

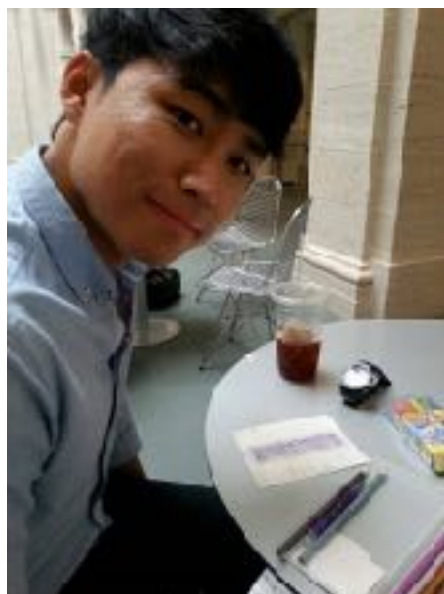


Regret bounds for meta Bayesian optimization with an **unknown** Gaussian process prior

Zi Wang

Microsoft Research AI Breakthroughs Workshop, Sep 18

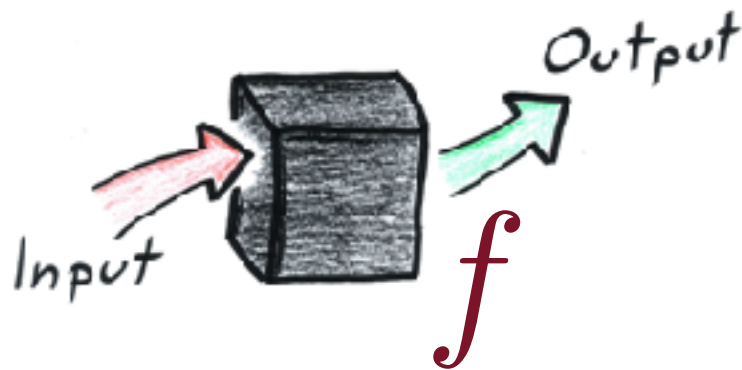
Joint work with Beomjoon Kim, Leslie Pack Kaelbling



Blackbox Function Optimization

a.k.a derivative-free optimization,
experimental design,
(continuous) multi-armed bandit

Goal: $x^* = \operatorname{argmax}_{\substack{\text{box } \mathcal{X} \subset \mathbb{R}^d \\ \text{or } |\mathcal{X}| = M}} f(x)$



Challenges:

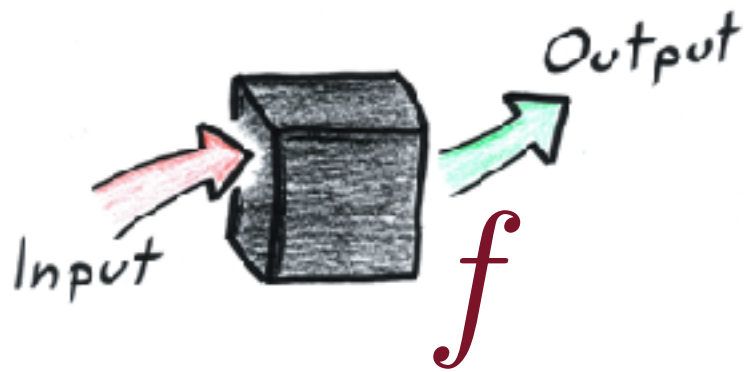
- f is expensive to evaluate
- f is multi-peak
- no gradient information
- evaluations can be noisy

(Kim et al., 2017; Snoek et al., 2012; Gonzalez et al., 2015)

Blackbox Function Optimization

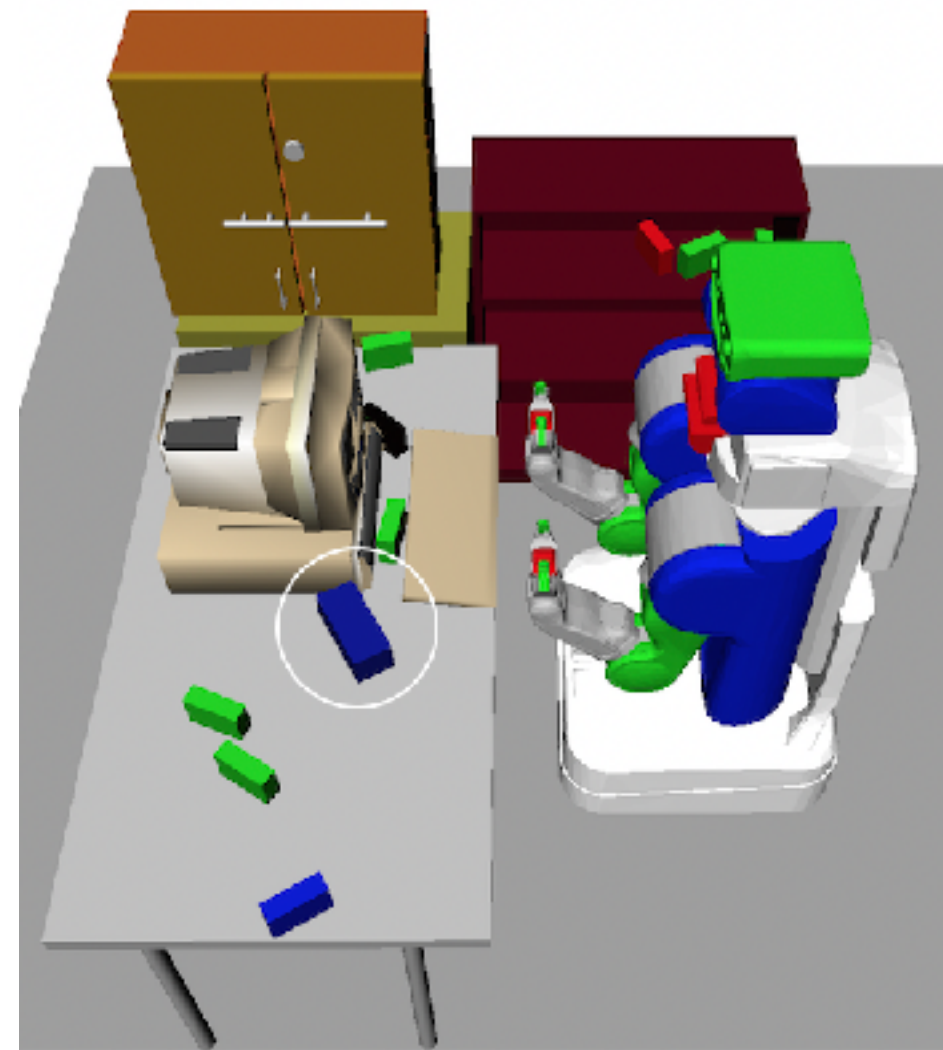
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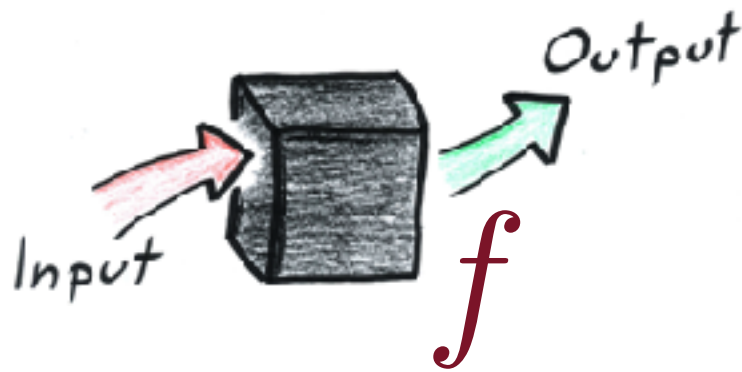


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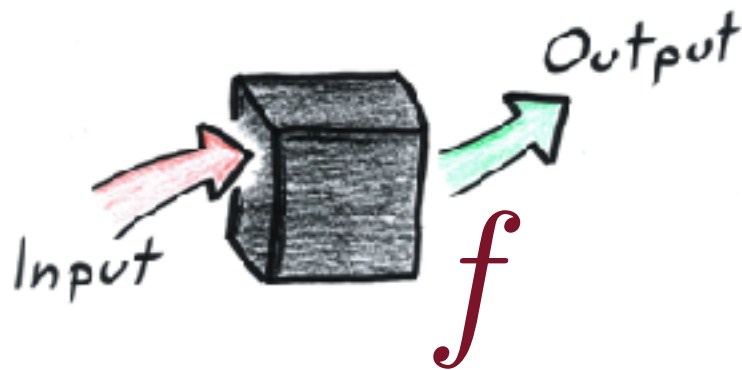


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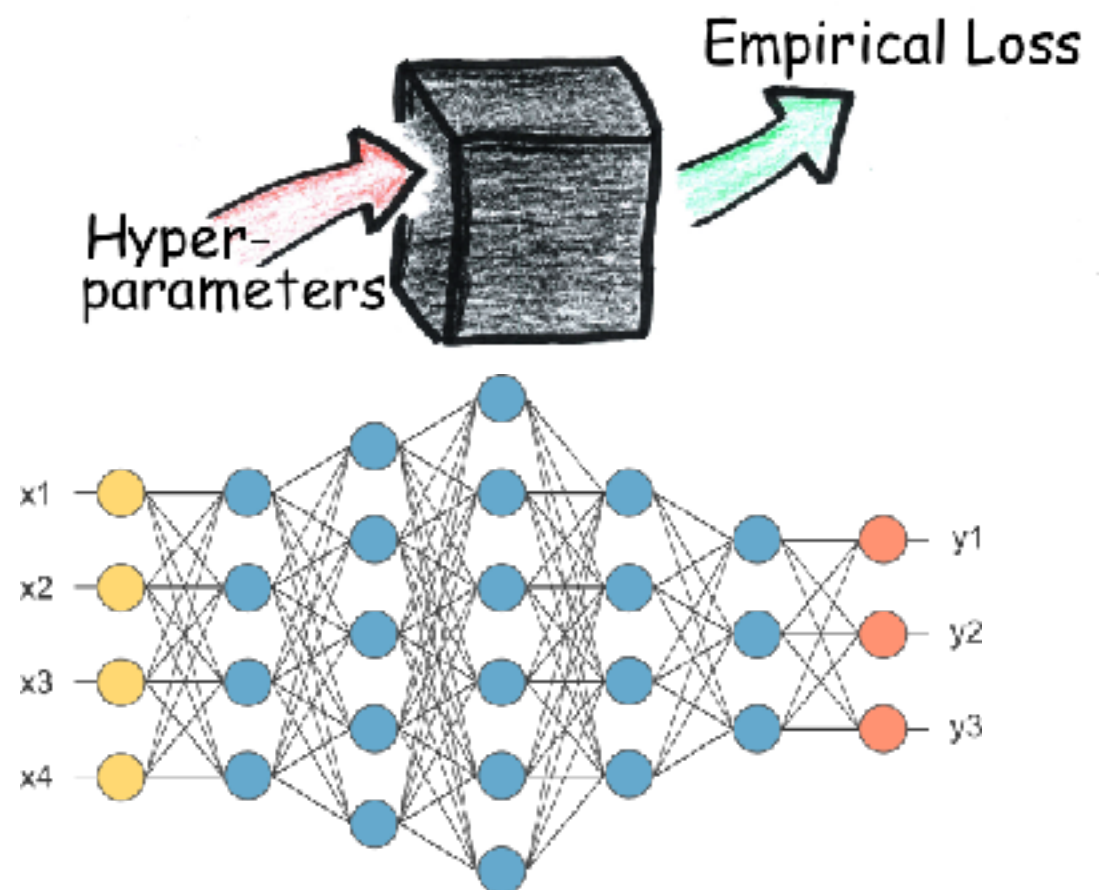
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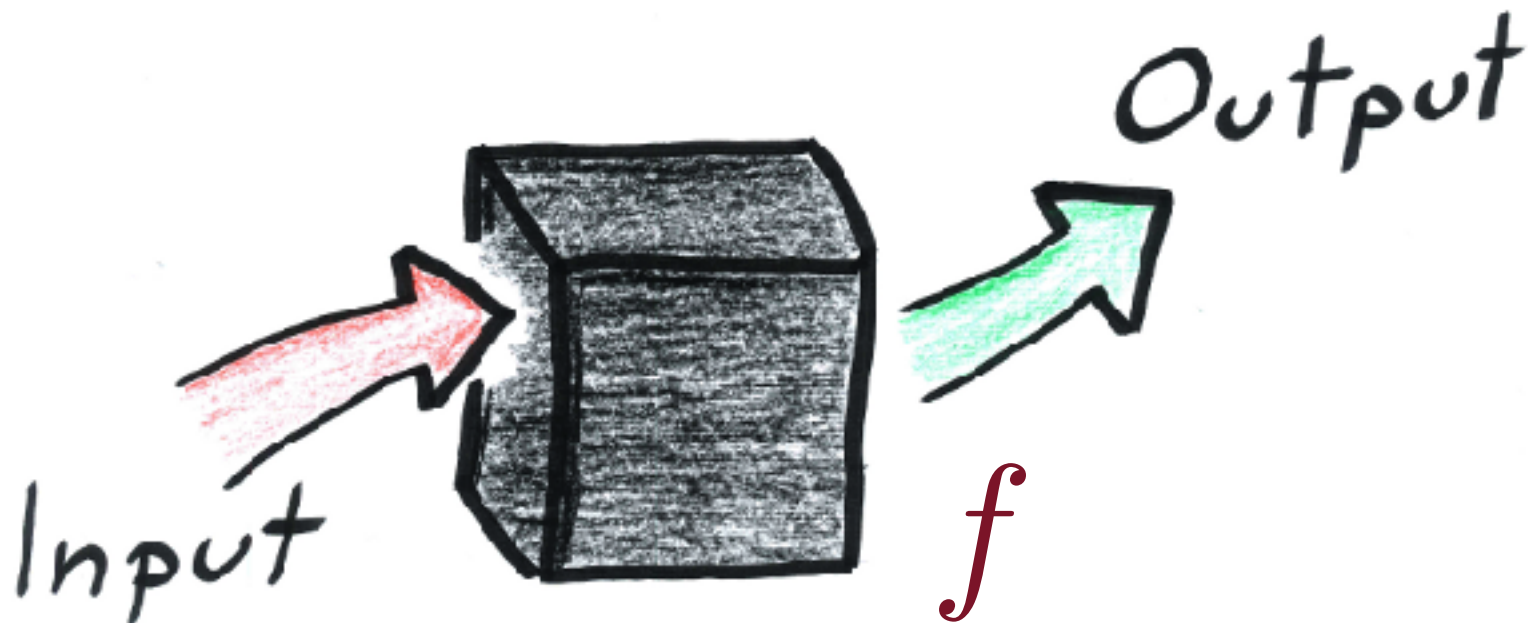
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Bayesian Optimization

Idea: build a **probabilistic model** of the function f

LOOP

- choose new query point(s) to evaluate
- update model

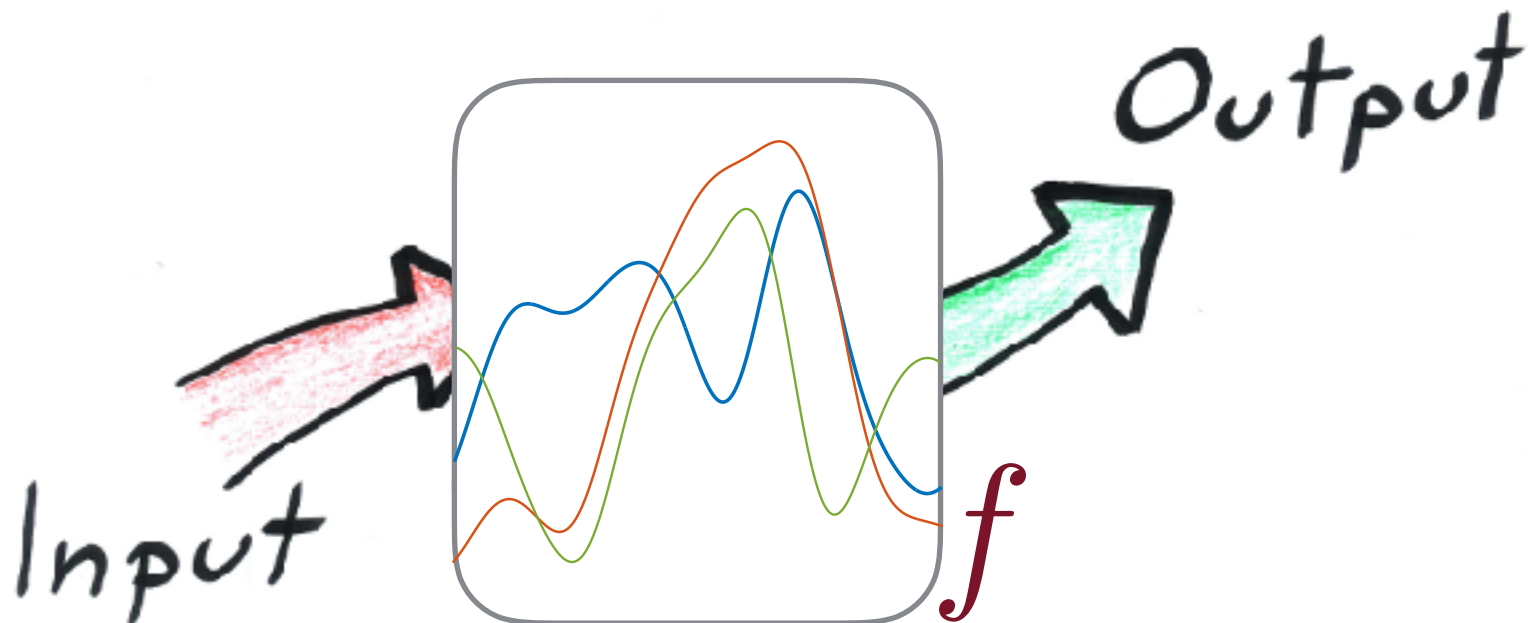


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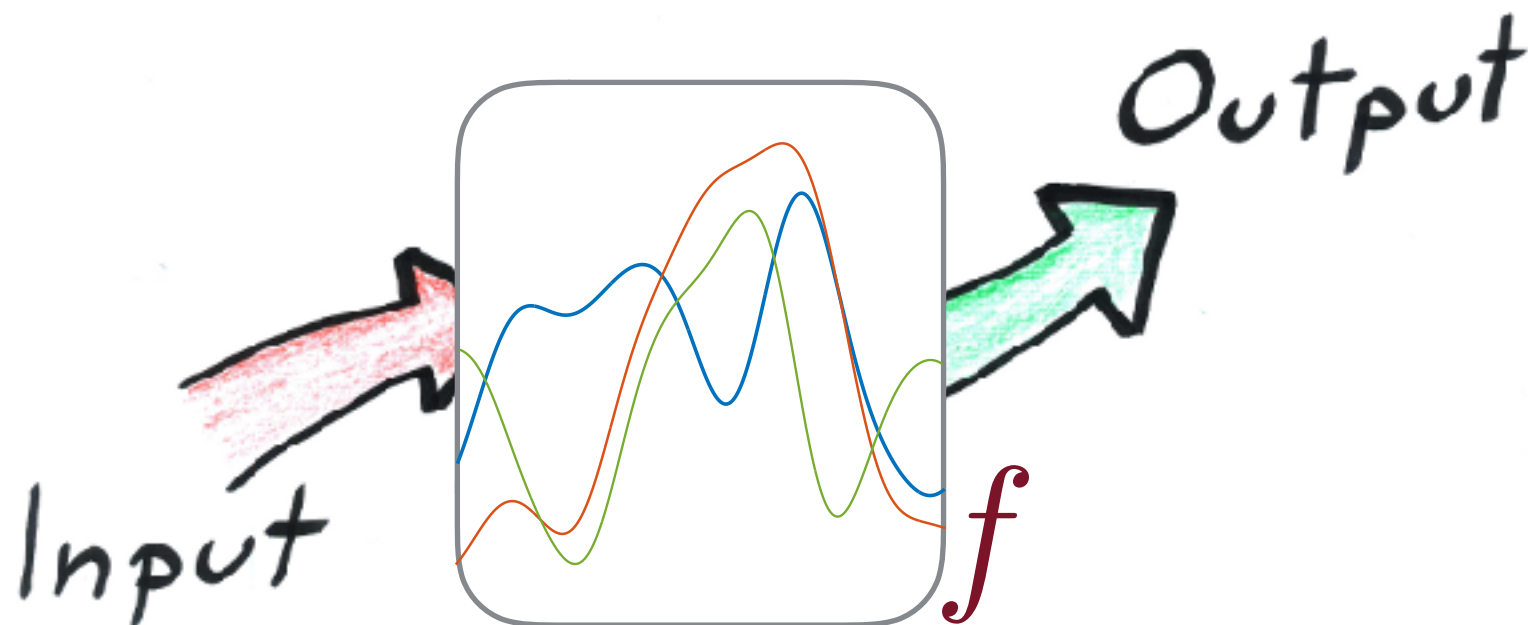


Bayesian Optimization

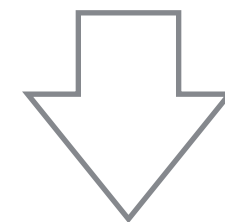
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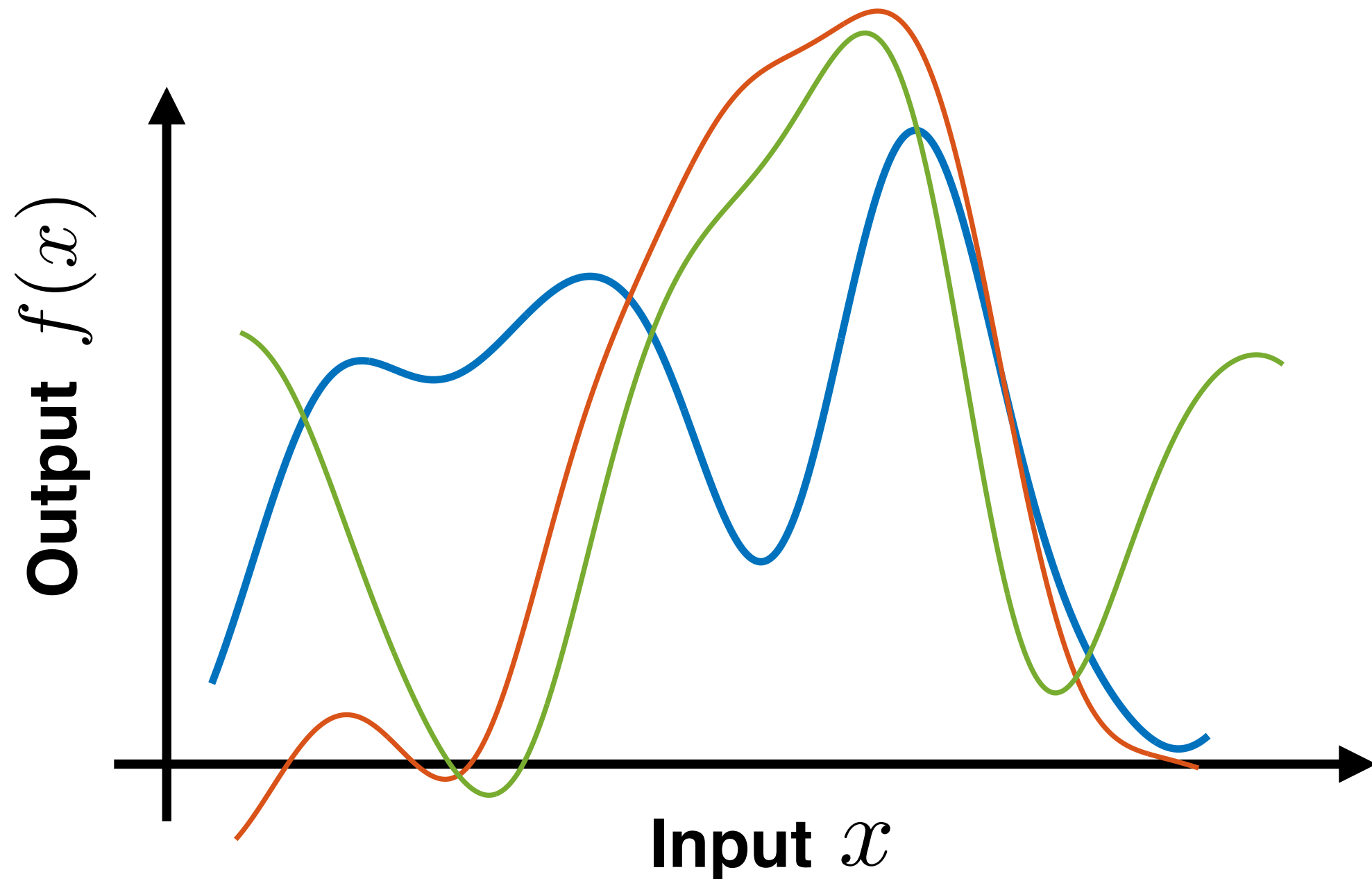


$$x_t = \operatorname{argmax}_{x \in \mathbb{R}^d} \alpha_t(x)$$

$$t = 1, \dots, T$$

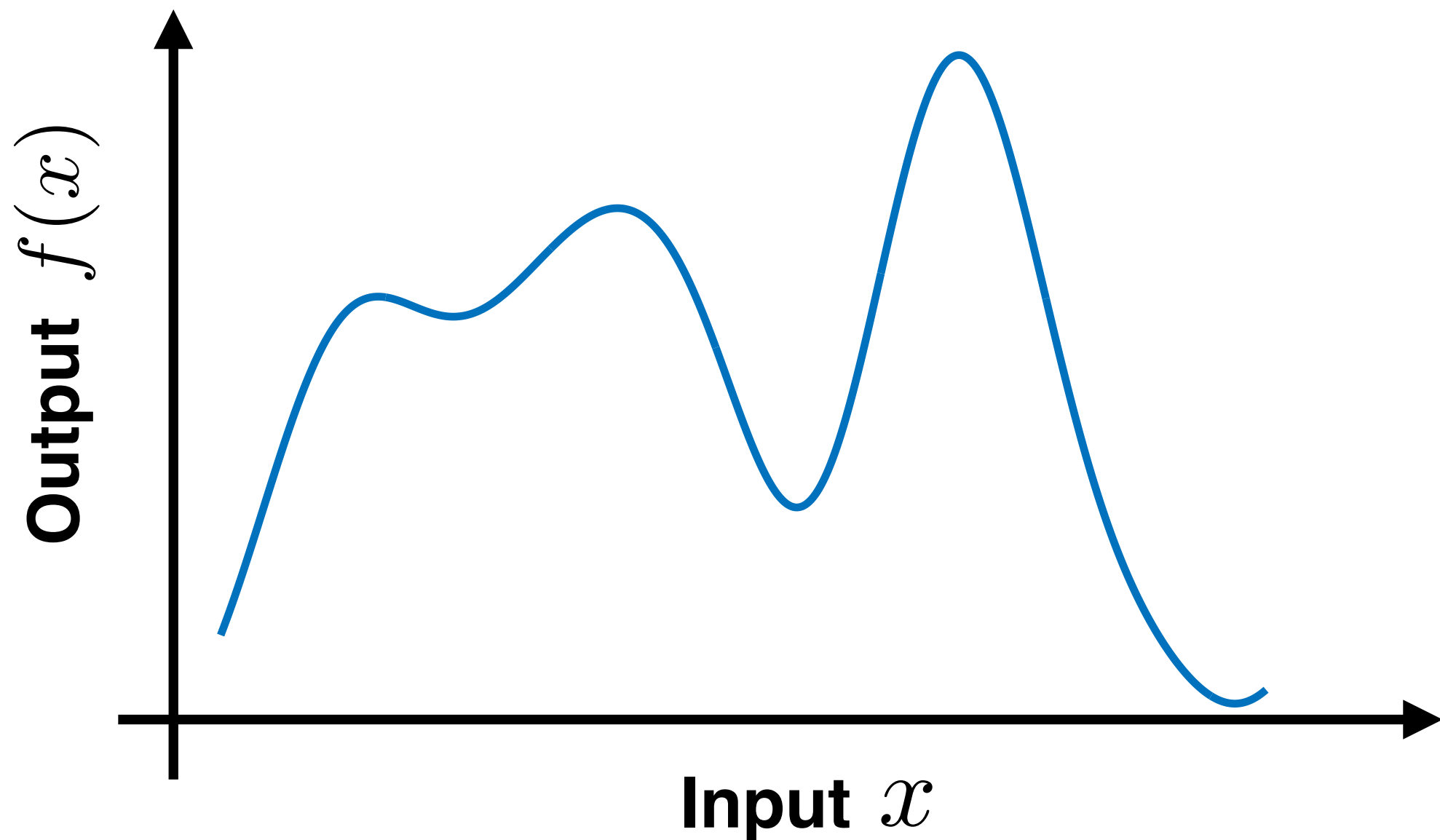
Gaussian Processes (GPs)

- probability distribution over functions
- any finite set of function values has a multivariate Gaussian distribution



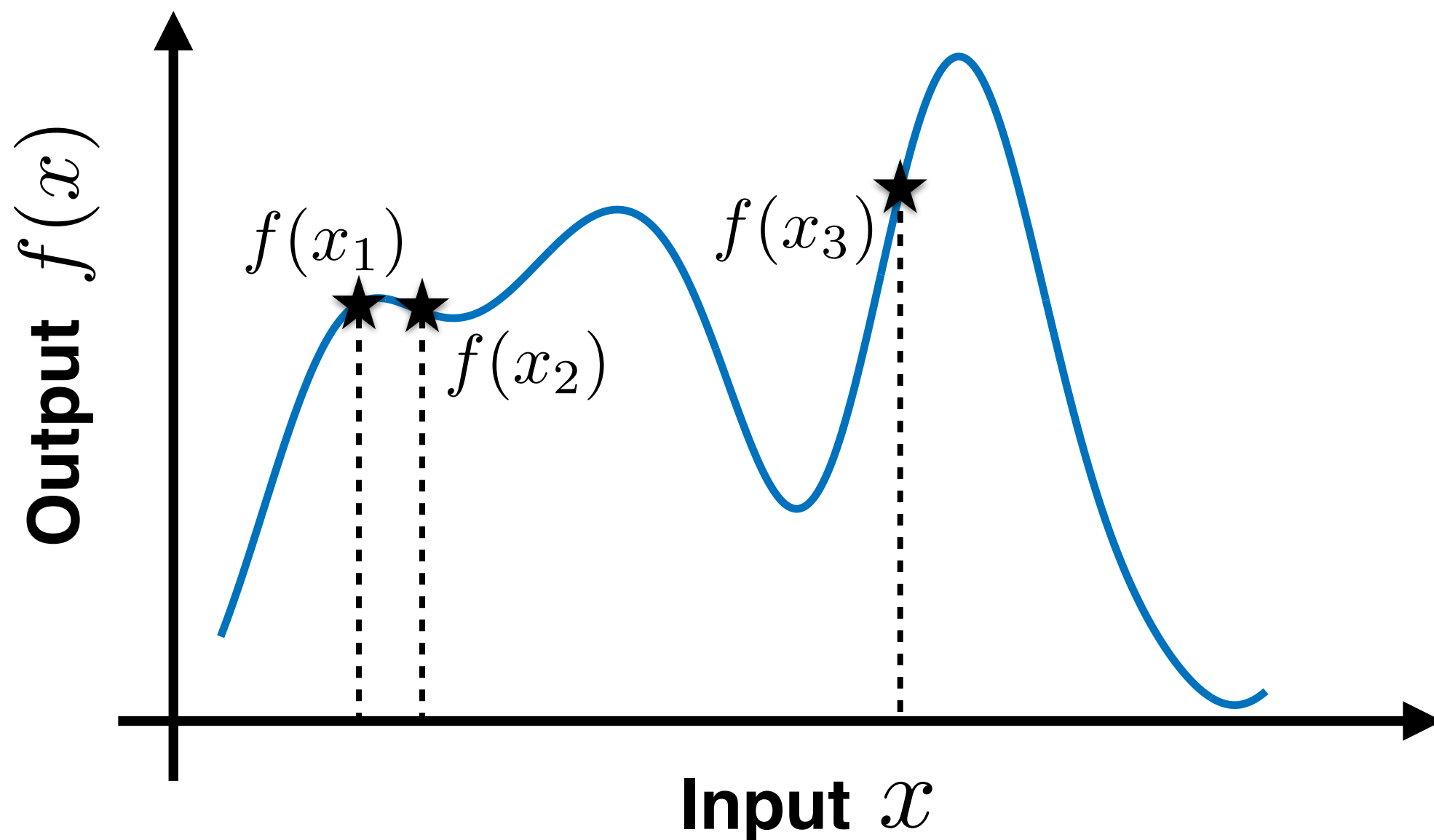
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- any finite set of function values has a multivariate Gaussian distribution
- kernel function $k(\cdot, \cdot)$; mean function $\mu(\cdot)$

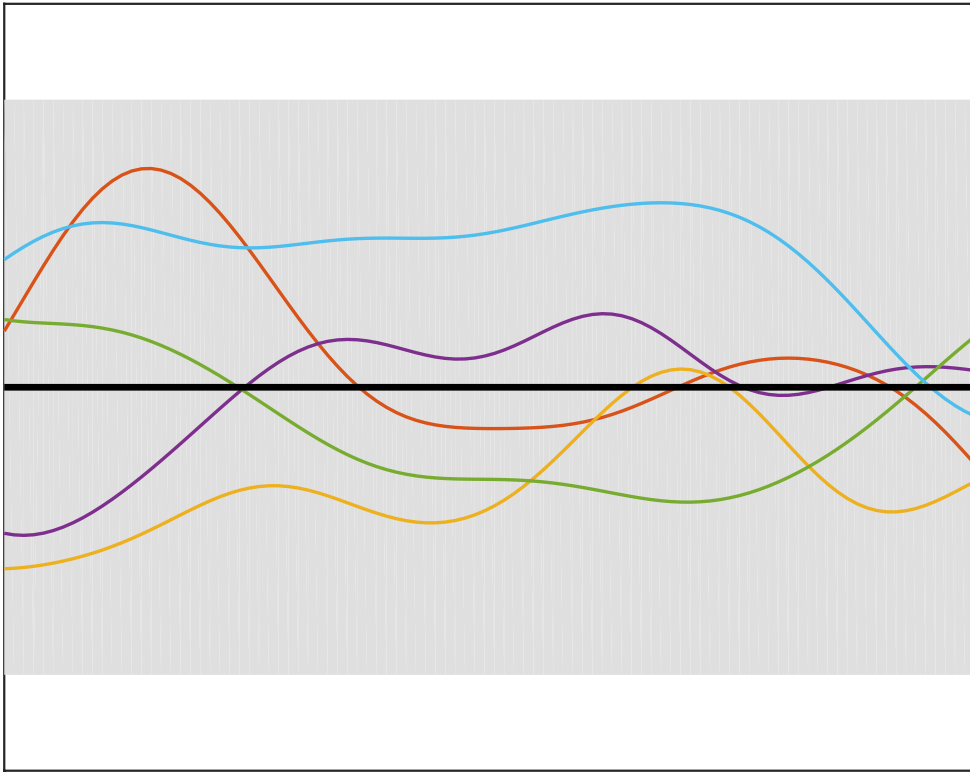
$$\begin{bmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu(x_1) \\ \vdots \\ \mu(x_n) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1), & \cdots, & k(x_1, x_n) \\ \vdots, & & \vdots \\ k(x_n, x_1), & \cdots, & k(x_n, x_n) \end{bmatrix} \right)$$

- function $f \sim GP(\mu, k)$; observe **noisy output** at x_τ

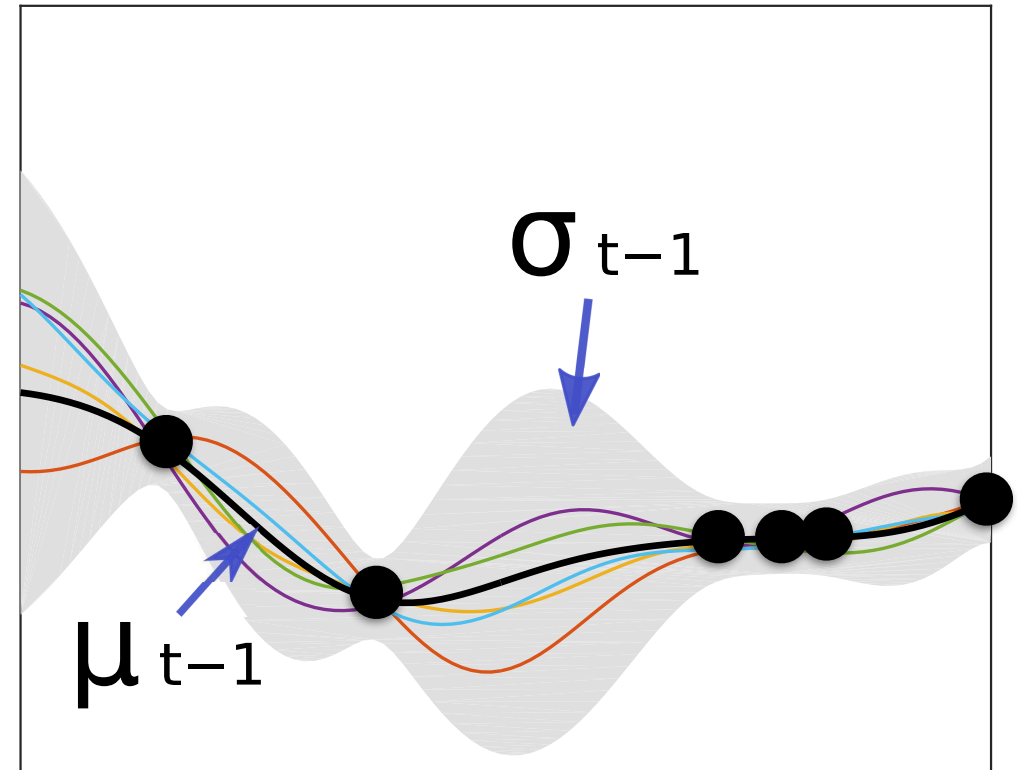
$$y_\tau = f(x_\tau) + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

Gaussian Processes (GPs)

Samples from the prior



Samples from the posterior



Given observations $D_t = \{(x_\tau, y_\tau)\}_{\tau=1}^{t-1}$, predict posterior mean and variance in **closed form** via conditional Gaussian

$$\mu_{t-1}(x) = k_{t-1}(x)^T (K_{t-1} + \sigma^2 I)^{-1} y_{t-1}$$

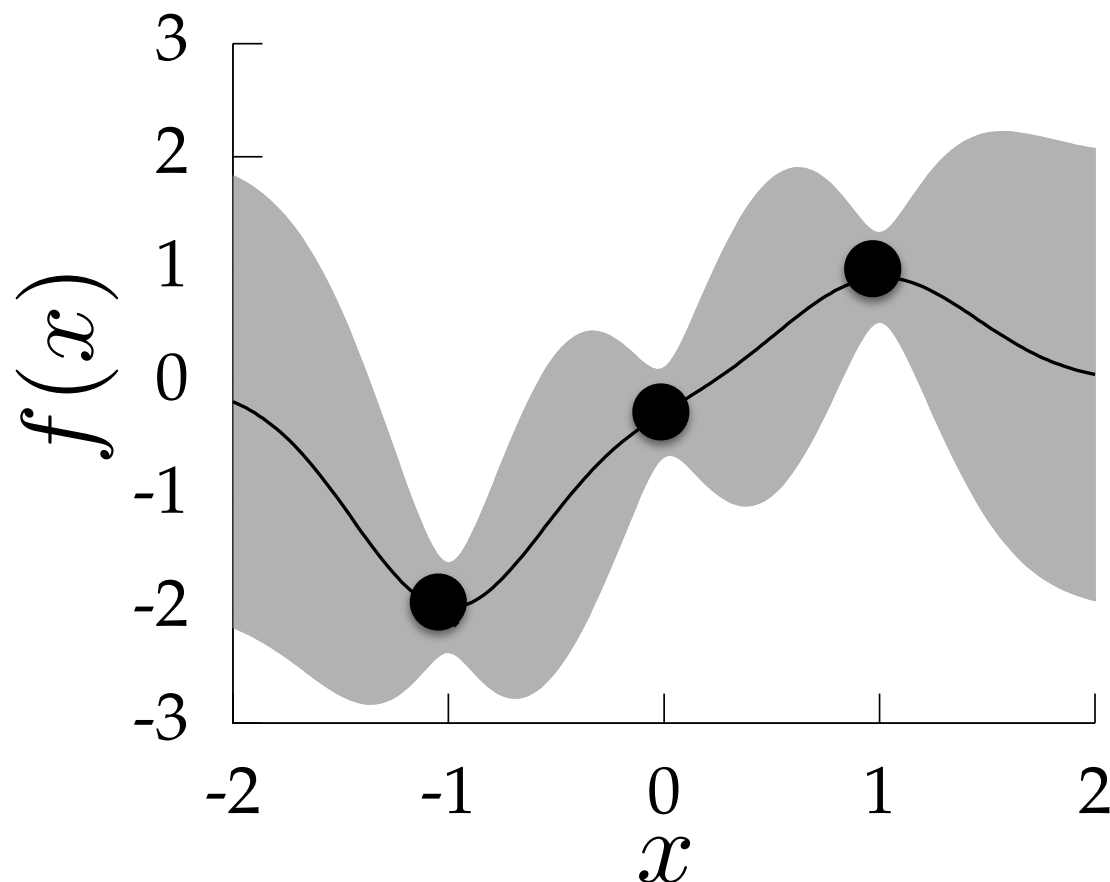
$$\sigma_{t-1}(x)^2 = k(x, x) - k_{t-1}(x)^T (K_{t-1} + \sigma^2 I)^{-1} k_{t-1}(x)$$

Bayesian Optimization

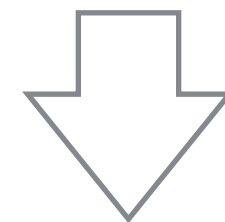
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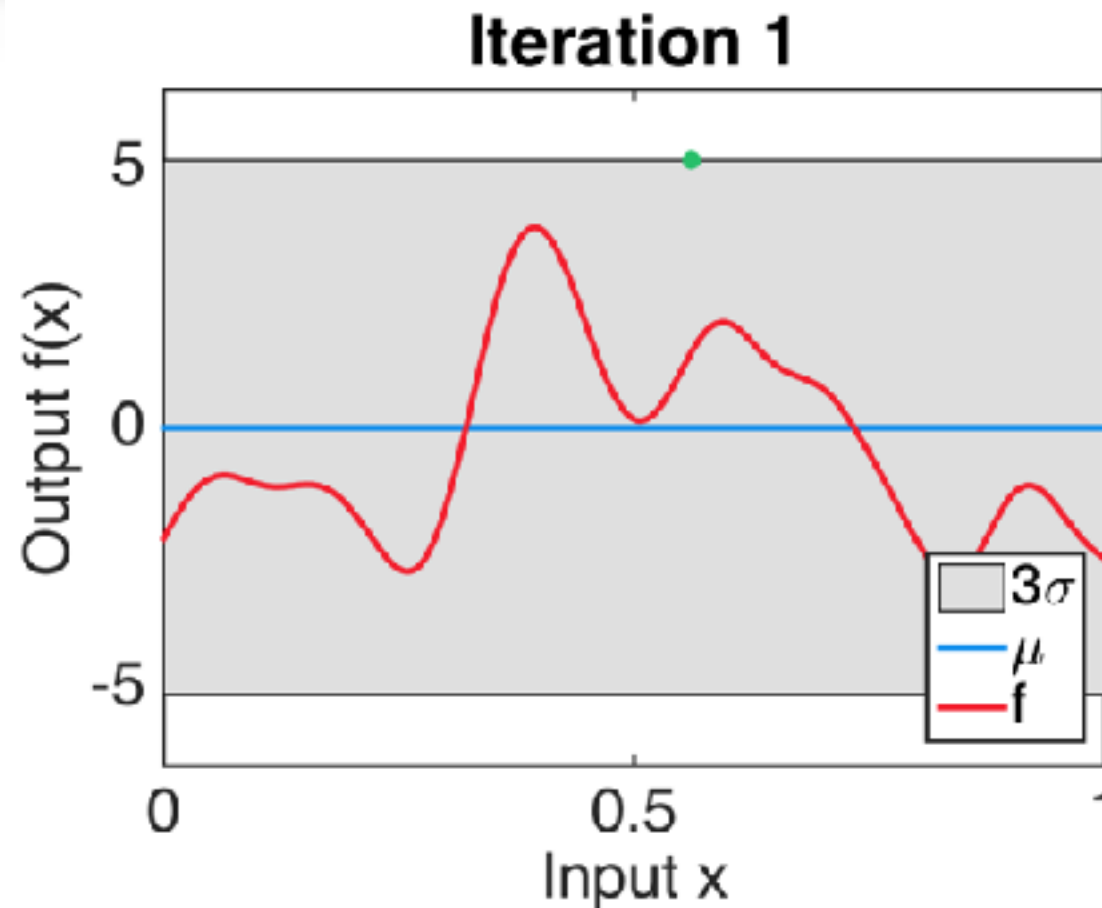
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$$t = 1, \dots, T$$

Gaussian process upper confidence bound



Prior: $f \sim GP(\mu, k)$

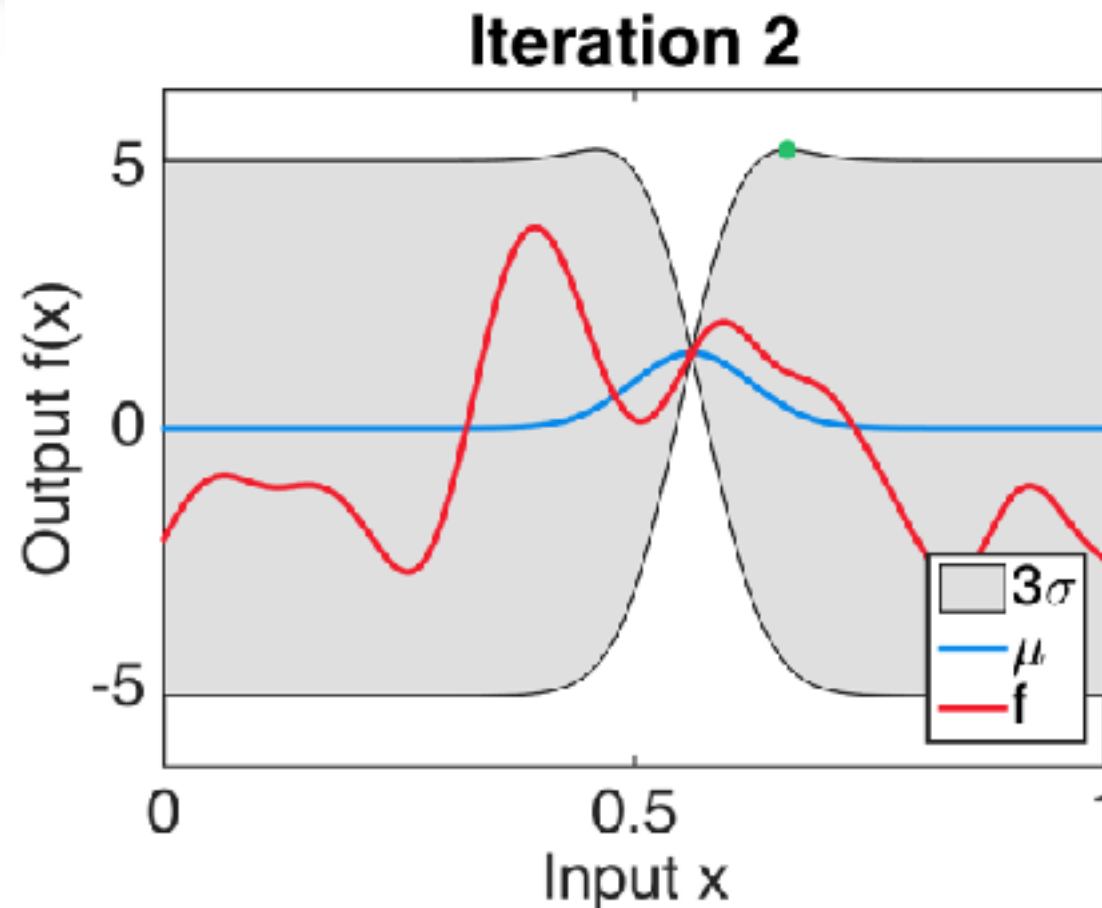
At iteration t ,

- predict the posterior $\mu_{t-1}(x)$ and $\sigma_{t-1}^2(x)$
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(Auer, 2002; Srinivas et al., 2010)

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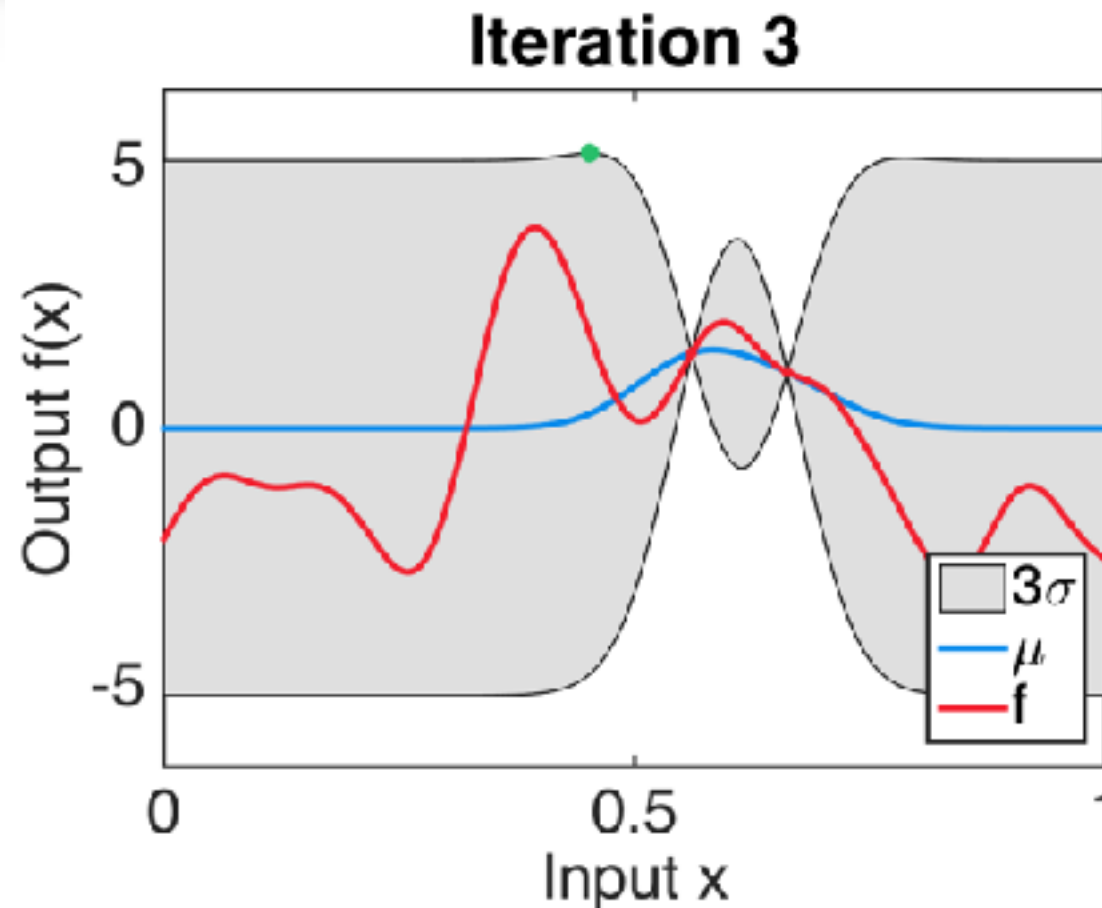
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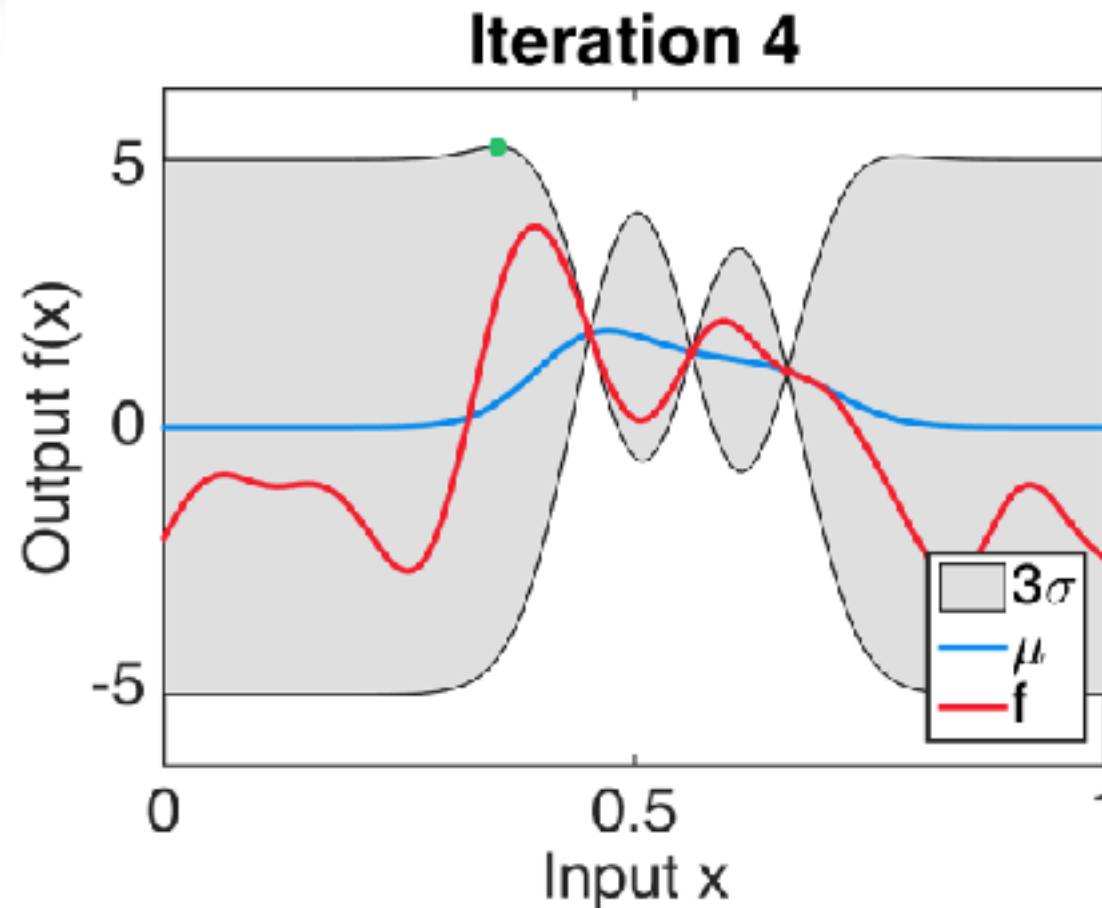
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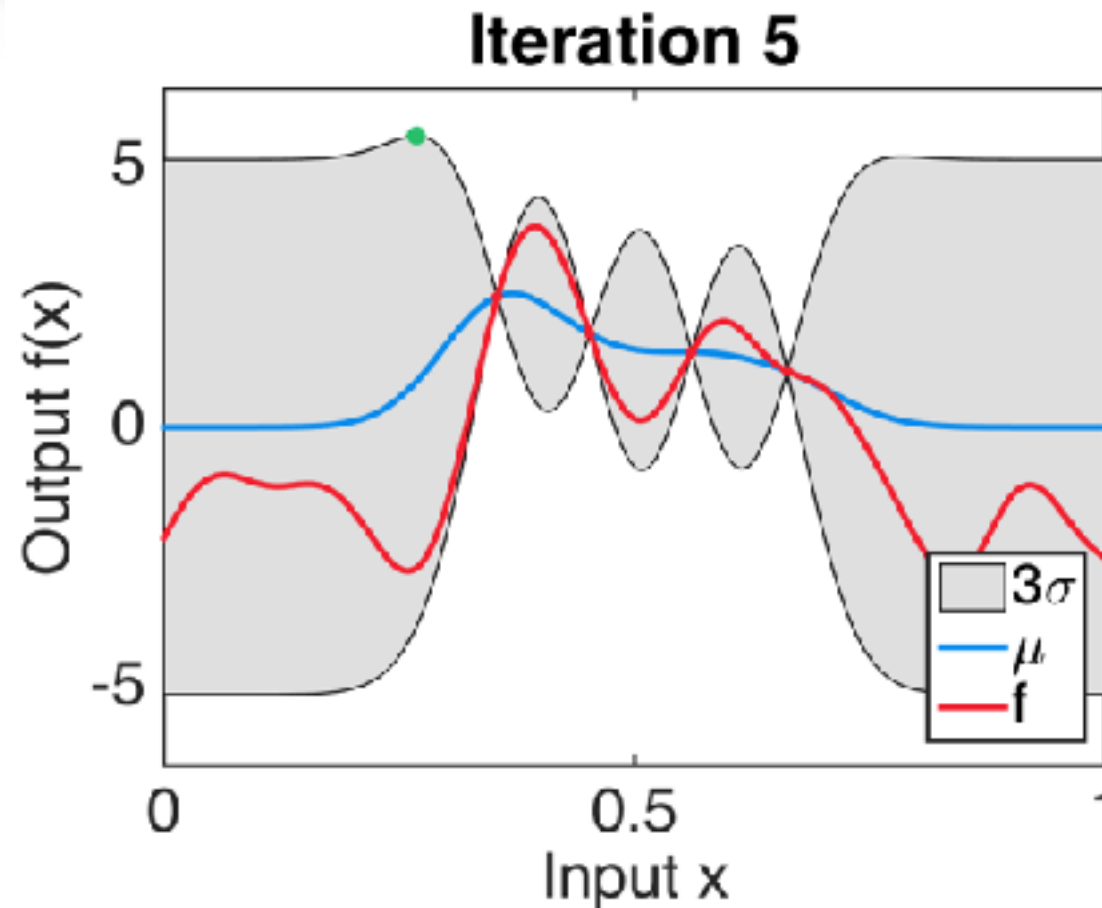
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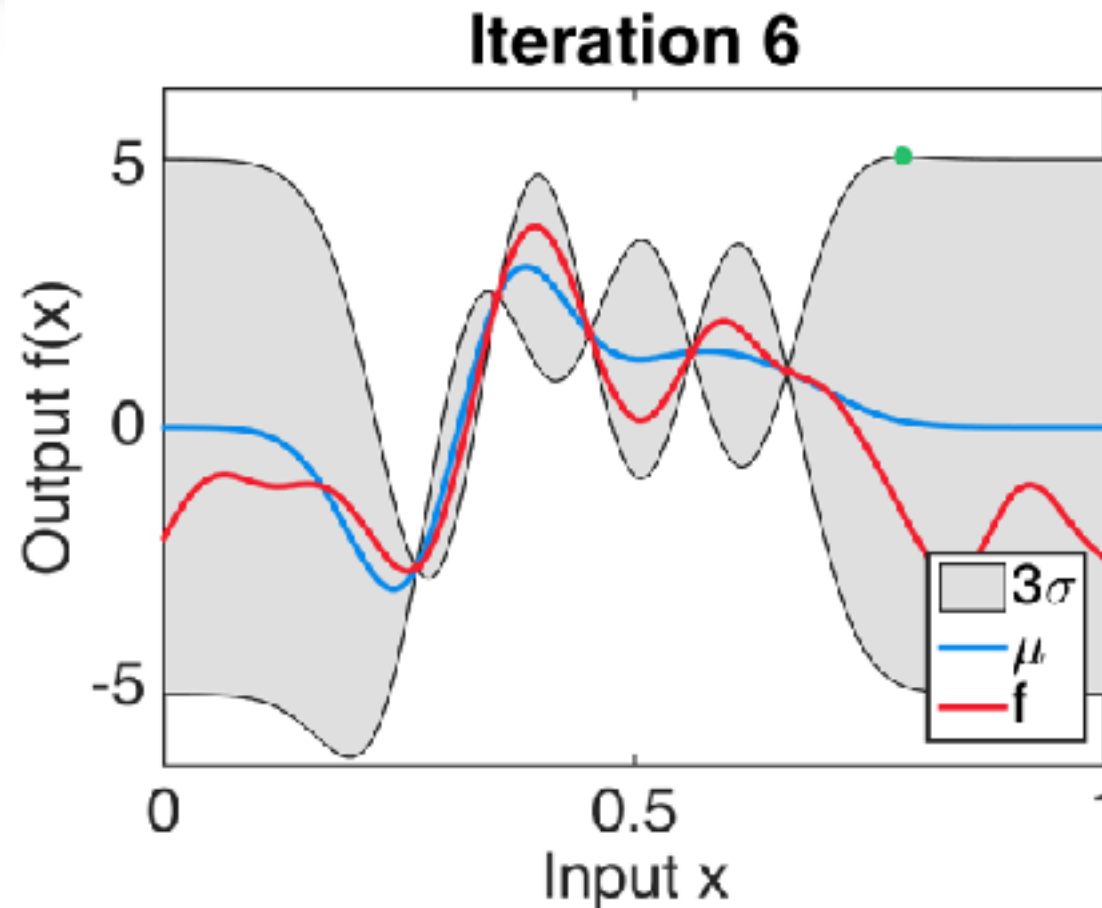
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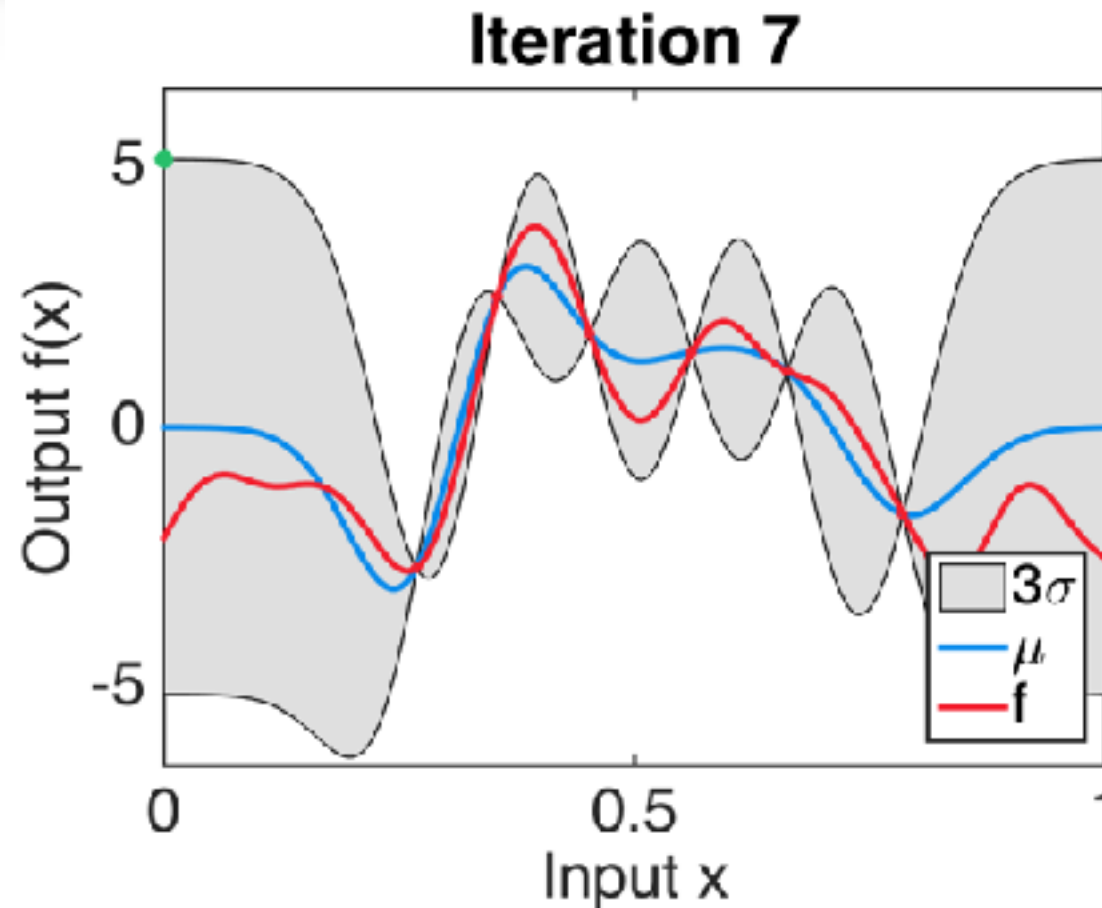
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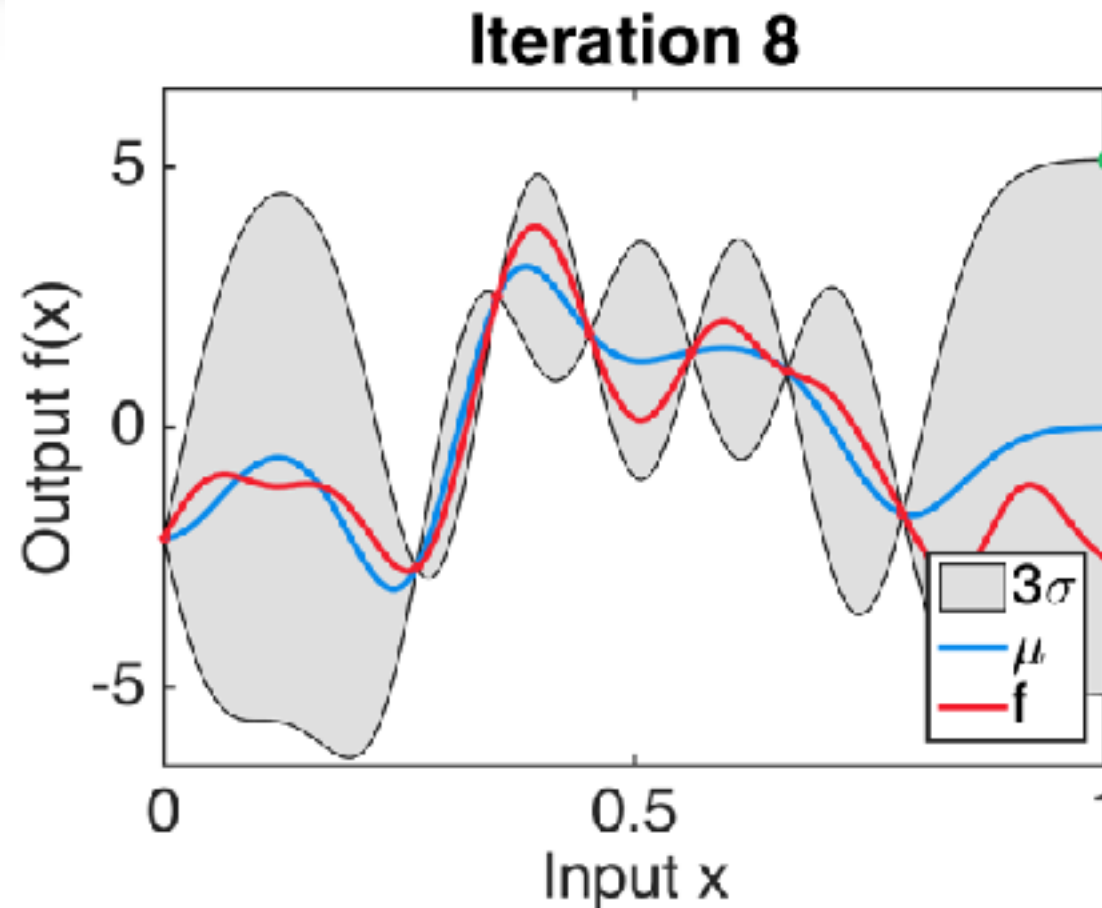
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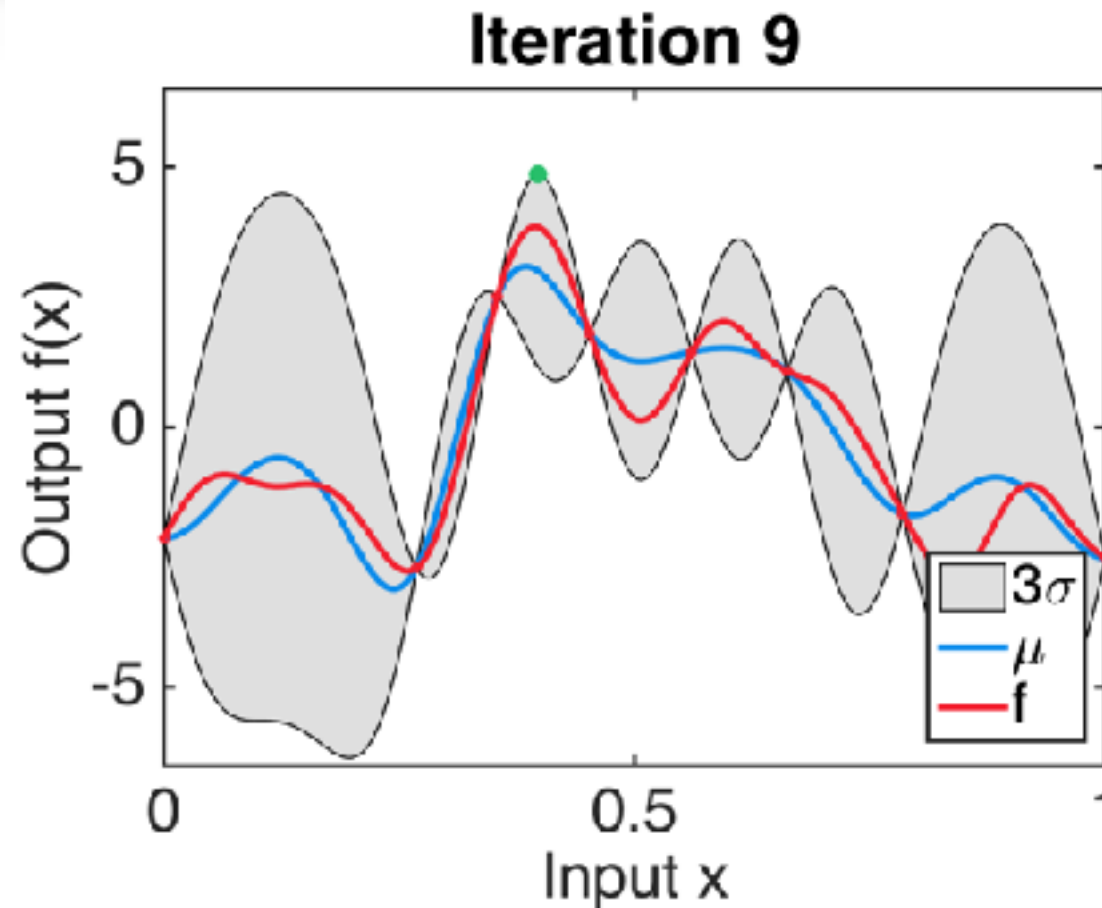
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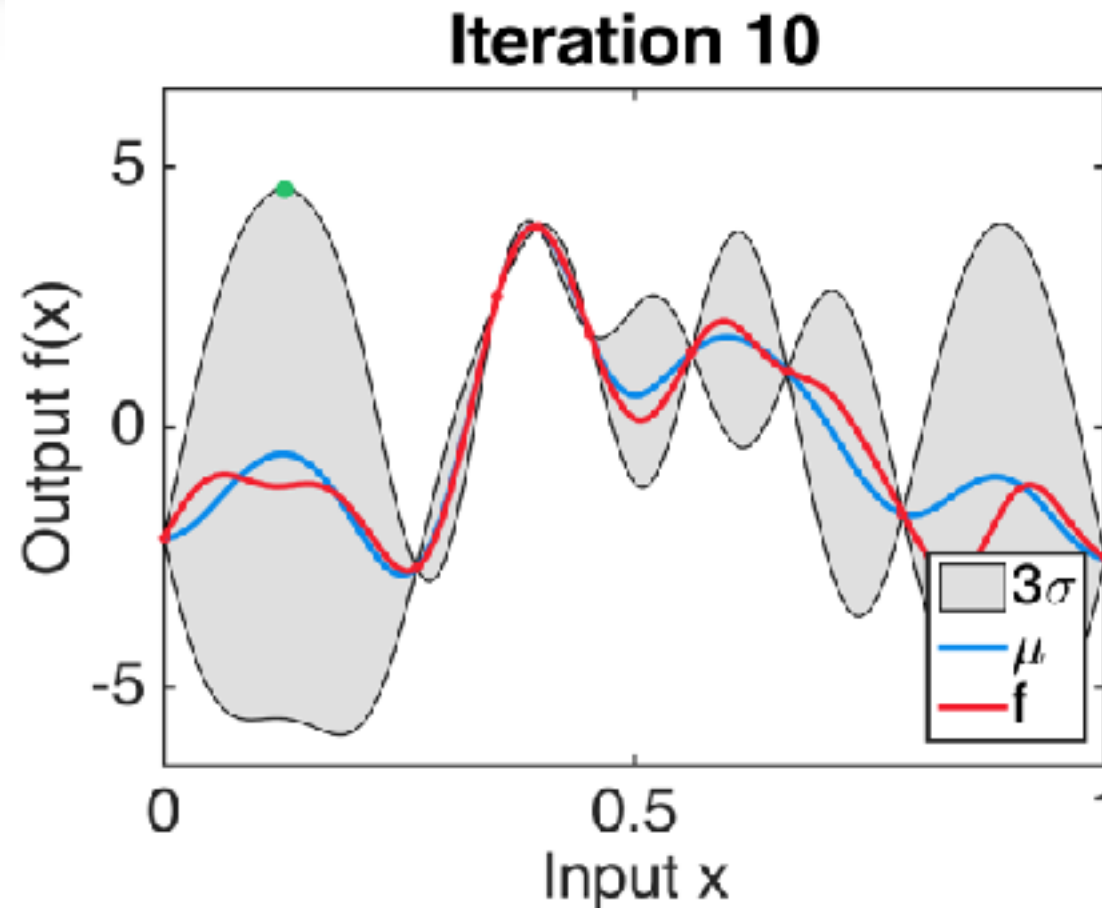
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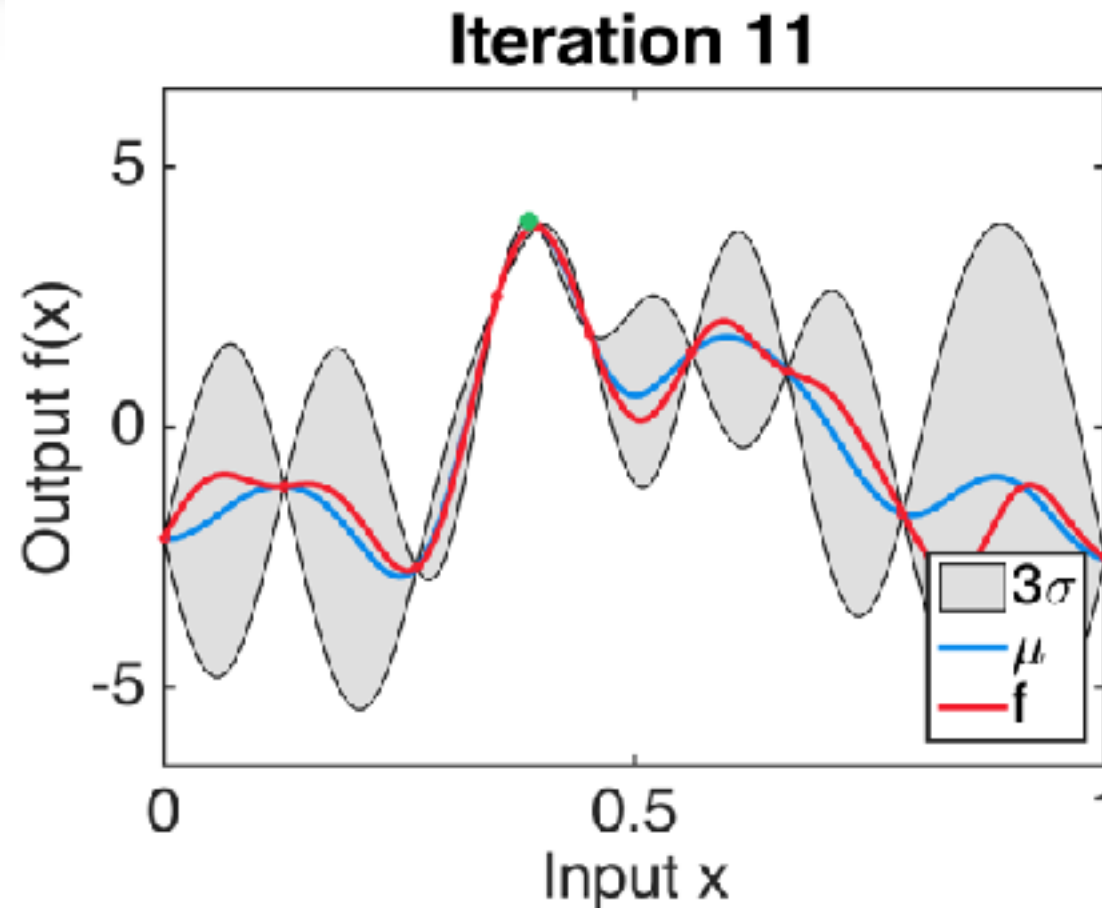
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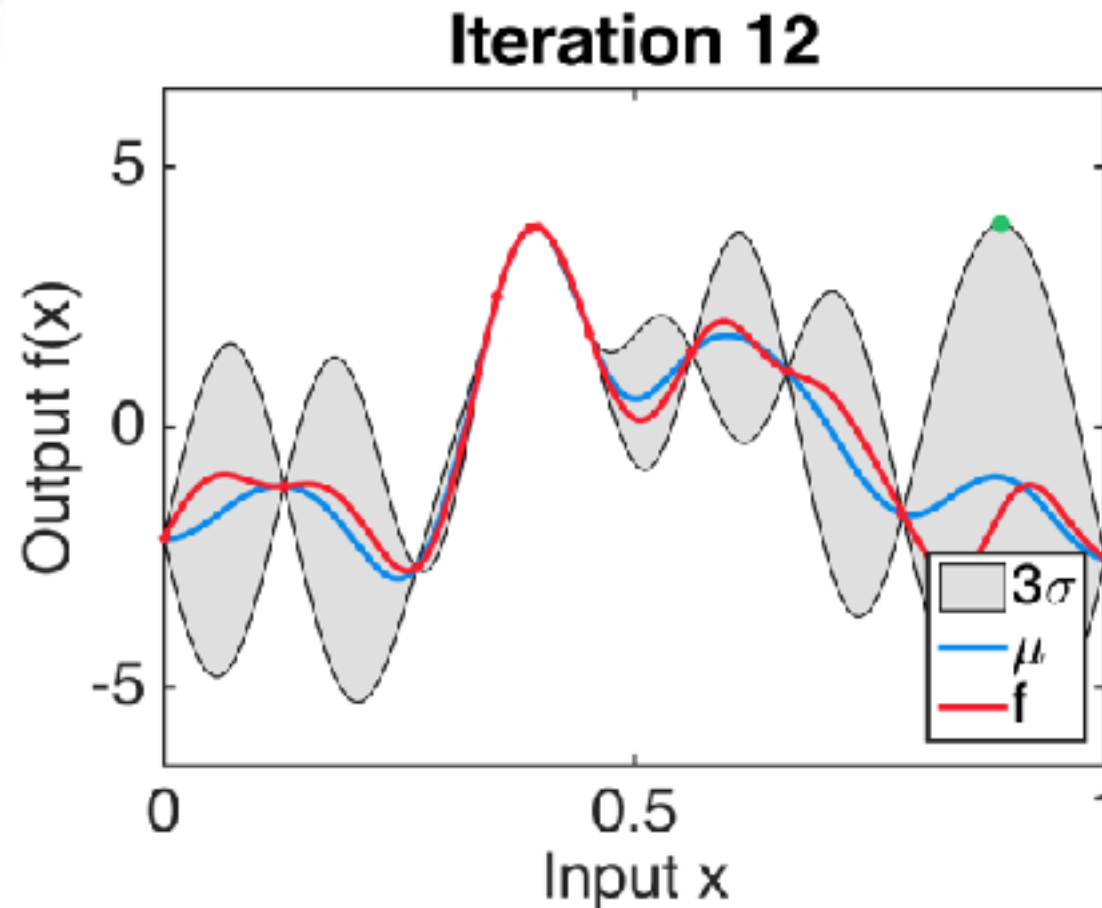
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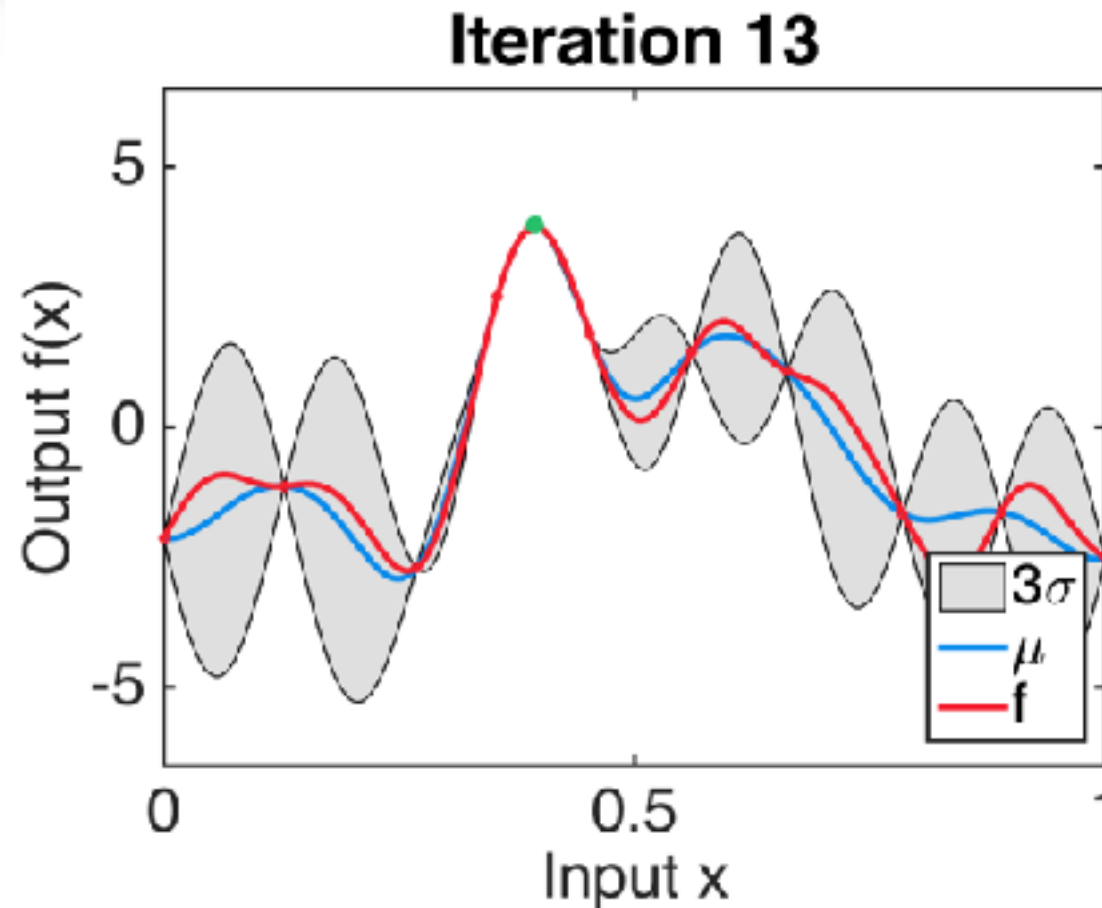
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Challenges in Bayesian optimization

- better acquisition function
- high dimensional input space
- large scale observations
- batch selection of queries
- prior estimation
- ...

Challenges in Bayesian optimization

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Optimization as Estimation with Gaussian Processes in Bandit Settings			Max-value Entropy Search for Efficient Bayesian Optimization	
Zi Wang MIT CSAIL	David Rosenberg MIT CSAIL	Stefano Jegelka MIT CSAIL	Zi Wang ¹ Stefano Jegelka ¹	
Abstract Recently, there has been rising interest in Bayesian optimization – the optimization of an unknown function with expensive queries guided by a Gaussian Process (GP) prior. We study an optimization strategy that directly accounts for the uncertainty of the function. This strategy offers both practical and theoretical advantages: no model parameter needs to be introduced; however, we establish strong connections to the popular GP-UCB and GP-PI strategies. Our approach can be understood as automatically and adaptively trading off exploration and exploitation in GP-UCB and GP-PI. We illustrate the effects of this adaptive trading via bounds on the regret as well as an experimentally-validated evaluation on robotics and vision tasks, demonstrating the effectiveness of this strategy for a range of performance criteria.			Abstract Entropy Search (ES) and Predictive Entropy Search (PES) are popular and empirically successful Bayesian Optimization techniques. Formally, as a competing information-theoretic motivation, and maximize the information gained about the true value of the unknown function; yet, both are plagued by the expensive computation for estimating entropies. We propose a new criterion, Max-value Entropy Search (MES), that instead uses the information about the maximum function value. We show relations of MES to other Bayesian optimization methods, and establish a regret bound. We observe that MES maintains or improves the good empirical performance of ES/PES, while tremendously lightening the computational burden. In particular, MES is much more robust to the number of samples used for computing the entropy, and hence more efficient for higher-dimensional problems.	
Batched High-dimensional Bayesian Optimization via Structural Kernel Learning			Batched Large-scale Bayesian Optimization in High-dimensional Space	
Zi Wang ¹ Chengxi Li ¹ Stefano Jegelka ¹ Prashant Kohli ²			Zi Wang MIT CSAIL	Chengxi Li MIT CSAIL
Abstract Optimization of high-dimensional black-box functions is an extremely challenging problem. While Bayesian optimization has emerged as a popular approach for optimizing black-box functions, its applicability has been limited to low-dimensional problems due to its computational and statistical challenges arising from high-dimensional settings. In this paper, we propose to tackle these challenges by (1) assuming a latent additive structure in the function and inferring it properly for more efficient and effective BO, and (2) performing multiple evaluations in parallel to reduce the number of iterations required for the method. Our novel approach leads to the latest state-of-the-art BO in sampling and/or non-sampling queries using deterministic noise processes. Large-scale validation on both synthetic and real-world datasets demonstrates the effectiveness of our method.			Abstract Bayesian optimization (BO) has become an effective approach for black-box function optimization problems when function evaluations are expensive and the optimum can be achieved within a relatively small number of queries. However, many cases, such as the ones with high-dimensional inputs, may require a much larger number of observations for optimization. Despite an abundance of theoretical results to guide their experiments, current BO techniques have been limited to merely a few thousand observations. In this paper, we propose a scalable Bayesian optimization (SBO) to address three current challenges in BO simultaneously: (1) large-scale observations; (2) high-dimensional input spaces; and (3) selection of batch size and batch selection method. We demonstrate the effectiveness of SBO on both synthetic and real-world datasets.	

[Wang&Jegelka, ICML 2017]

[Wang&Zhou&Jegelka, oral@AISTATS 2016]

[Wang&Gehring&Kohli&Jegelka, AISTATS 2018]

[Wang*&Li*&Jegelka&Kohli, ICML 2017]

Challenges in Bayesian optimization

check out ziw.fyi

- better acquisition function
- high dimensional input space
- large scale observations
- batch selection of queries

- prior estimation

- ... this talk

[Wang*&Kim*&Kaelbling, spotlight@NIPS 2018]

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[Wang&Gehring&Kohli&Jegelka, AISTATS 2018]

[Wang*&Li*&Jegelka&Kohli, ICML 2017]

Bayesian optimization with an unknown prior

Estimate “prior” from data

- maximum likelihood
- hierarchical Bayes

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Data or prior?



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Ben Recht
@beenwrekt

Bayesian Optimization and other bad ideas for tuning hyperparameters.

arg min blog

About

Embracing the Random

Kevin Jamieson and Ben Recht • Jun 23, 2016

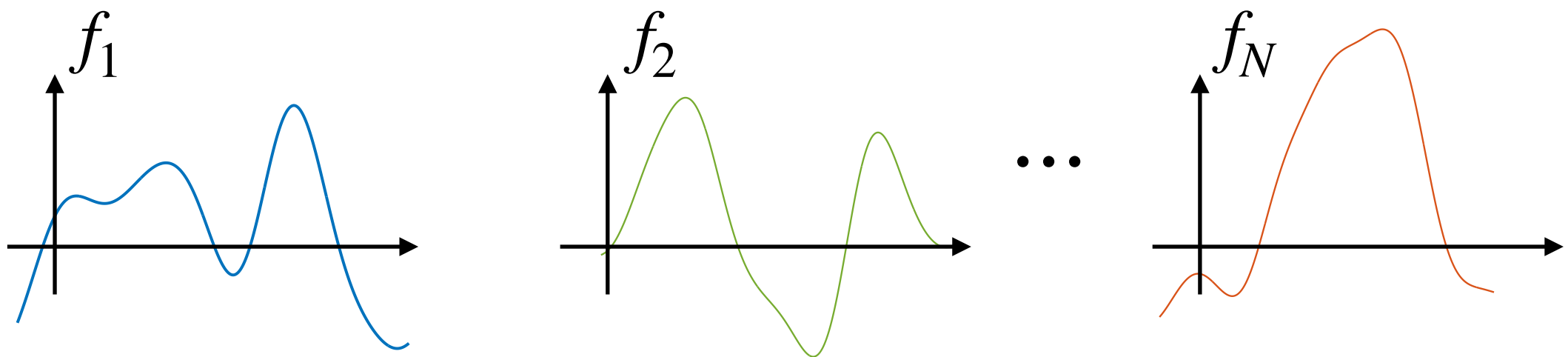
Bayesian optimization with an unknown prior

- Our idea: learn the “prior” from past experience with similar functions
- Assumption: we can collect data on functions sampled from the same prior

[Wang*&Kim*&Kaelbling, NIPS 2018]

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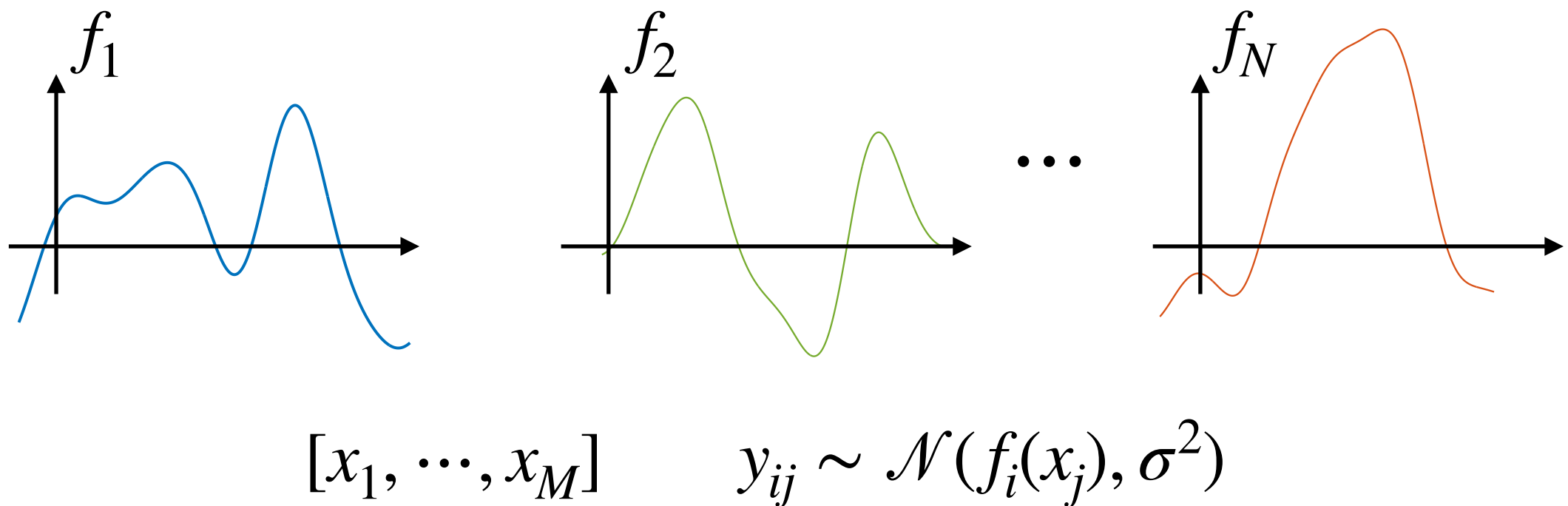
- Our idea: learn the “prior” from past experience with similar functions
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[Wang* & Kim* & Kaelbling, NIPS 2018]

Bayesian optimization with an unknown prior

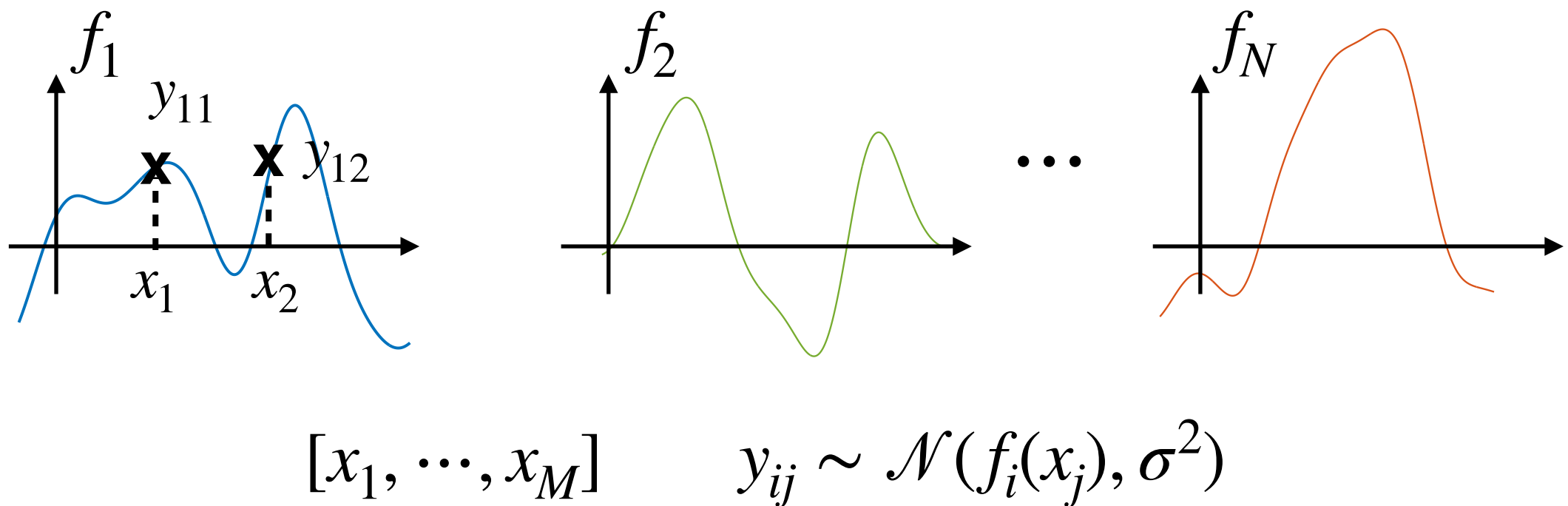
- Our idea: learn the “prior” from past experience with similar functions
- Assumption: we can collect data on functions sampled from the same prior $f_1, f_2, \dots, f_N \sim GP(\mu, k)$



[Wang*&Kim*&Kaelbling, NIPS 2018]

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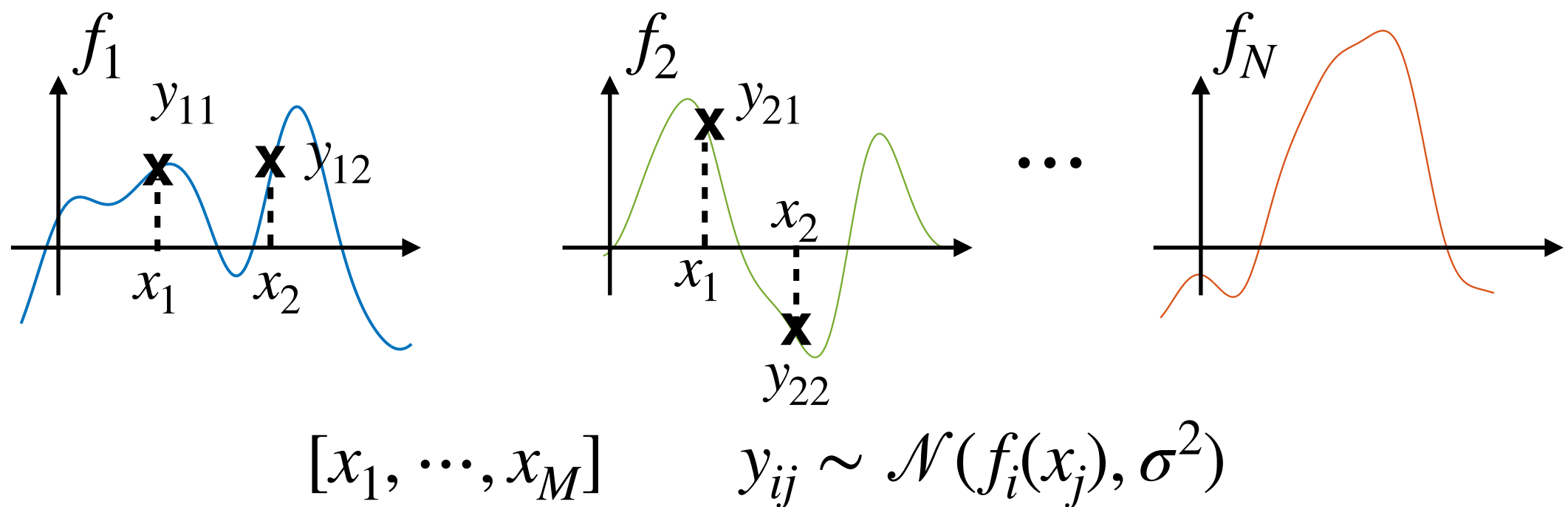
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[Wang*&Kim*&Kaelbling, NIPS 2018]

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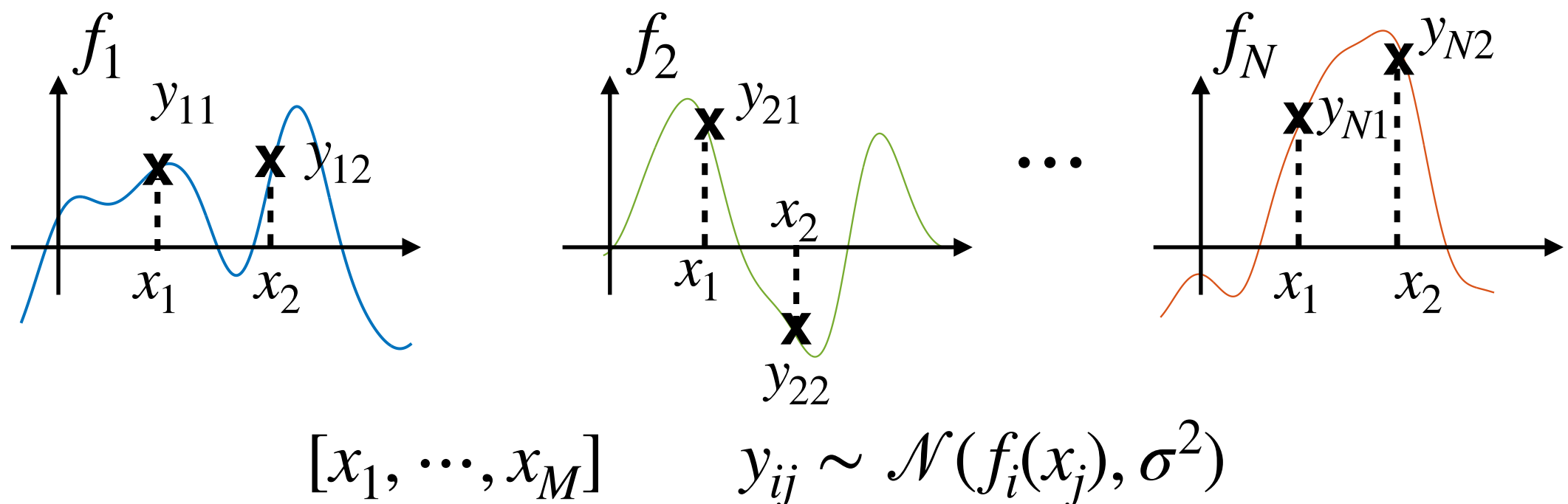
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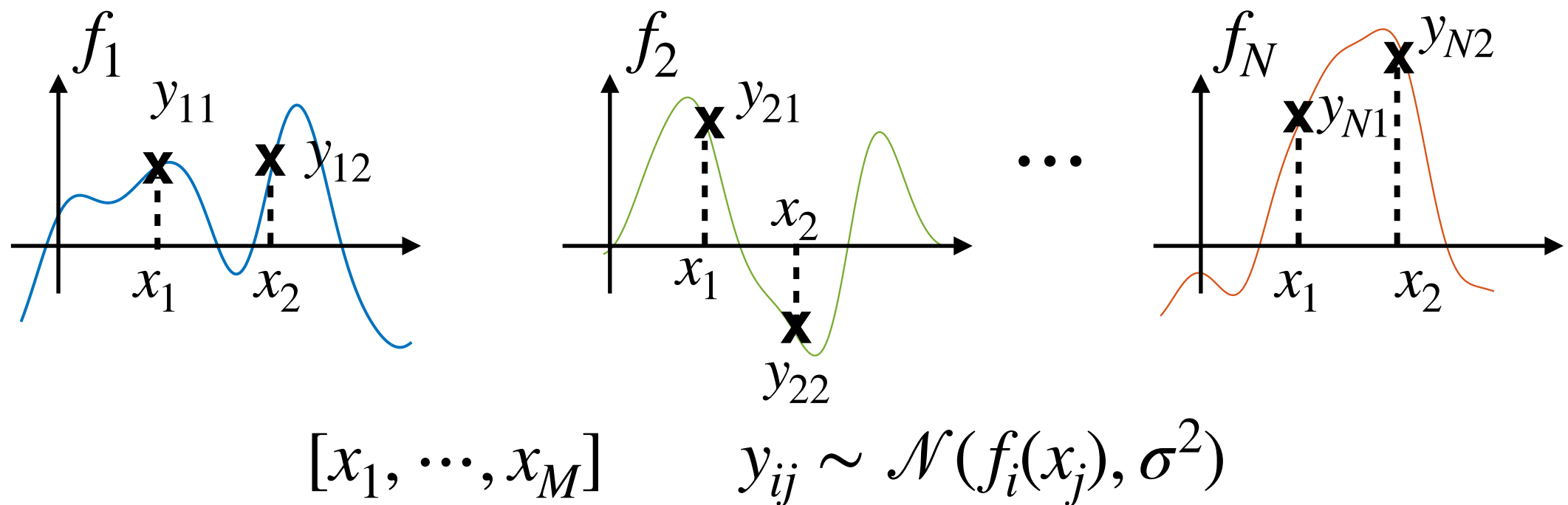


[Wang*&Kim*&Kaelbling, NIPS 2018]

Bayesian optimization with an unknown prior

meta / multi-task / transfer learning

- Our idea: learn the “prior” from past experience with similar functions
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[Wang*&Kim*&Kaelbling, NIPS 2018]

Bayesian optimization with an unknown prior

Generic knowledge on functions

distribution over functions

$GP(\mu, k)$

$f_1, f_2, \dots, f_N, f \sim GP(\mu, k)$

function 1

f_1

x_1, y_{11} x_2, y_{12} ...

function 2

f_2

x_1, y_{21} x_2, y_{22} ...

...

new
function

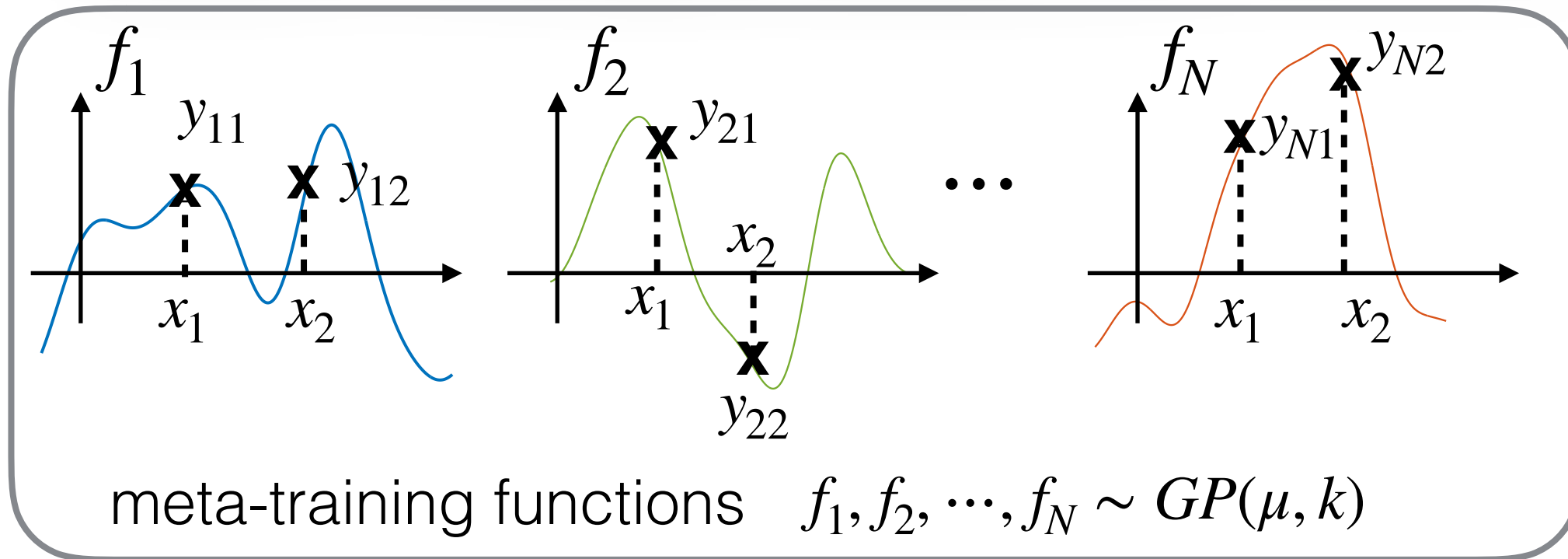
f

?? ?? ...

observations of
function values

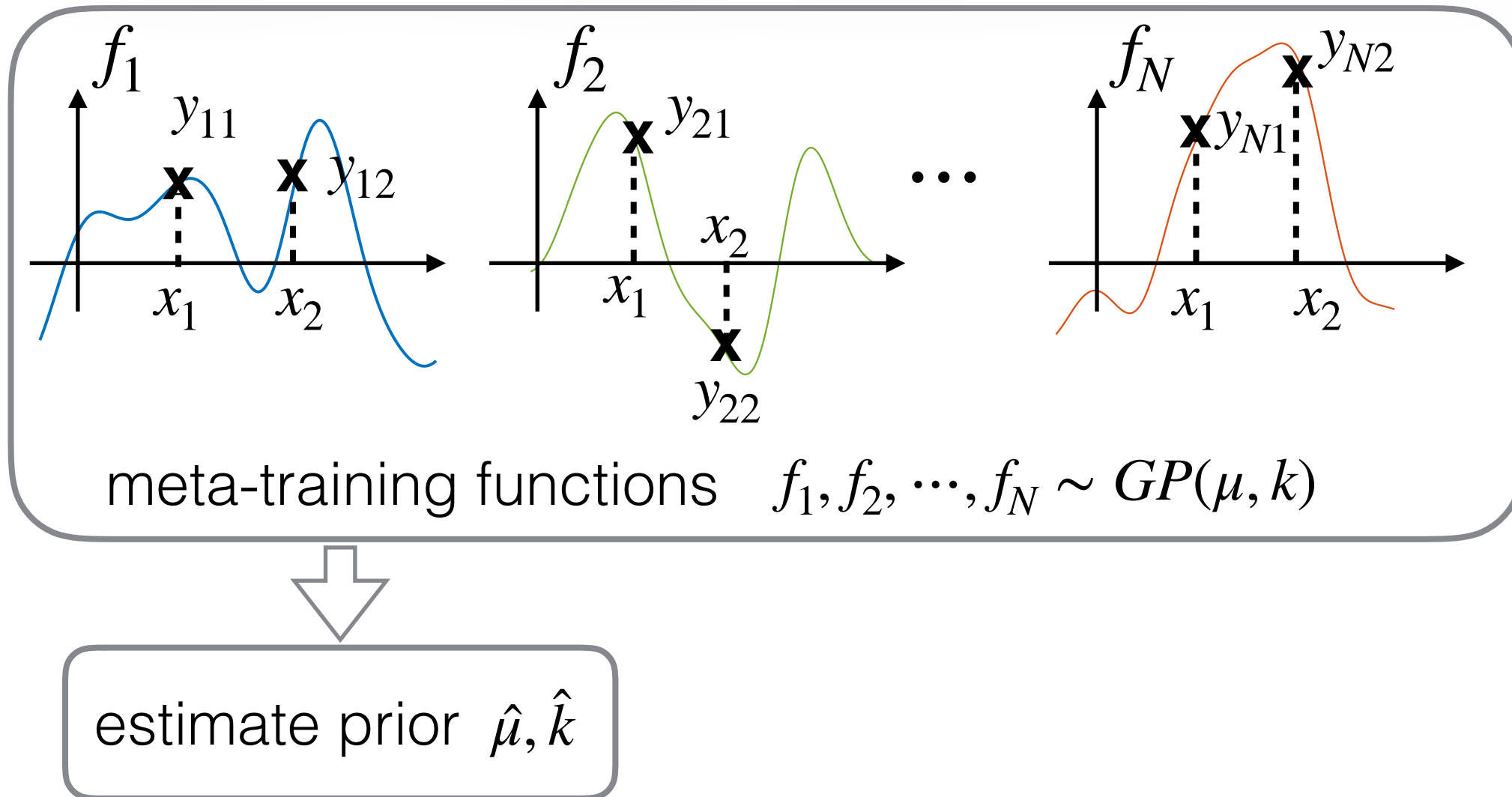
[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



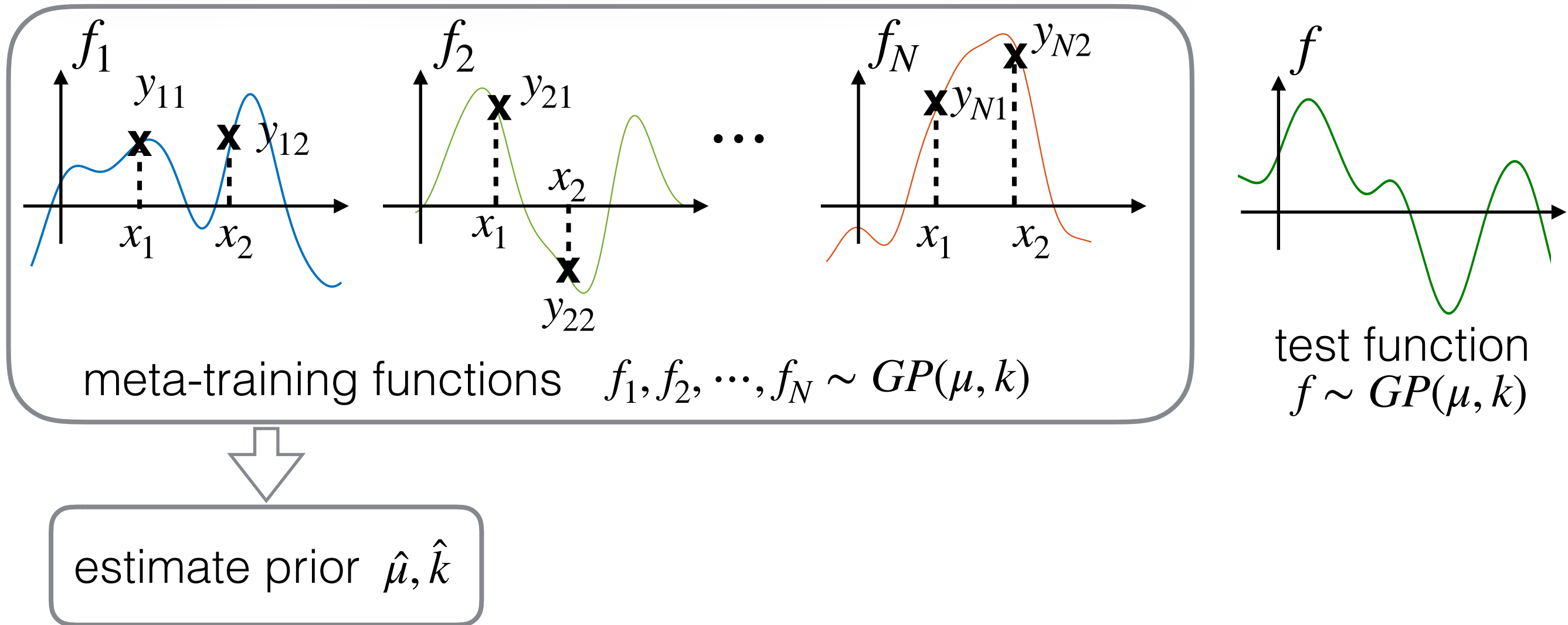
[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



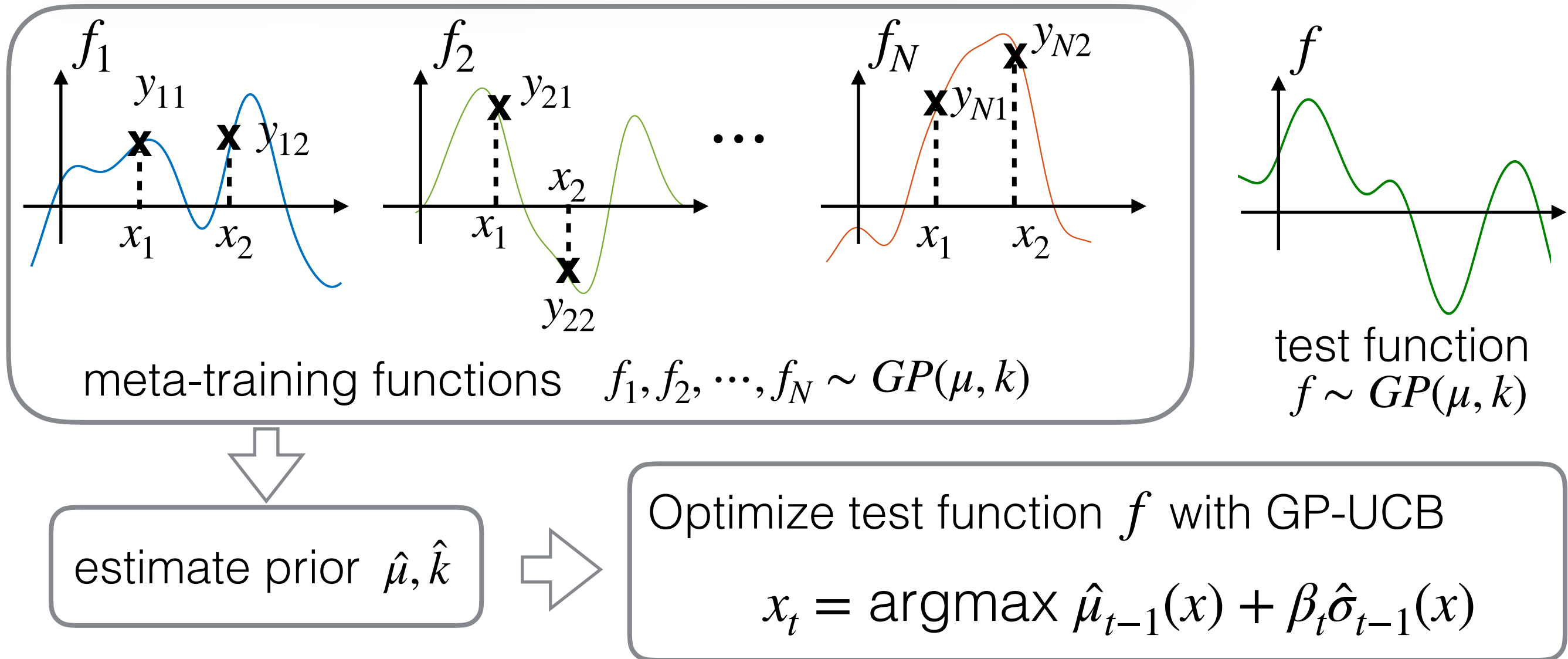
[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



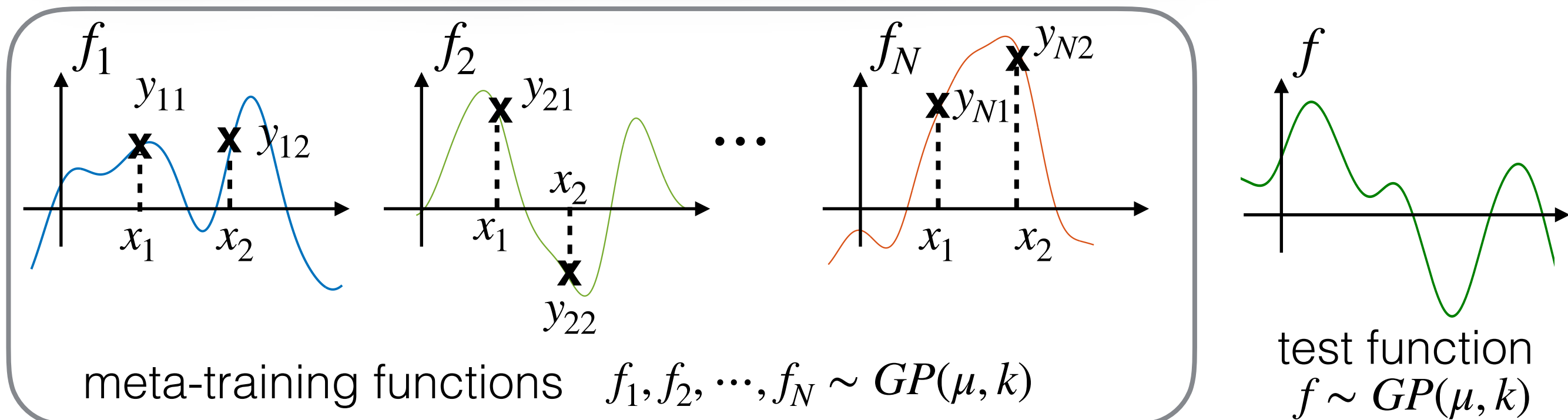
[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



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

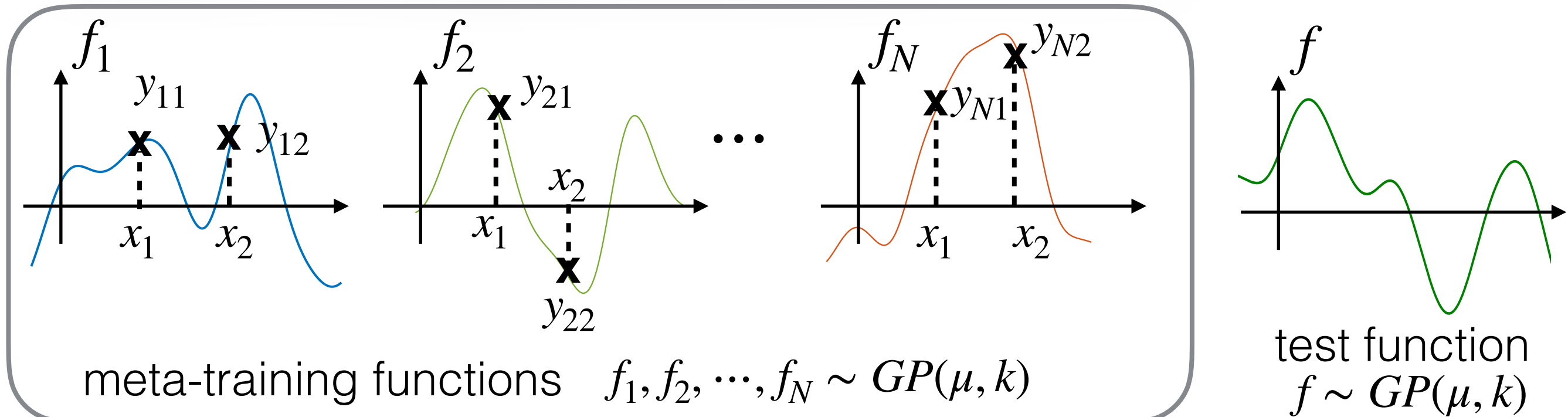
Optimize test function f with GP-UCB

$$x_t = \operatorname{argmax} \hat{\mu}_{t-1}(x) + \beta_t \hat{\sigma}_{t-1}(x)$$

$$\beta_t = \frac{\left(6(N-3+t+2\sqrt{t \log \frac{6}{\delta}} + 2 \log \frac{6}{\delta}) / (\delta N(N-t-1)) \right)^{\frac{1}{2}} + (2 \log(\frac{3}{\delta}))^{\frac{1}{2}}}{(1 - 2(\frac{1}{N-t} \log \frac{6}{\delta})^{\frac{1}{2}})^{\frac{1}{2}}}$$

[Wang* & Kim* & Kaelbling, NIPS 2018]

Meta Bayesian optimization with an unknown prior



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N	δ	t	$\beta_t(N, \delta)$
50	0.01	10	19.0
100	0.01	10	9.7
1000	0.01	10	4.5

[Wang*&Kim*&Kaelbling, NIPS 2018]

Regret bound for meta BO with unknown prior

Theorem (informal)

simple regret: $r_T = \max_{x \in \mathcal{X}} f(x) - \max_{t \in [T]} f(x_t)$

Important assumptions:

- meta-training functions come from the same prior
- enough number of meta-training functions $N \geq O(\max(T, M))$
- kernel function is bounded

[Wang*&Kim*&Kaelbling, NIPS 2018]

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↑
#observations on each
training function

[Wang* & Kim* & Kaelbling, NIPS 2018]

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T observations on the test function f

[Wang* & Kim* & Kaelbling, NIPS 2018]

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#observations on each
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Given T observations on the test function f , with probability $1 - \delta$,

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

[Wang* & Kim* & Kaelbling, NIPS 2018]

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constant
depending on δ

[Wang* & Kim* & Kaelbling, NIPS 2018]

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constant
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linear kernel

↑
observation noise

[Wang*&Kim*&Kaelbling, NIPS 2018]

Discrete input space $|\mathcal{X}| = M$

Prior estimation with meta training data $\{[(x_j, y_{ij})]_{j=1}^M\}_{i=1}^N$

$$Y = \begin{bmatrix} y_{11} & \cdots & y_{1M} \\ \cdots & & \cdots \\ y_{N1} & \cdots & y_{NM} \end{bmatrix}$$

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unbiased prior estimator

$$\hat{\mu}(\mathcal{X}) = \frac{1}{N} Y^T \mathbf{1}_N \sim \mathcal{N}(\mu(\mathcal{X}), \frac{1}{N} (k(\mathcal{X}) + \sigma^2 \mathbf{I}))$$

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unbiased posterior estimator

$$\hat{\mu}_t(x) = \hat{\mu}(x) + \hat{k}(x, \mathbf{x}_t) \hat{k}(\mathbf{x}_t, \mathbf{x}_t)^{-1} (y_t - \hat{\mu}(\mathbf{x}_t))$$

$$\hat{\sigma}_t^2(x, x') = \frac{N-1}{N-t-1} \left(\hat{k}(x, x') - \hat{k}(x, \mathbf{x}_t) \hat{k}(\mathbf{x}_t, \mathbf{x}_t)^{-1} \hat{k}(\mathbf{x}_t, x') \right)$$

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$$\hat{\mu}_t(x) = \text{can bound } |\hat{\mu}_t(x) - \mu_t(x)|$$

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bias correction

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$\sim$ **Wishart distribution**

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unbiased posterior estimator

$$\hat{\mu}_t(x) = \text{can bound } |\hat{\mu}_t(x) - \mu_t(x)|$$

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Continuous input space

assume basis functions are given!

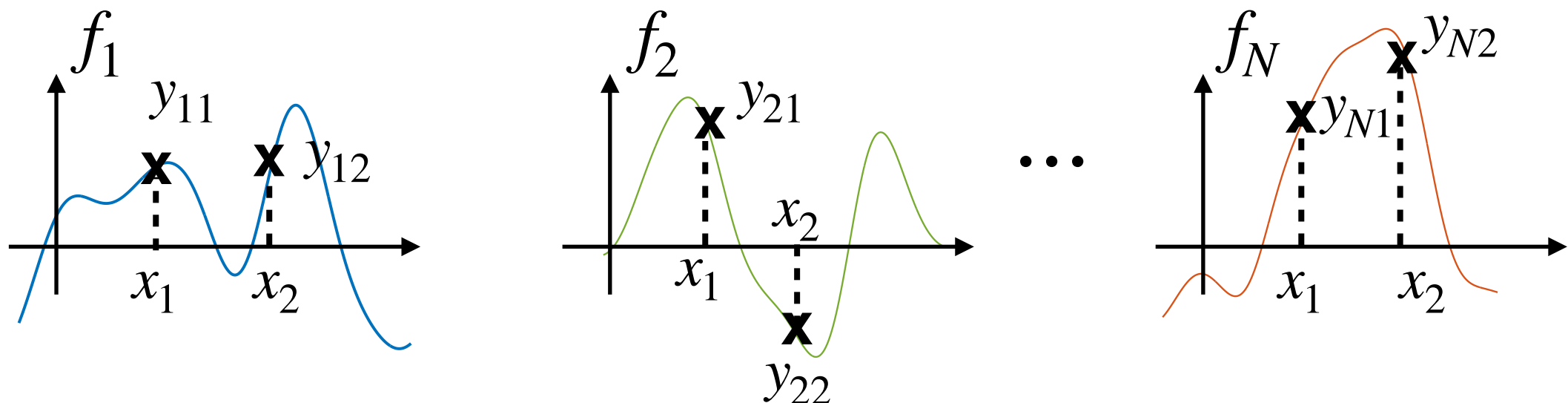
basis functions

mean parameter

covariance parameter

$$f = \Phi(x)^T W \sim GP(\mu, k) \quad W \sim \mathcal{N}(\mathbf{u}, \Sigma)$$

$$\mu(x) = \Phi(x)^T \mathbf{u} \quad k(x, x') = \Phi(x)^T \Sigma \Phi(x')$$

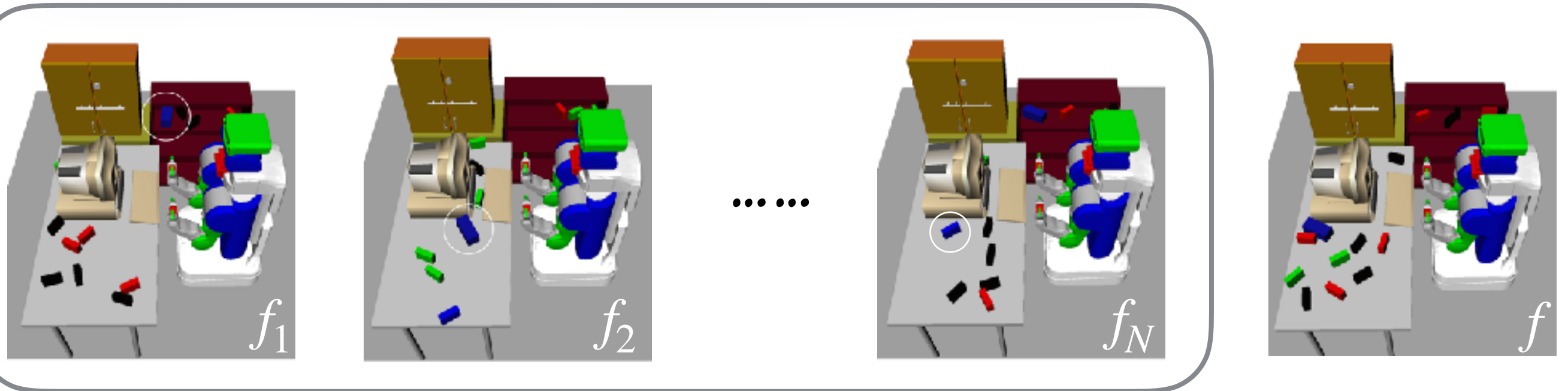


$$\Phi(X)^T W_i = Y_i \implies W_i = (\Phi(X)\Phi(X)^T)^{-1} \Phi(X) Y_i$$

estimate its mean and covariance to construct GP prior

[Neal, 1996; Wang*&Kim*&Kaelbling, NIPS 2018]

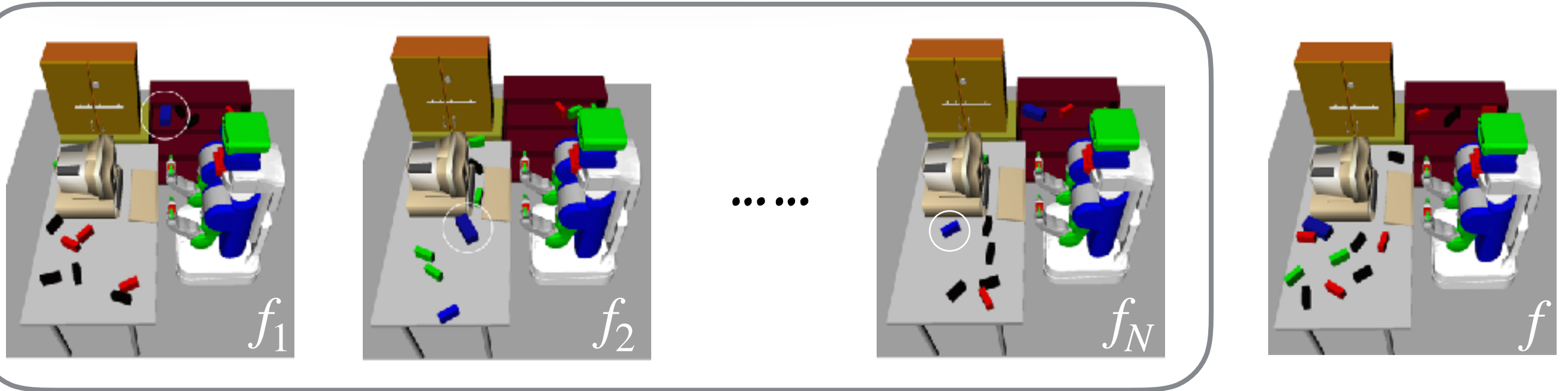
Empirical results on block picking and placing



meta-training data $N = 1500, M = 1000$

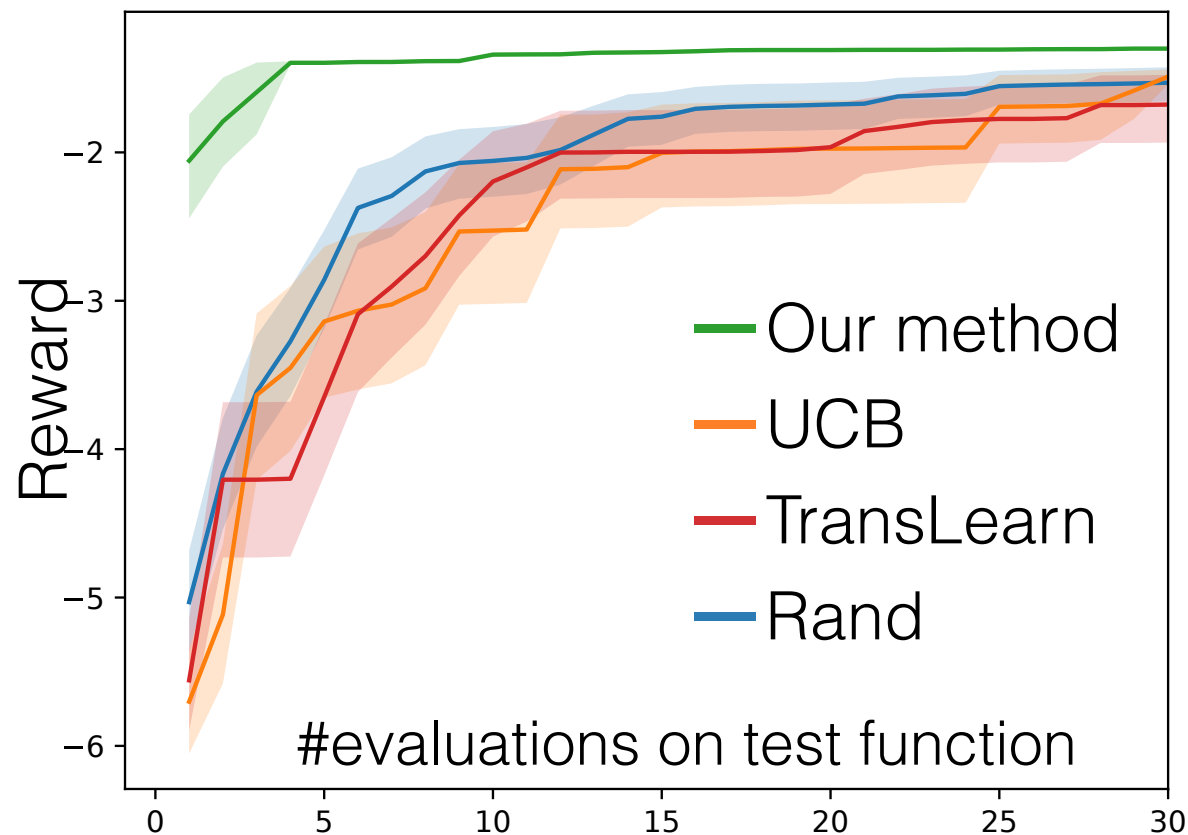
test function

Empirical results on block picking and placing

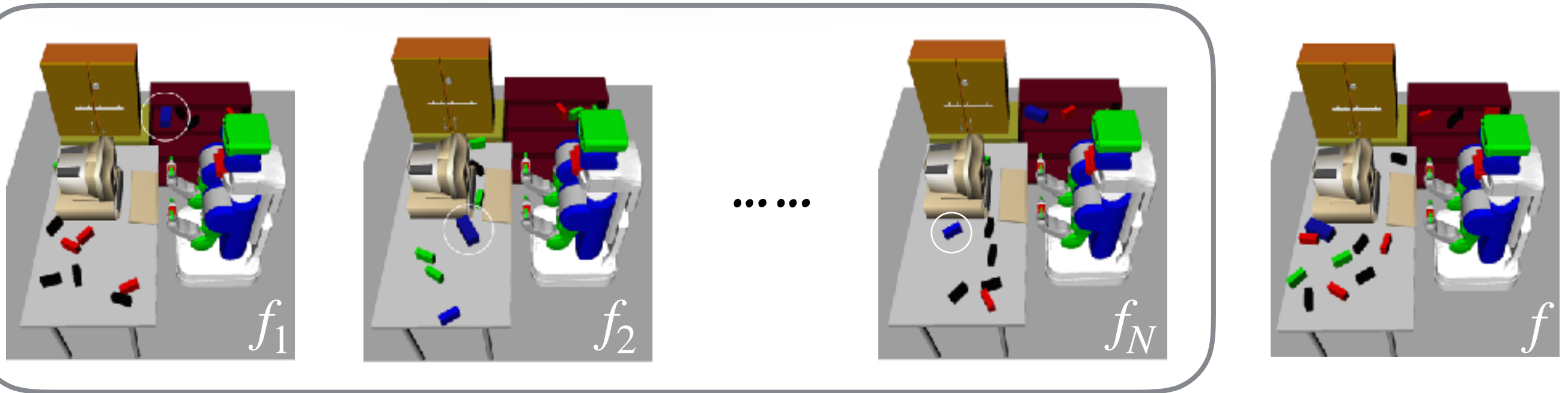


meta-training data $N = 1500, M = 1000$

test function

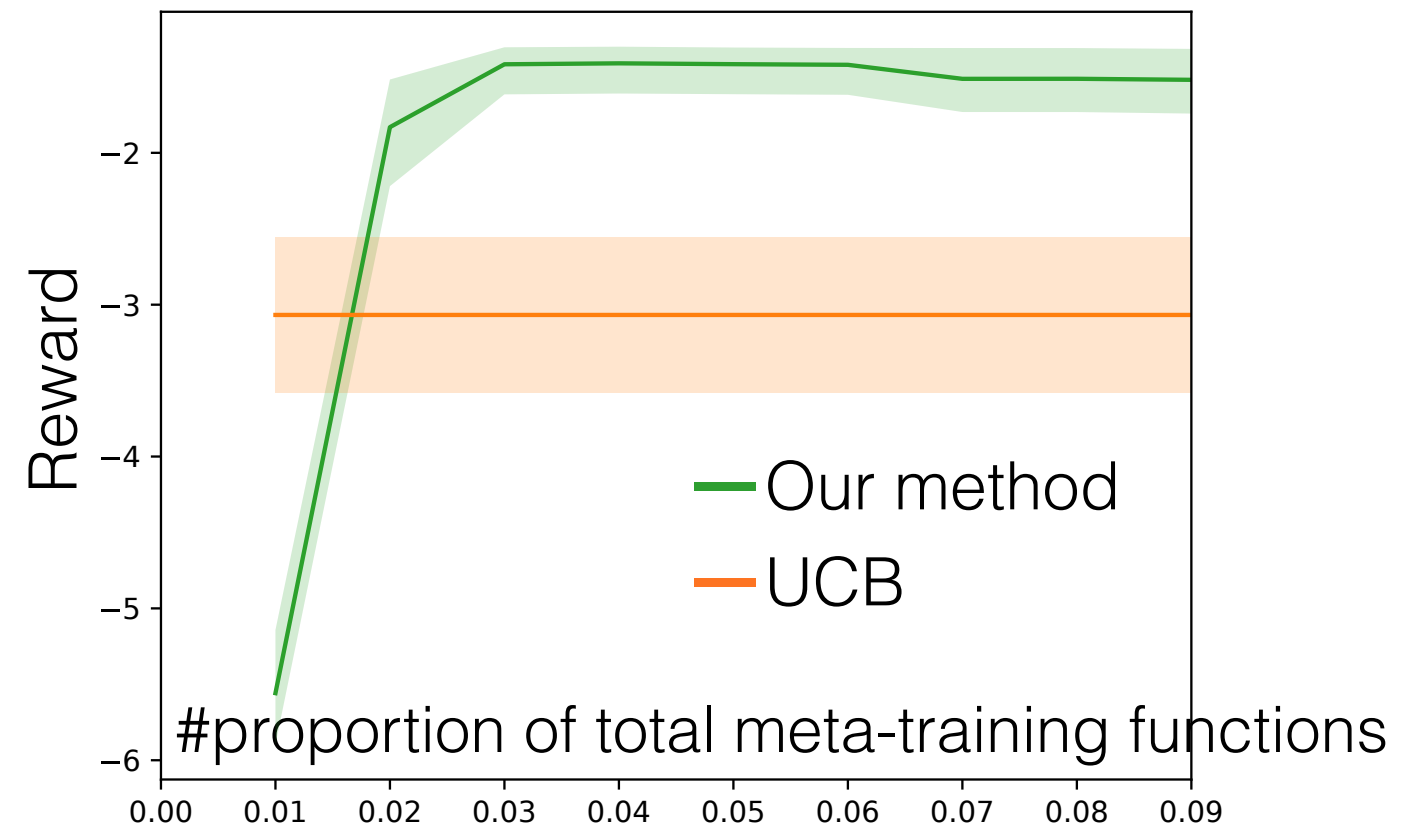
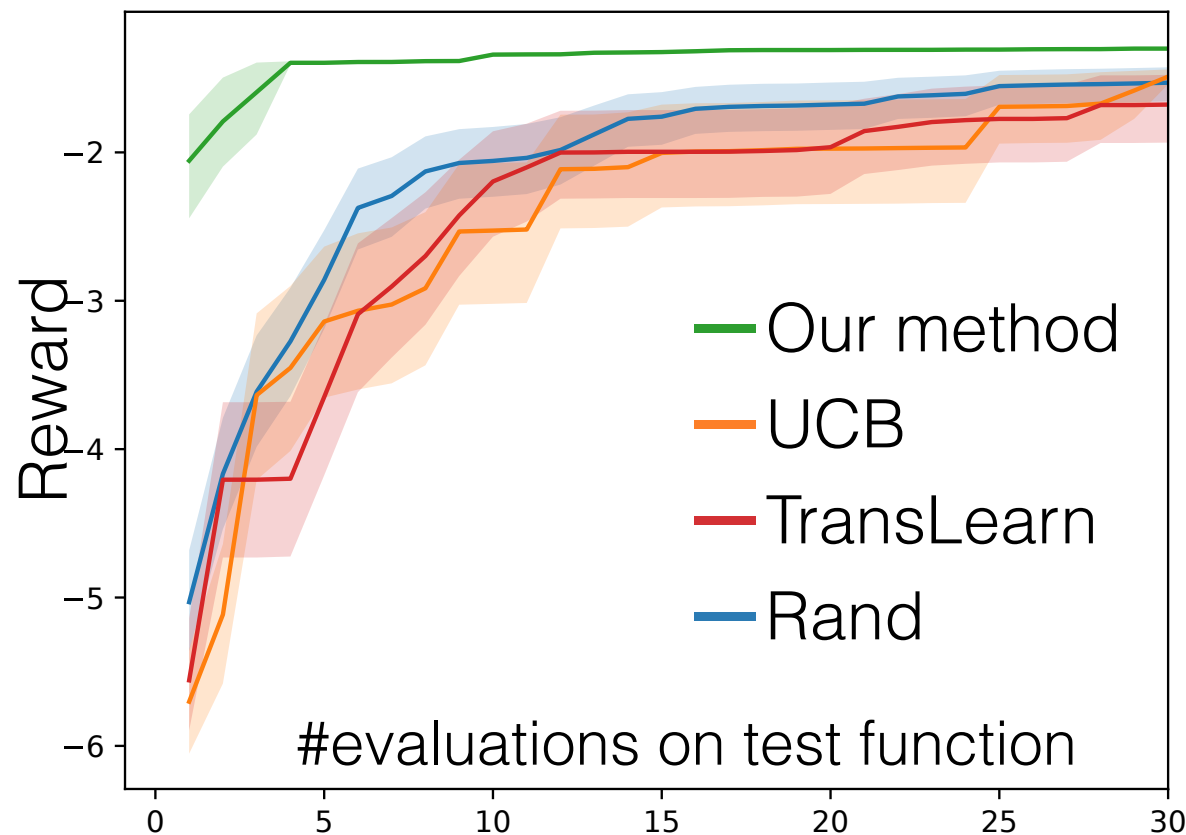


Empirical results on block picking and placing



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test function



Summary

- a regret bound for meta Bayesian optimization with an unknown prior but with assumptions on available data
- future directions
 - what if basis functions are unknown?
 - goodness-of-fit test for functions?
 - how to reduce the dependency on large N ?
$$N = O(\max(T, M))$$
- are there better estimators than unbiased ones?