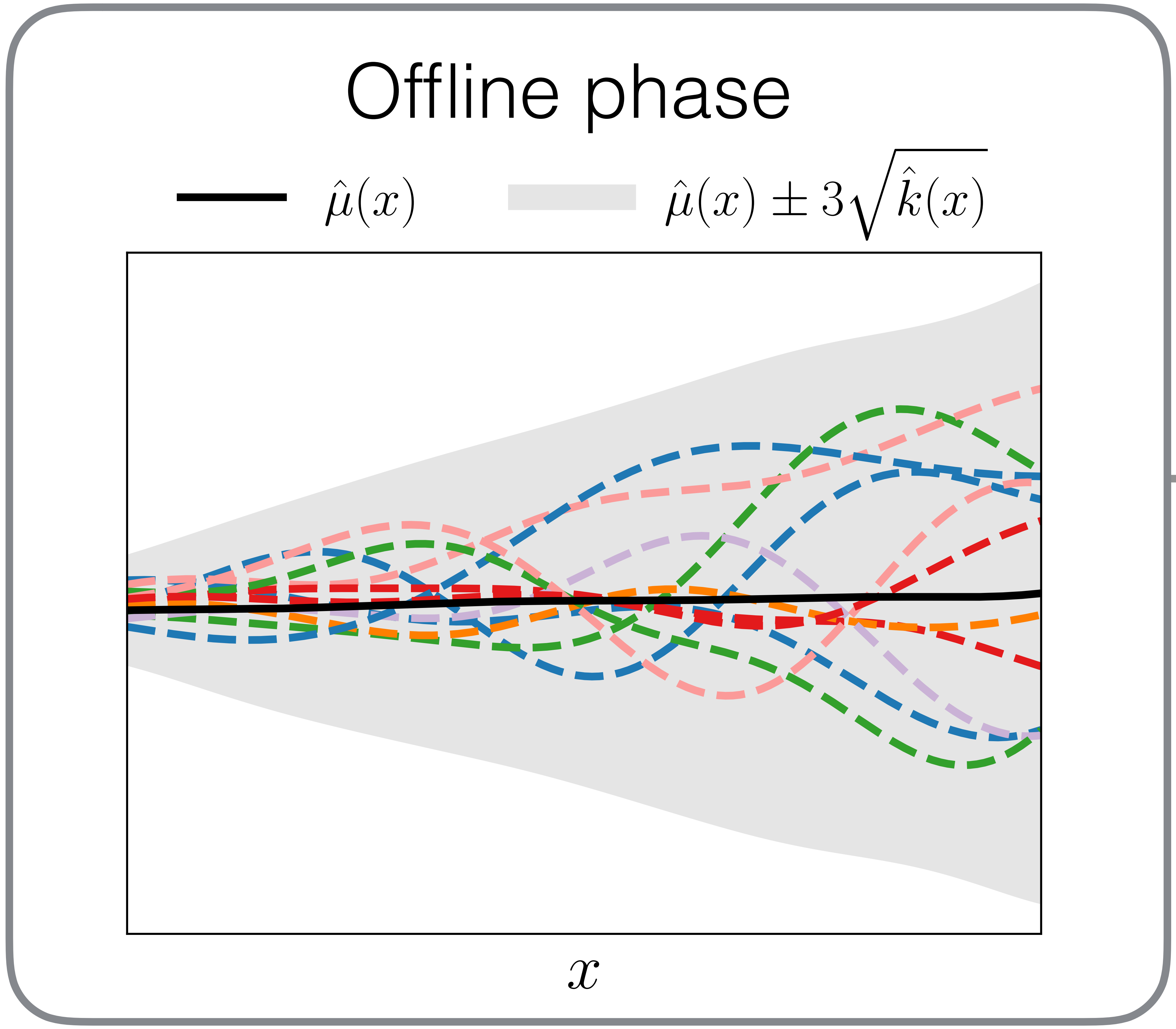
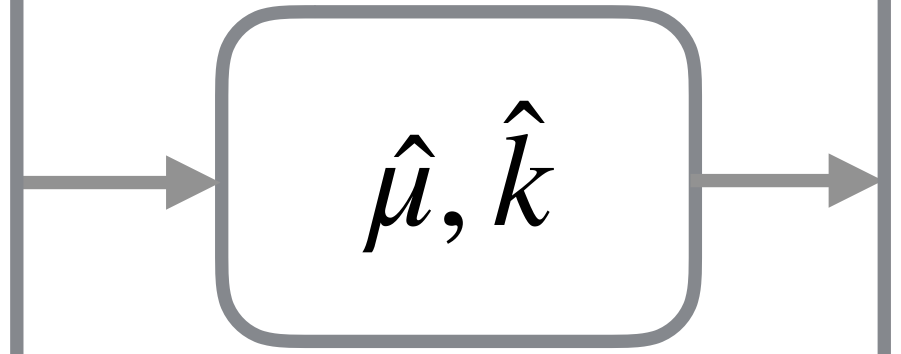
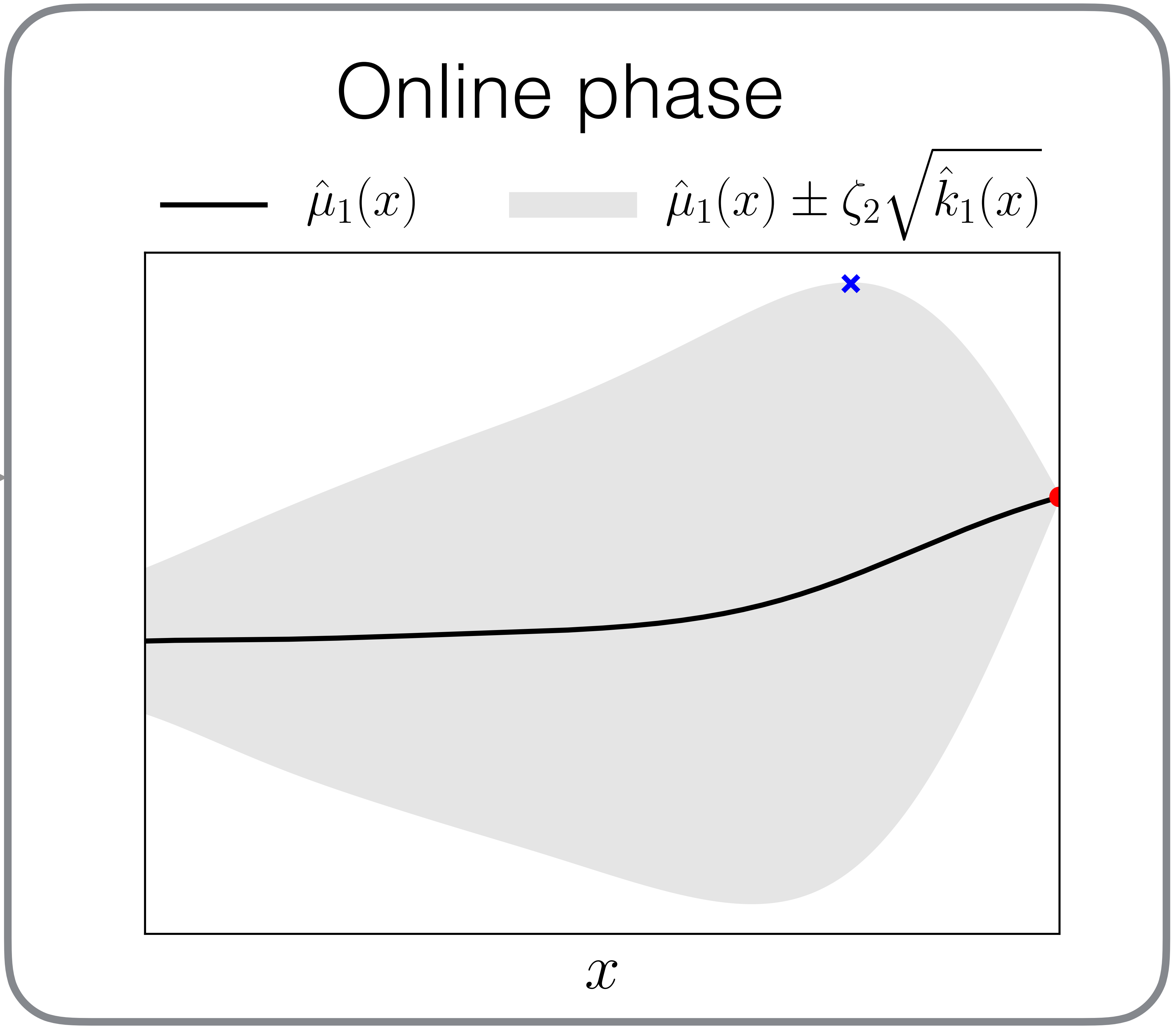


Estimated prior





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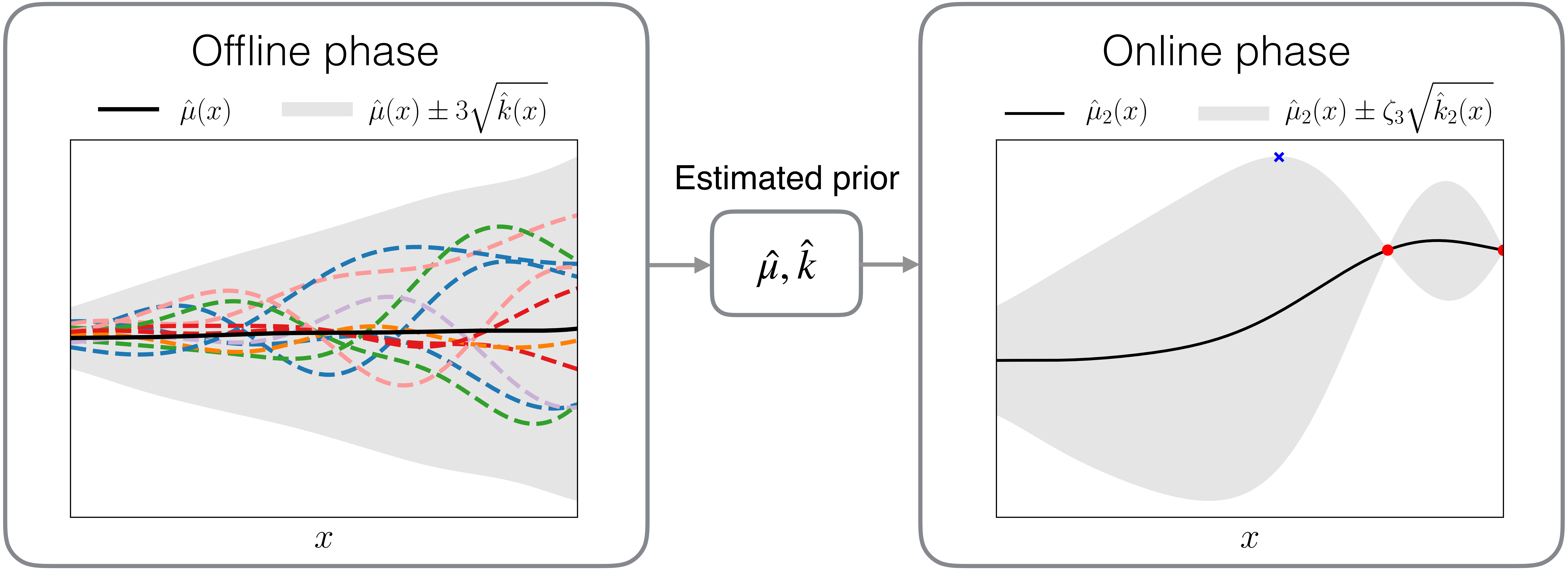

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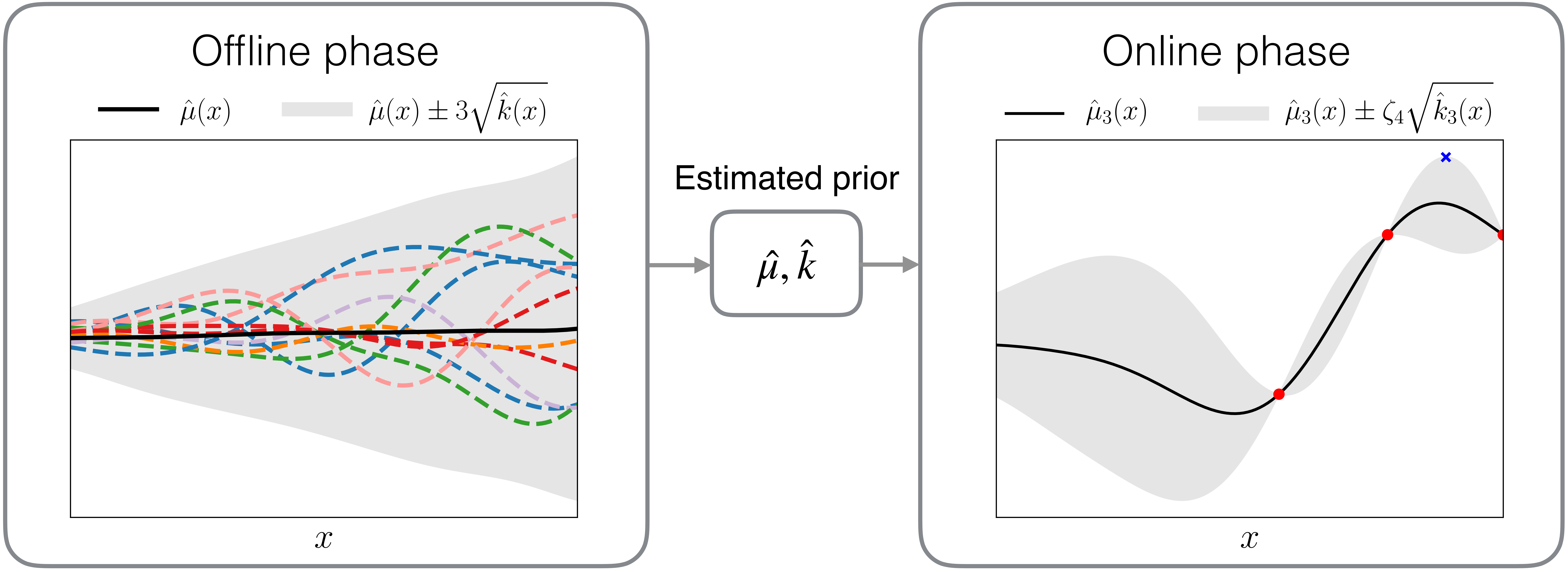

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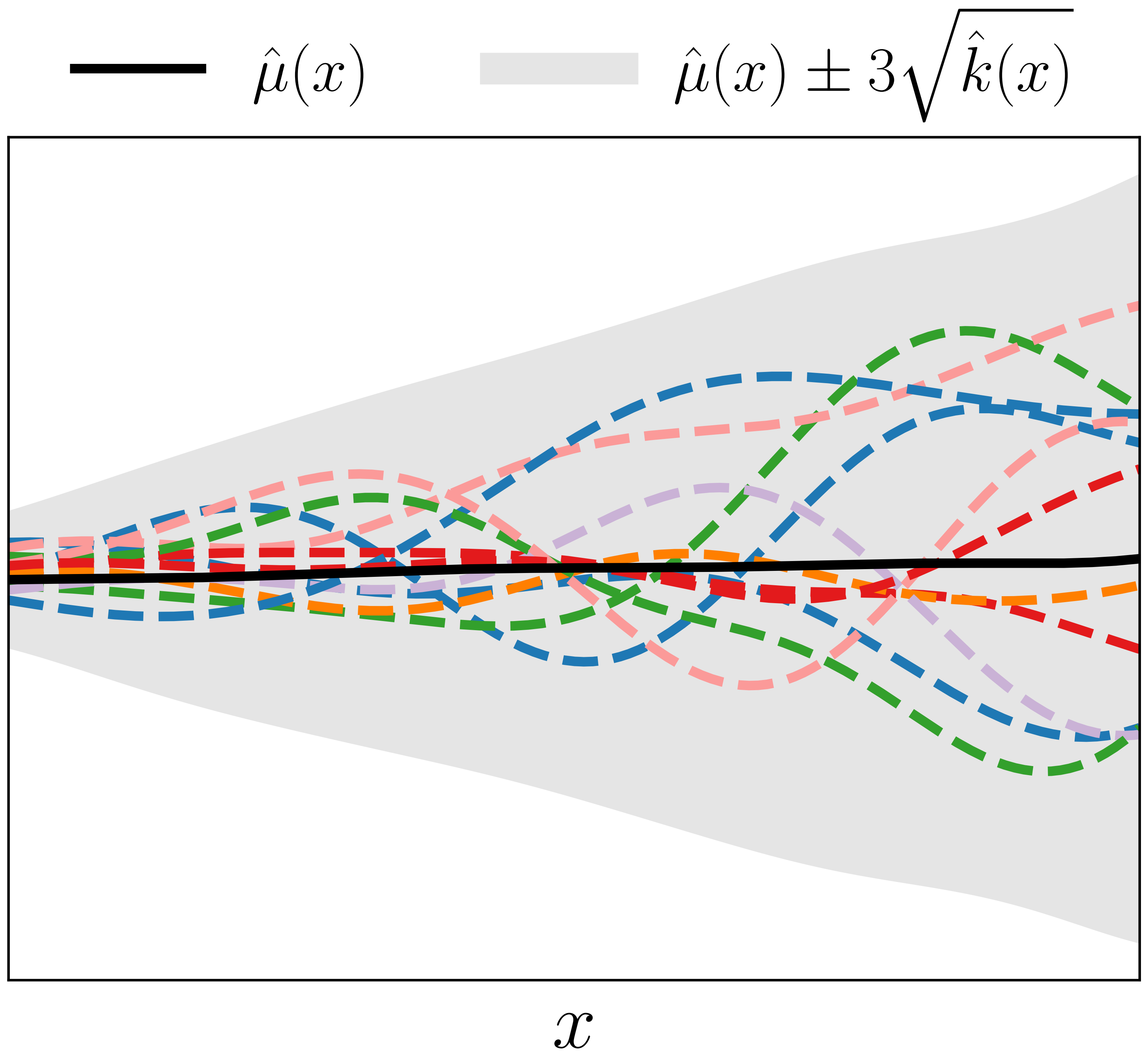
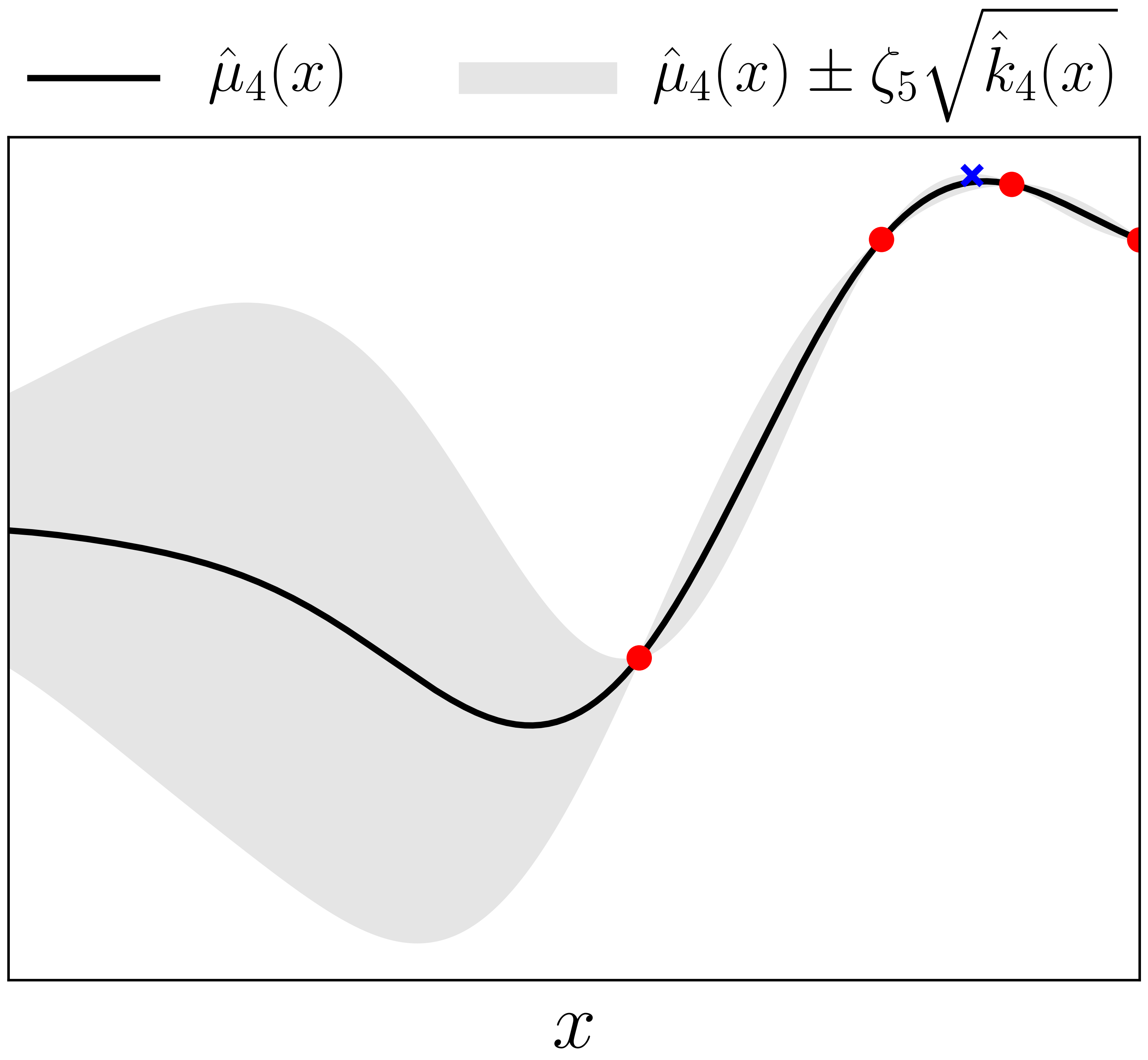


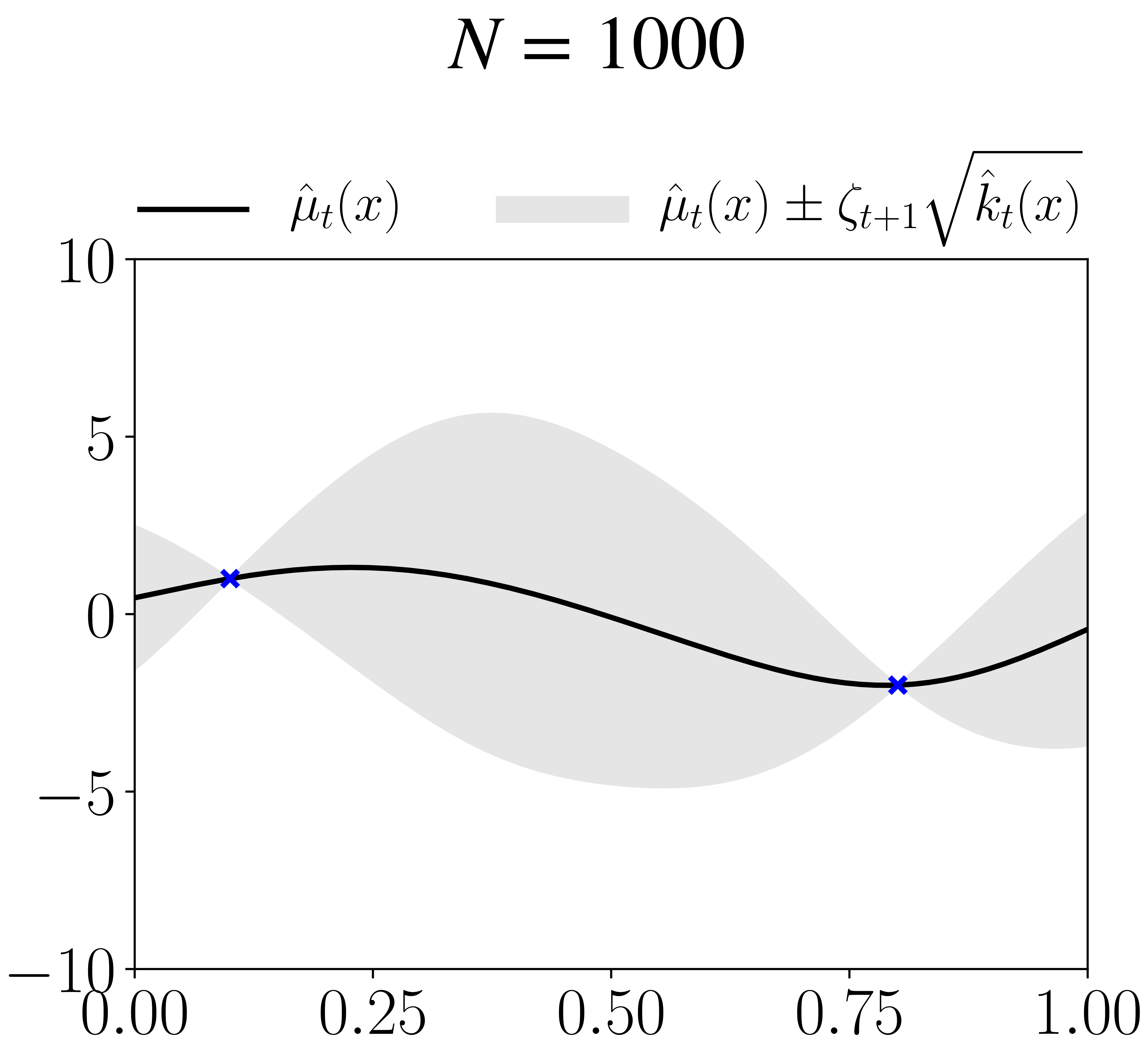
Estimated prior

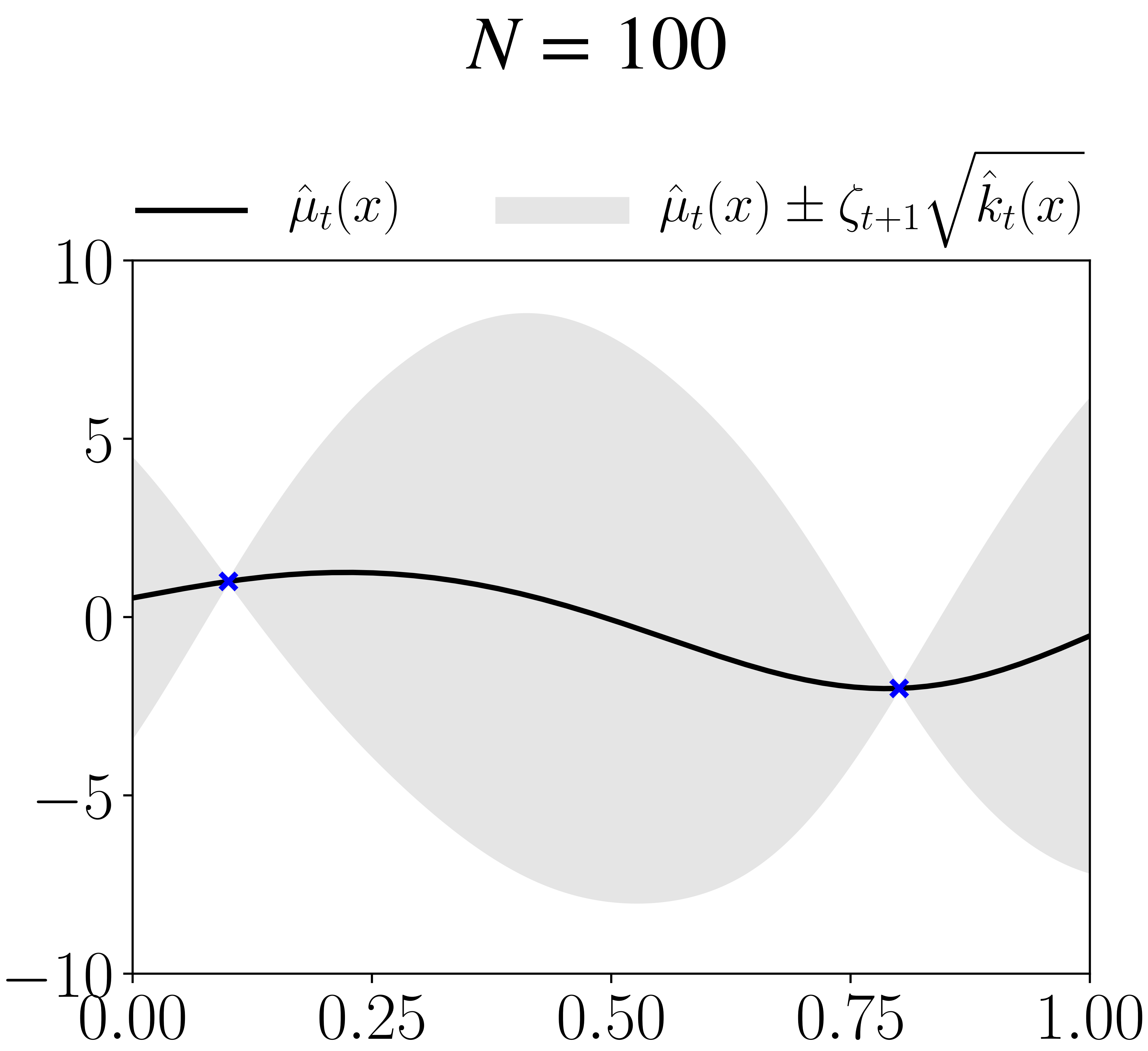
$\hat{\mu}, \hat{k}$

Online phase



Effect of N, the number of meta training functions





Bounding the regret of meta BO with an unknown GP prior

Results for continuous input space @ poster #22

Theorem (finite input space)

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,

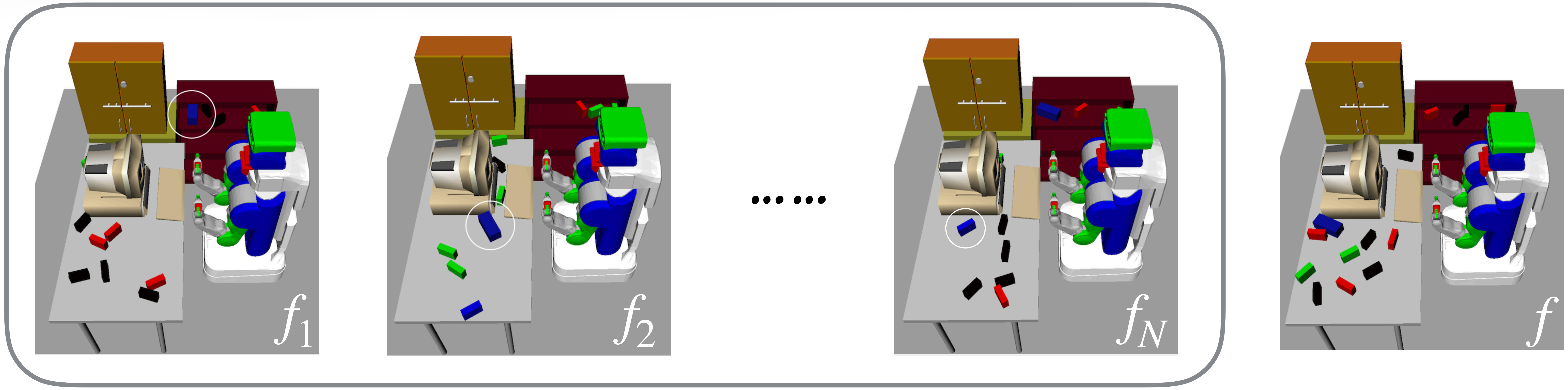
simple regret $$R_T \lesssim \left(O\left(\sqrt{\frac{1}{N-T}}\right) + C \right)\left(\sqrt{O\left(\frac{\log T}{T}\right) + \sigma^2} \right) \to C\sigma$$

constant ≈ 10

linear kernel

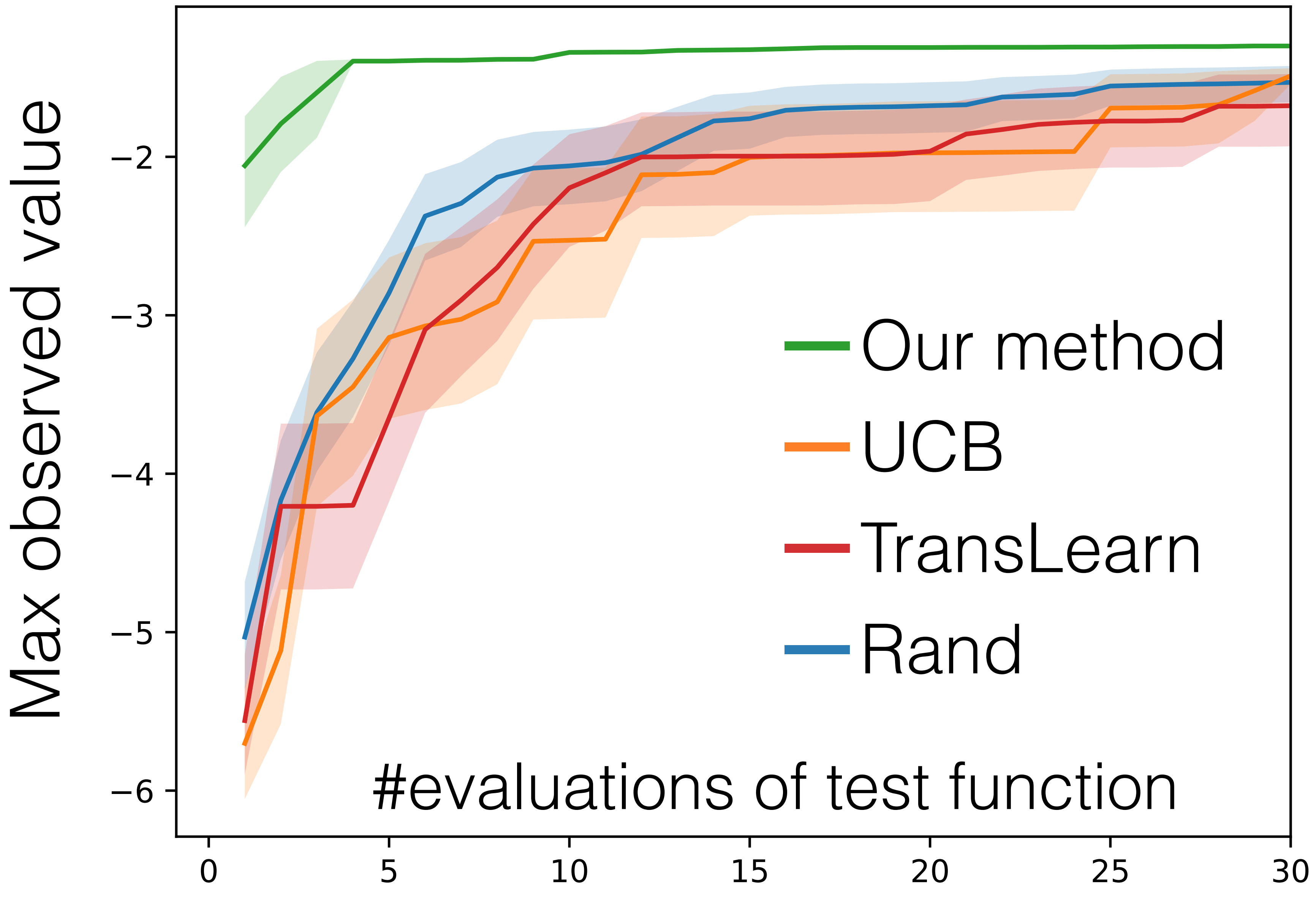
observation noise

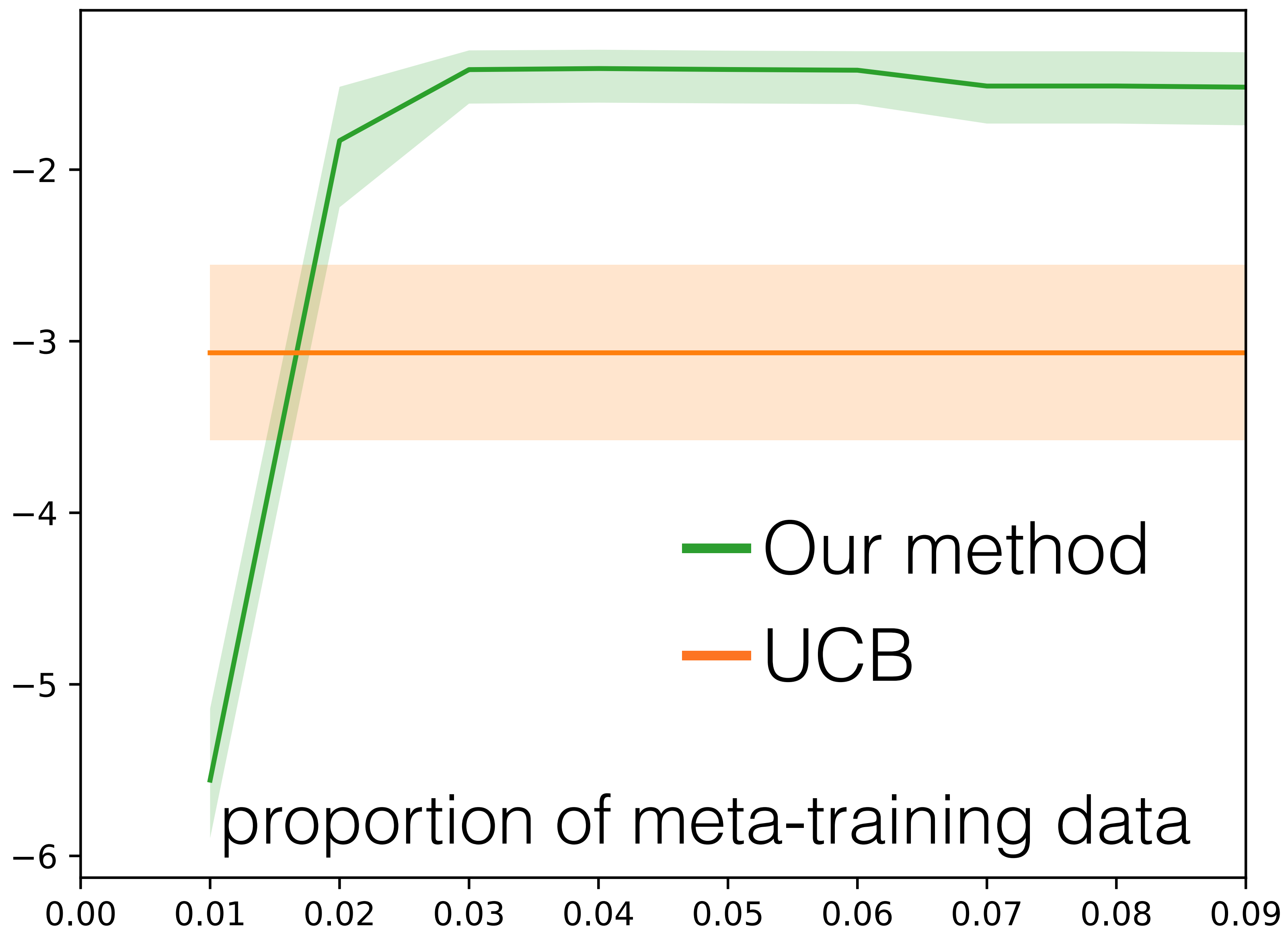
Empirical results on block picking and placing



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