Scalable Bandit Methods for Hyper-parameter Tuning

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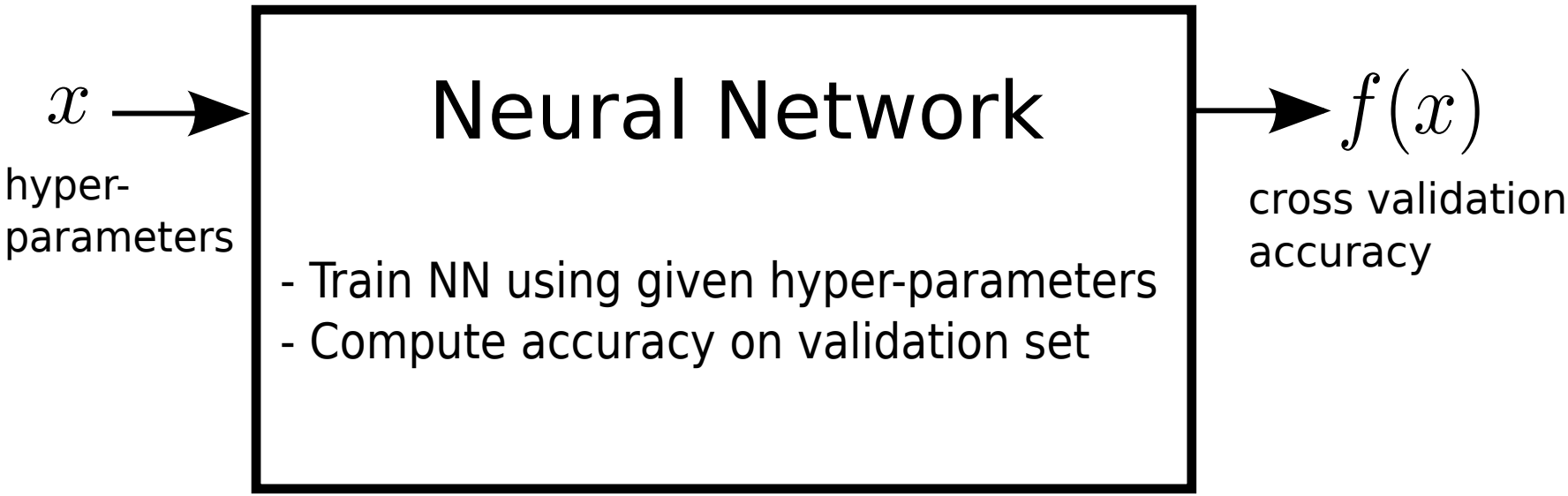
Carnegie Mellon University

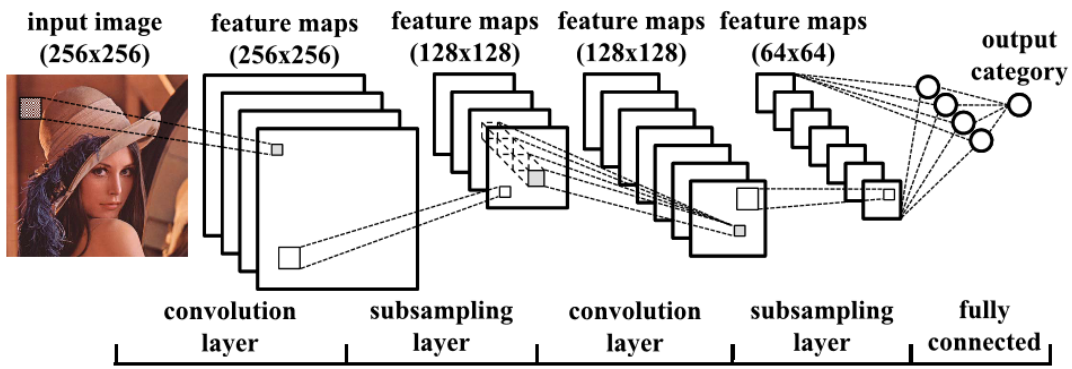
Guest Lecture - Scalable Machine Learning for Big Data Biology

University of Pittsburgh, Pittsburgh, PA

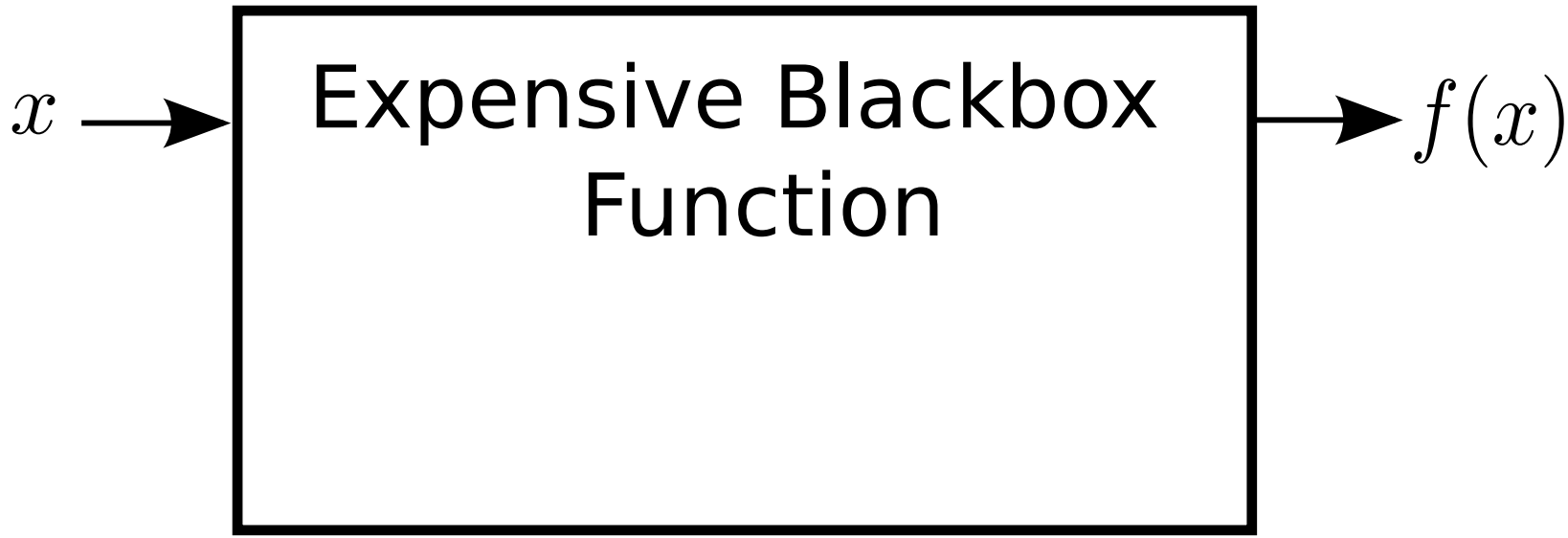
November 3, 2017

Hyper-parameter Tuning

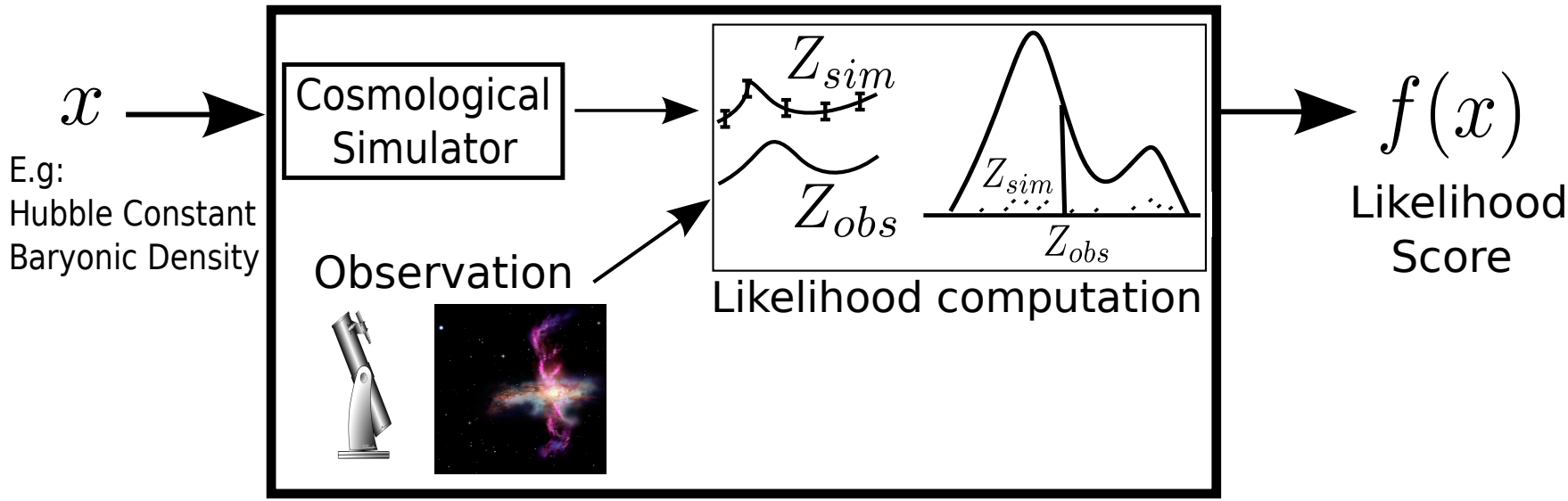


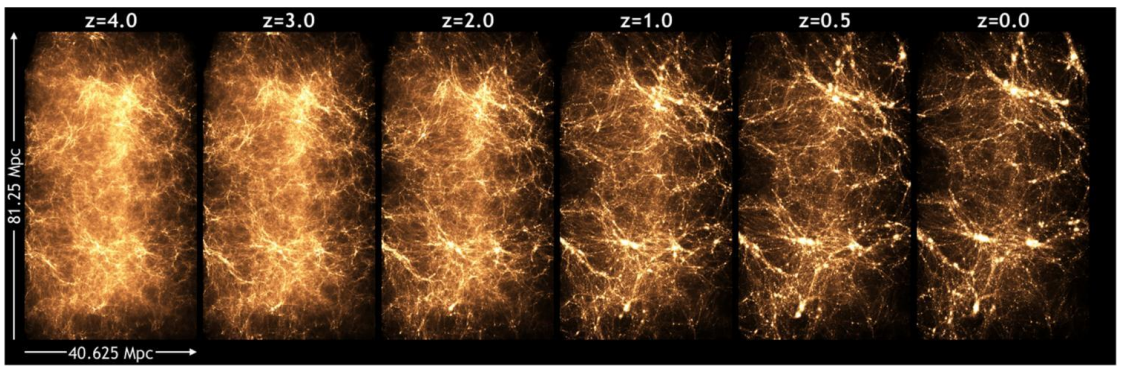


Black-box Optimisation



Maximum Likelihood estimation in Astrophysics





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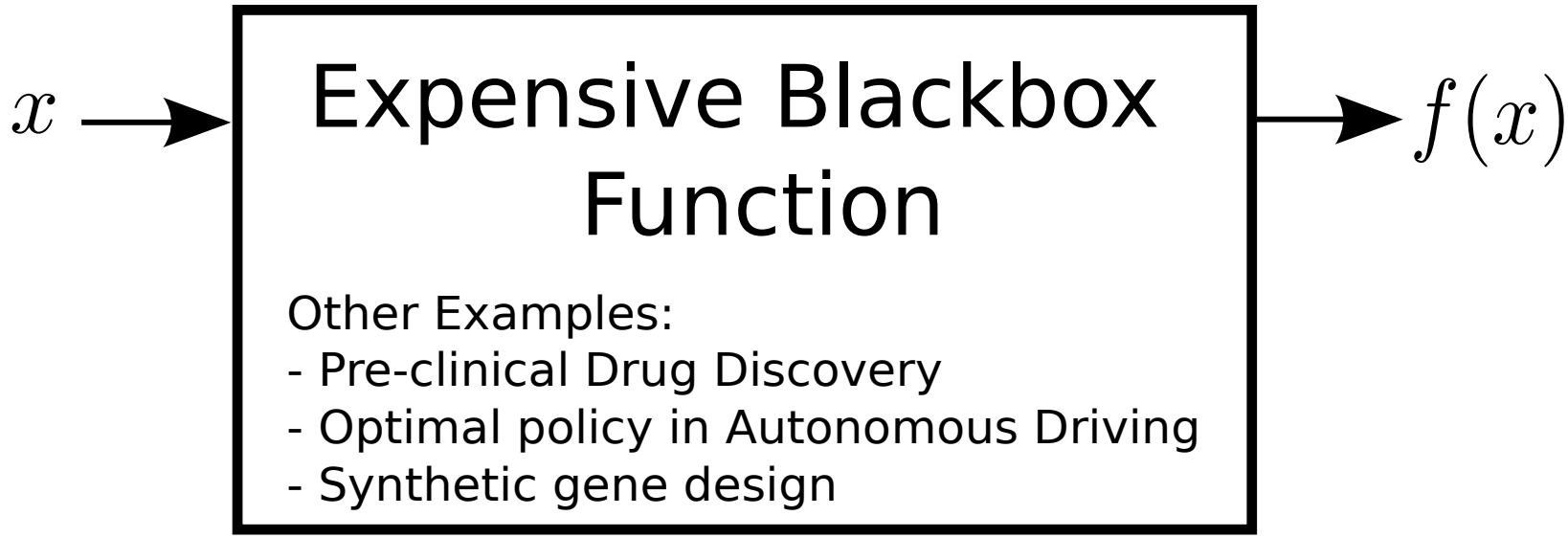
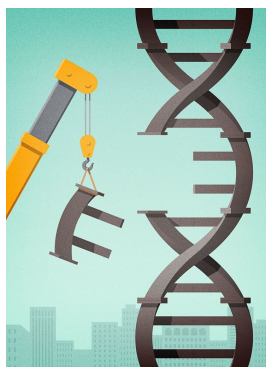
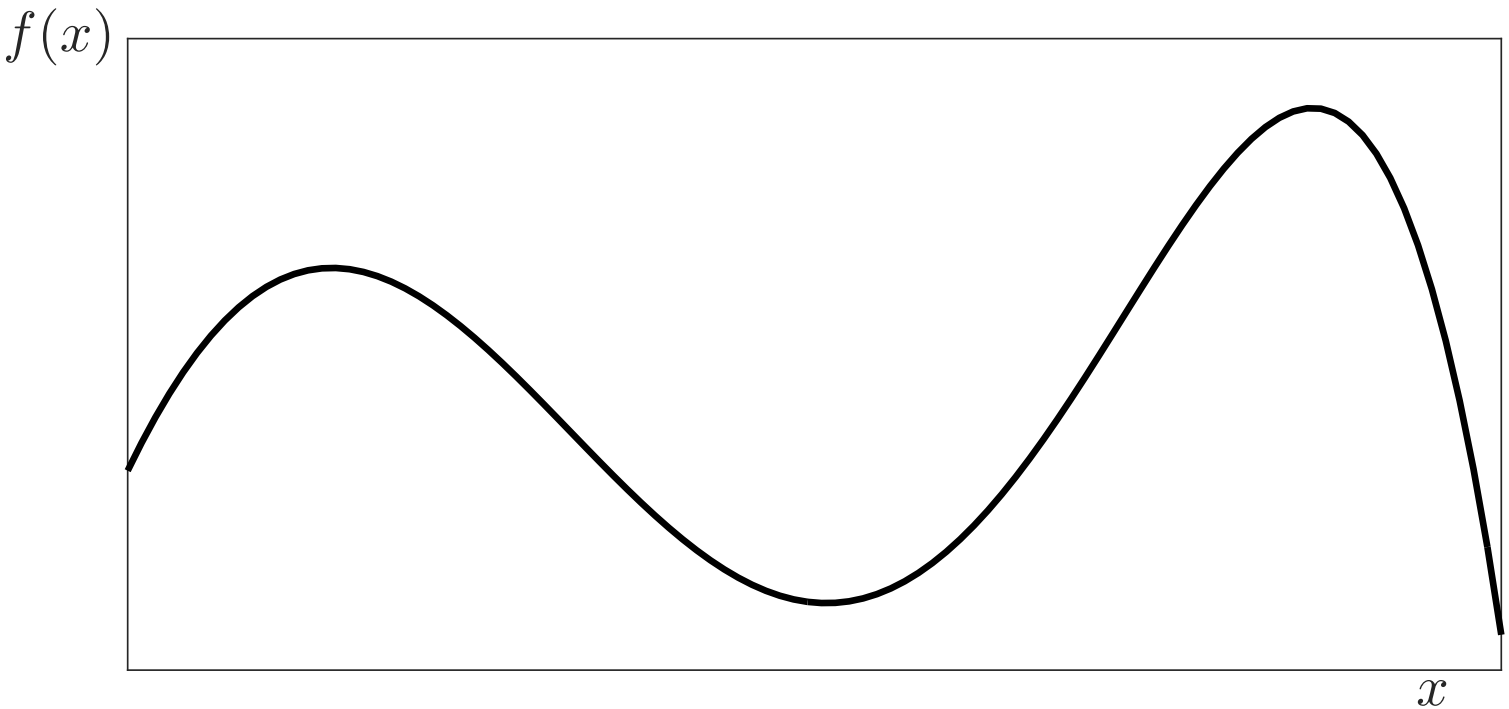




Black-box Optimisation

$f : \mathcal{X} \to \mathbb{R}$ is a black-box function that is accessible only via noisy evaluations.



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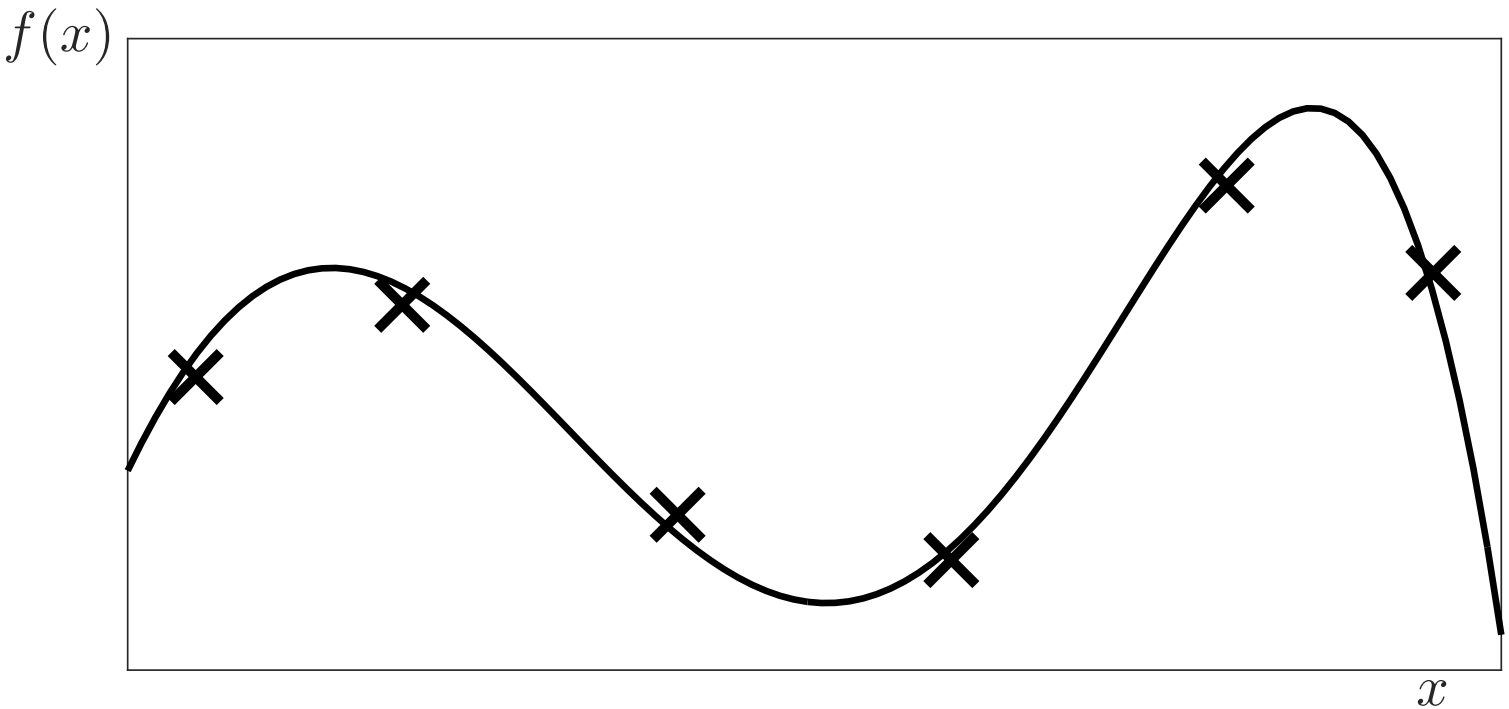

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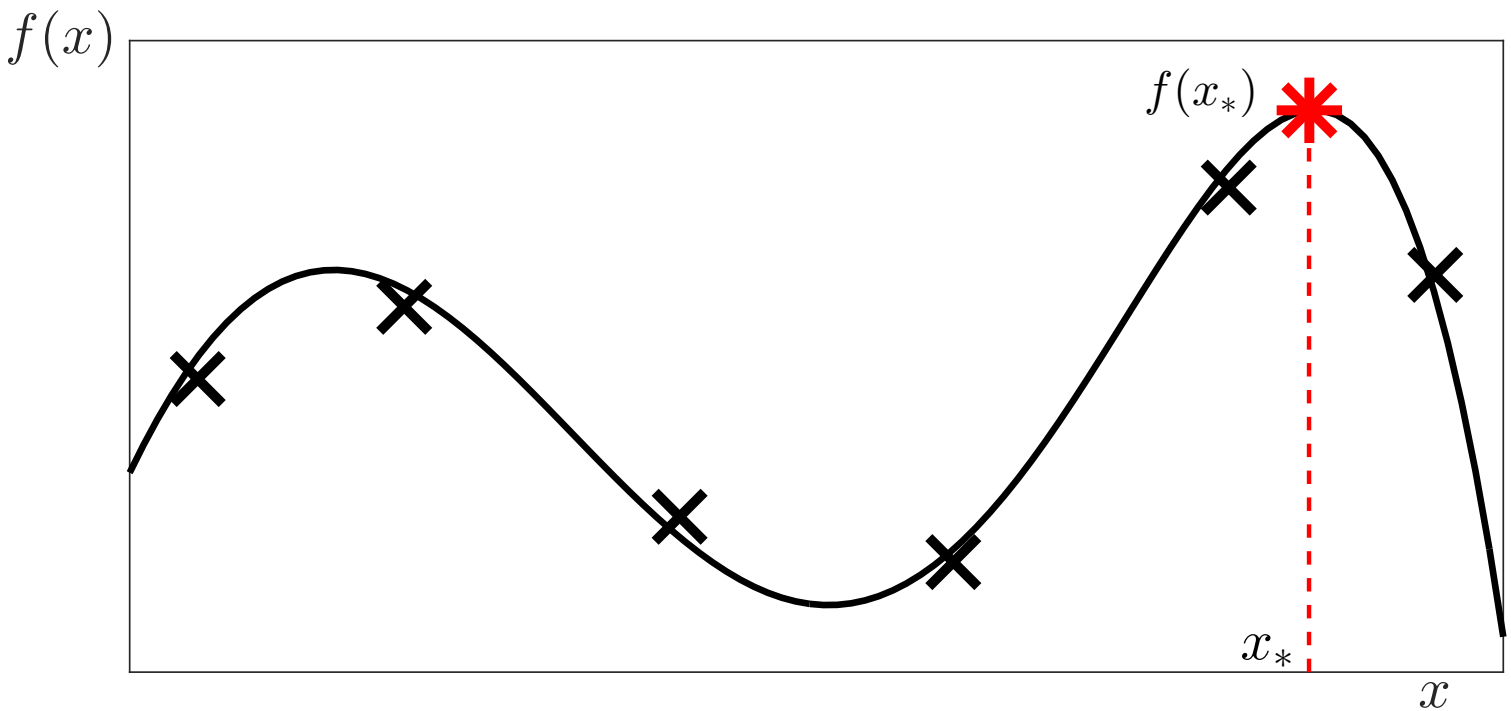

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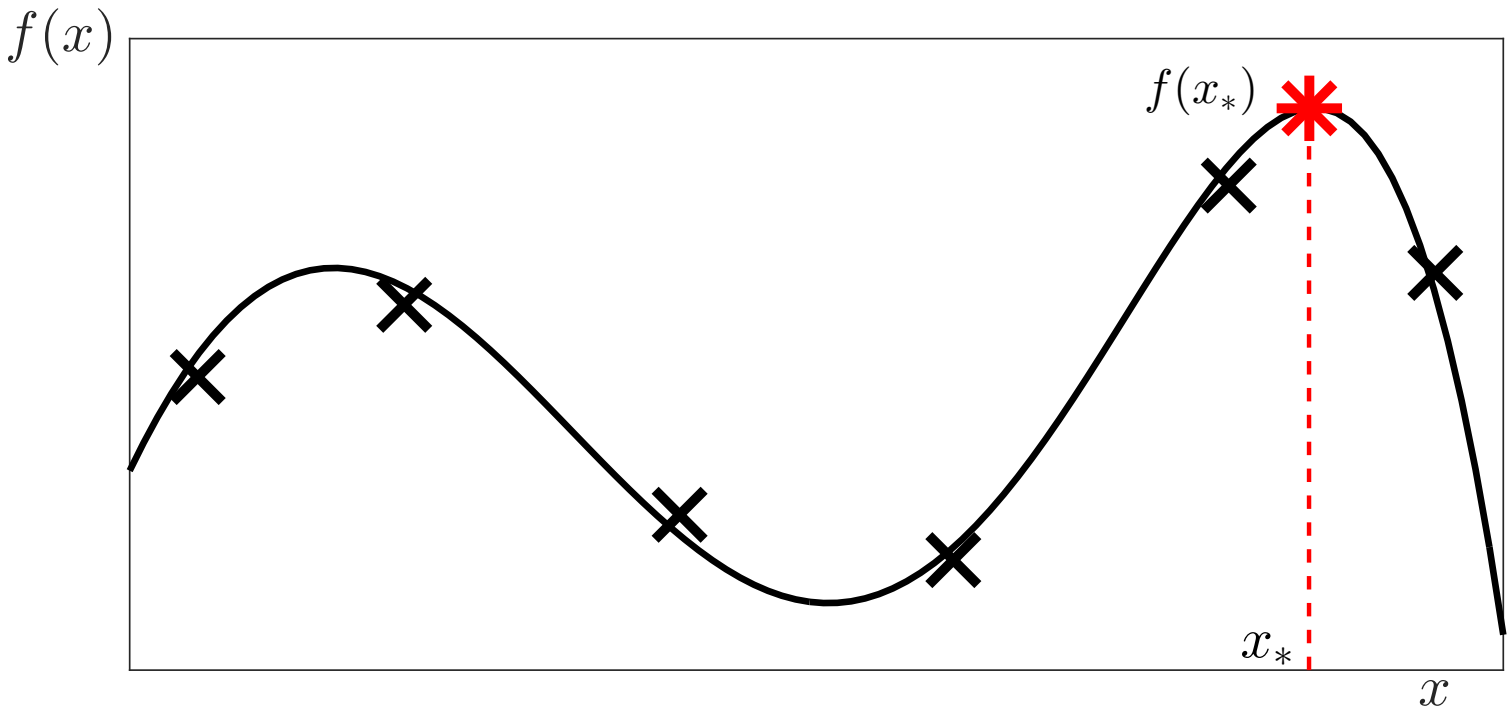

Simple Regret after n evaluations

$$S_n = f(x_\star) - \max_{t=1,\ldots,n} f(x_t).$$

Outline

- Part I: Bandits in the Bayesian Paradigm
  1. Gaussian processes
  2. Algorithms: Upper Confidence Bound (UCB) & Thompson Sampling (TS)
- Part II: Scaling up Bandits
  1. Multi-fidelity bandit: cheap approximations to an expensive experiment
  2. Parallelising function evaluations
  3. High dimensional input spaces

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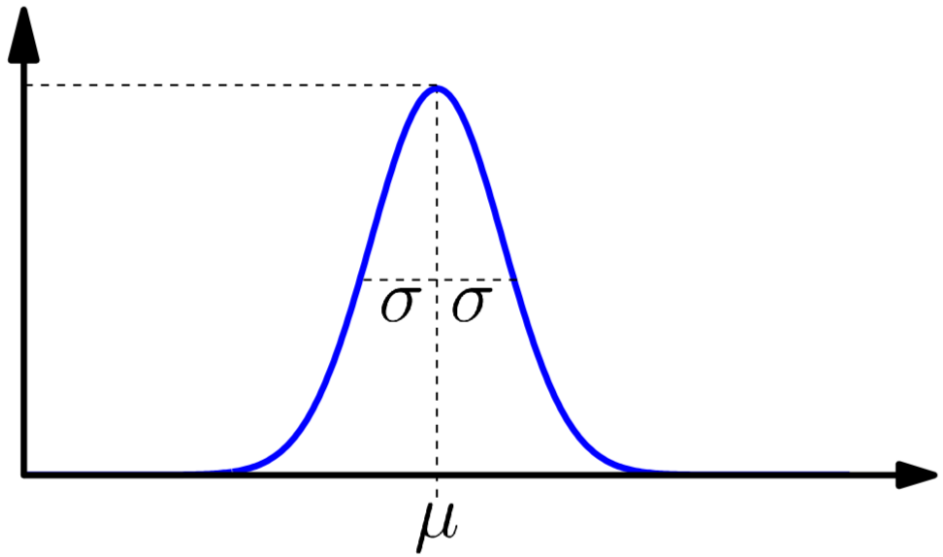
Gaussian (Normal) distribution $\mathcal{N}(\mu, \sigma^2)$



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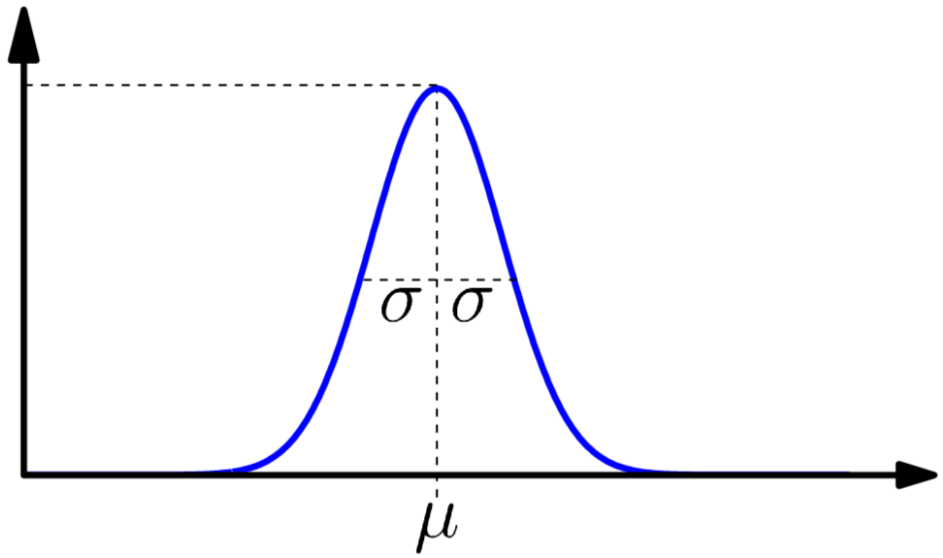

- A probability distribution for real valued random variables.
- Mean μ and variance σ^2 completely characterises distribution.
- For samples $X_1, \ldots, X_n$, let $\hat{\mu} = \frac{1}{n}\sum_i X_i$ be the sample mean. Then, $\hat{\mu} \pm 1.96\frac{\sigma}{\sqrt{n}}$ is a 95% confidence interval for μ.
- Can draw samples (e.g. in Matlab: `mu + sigma * randn()`).

Gaussian Processes ($\mathcal{GP}$)

$\mathcal{GP}(\mu, \kappa)$: A distribution over functions from $\mathcal{X}$ to $\mathbb{R}$.

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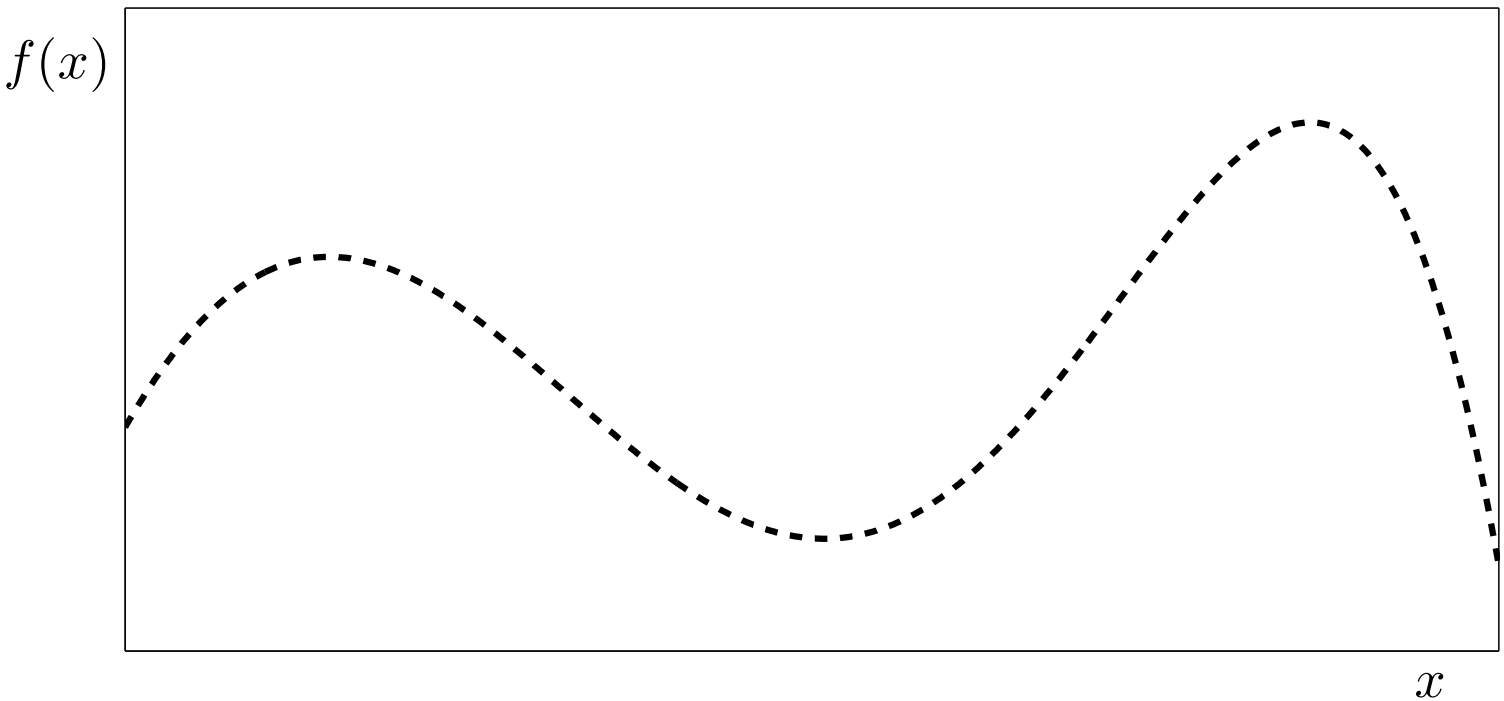
Functions with no observations



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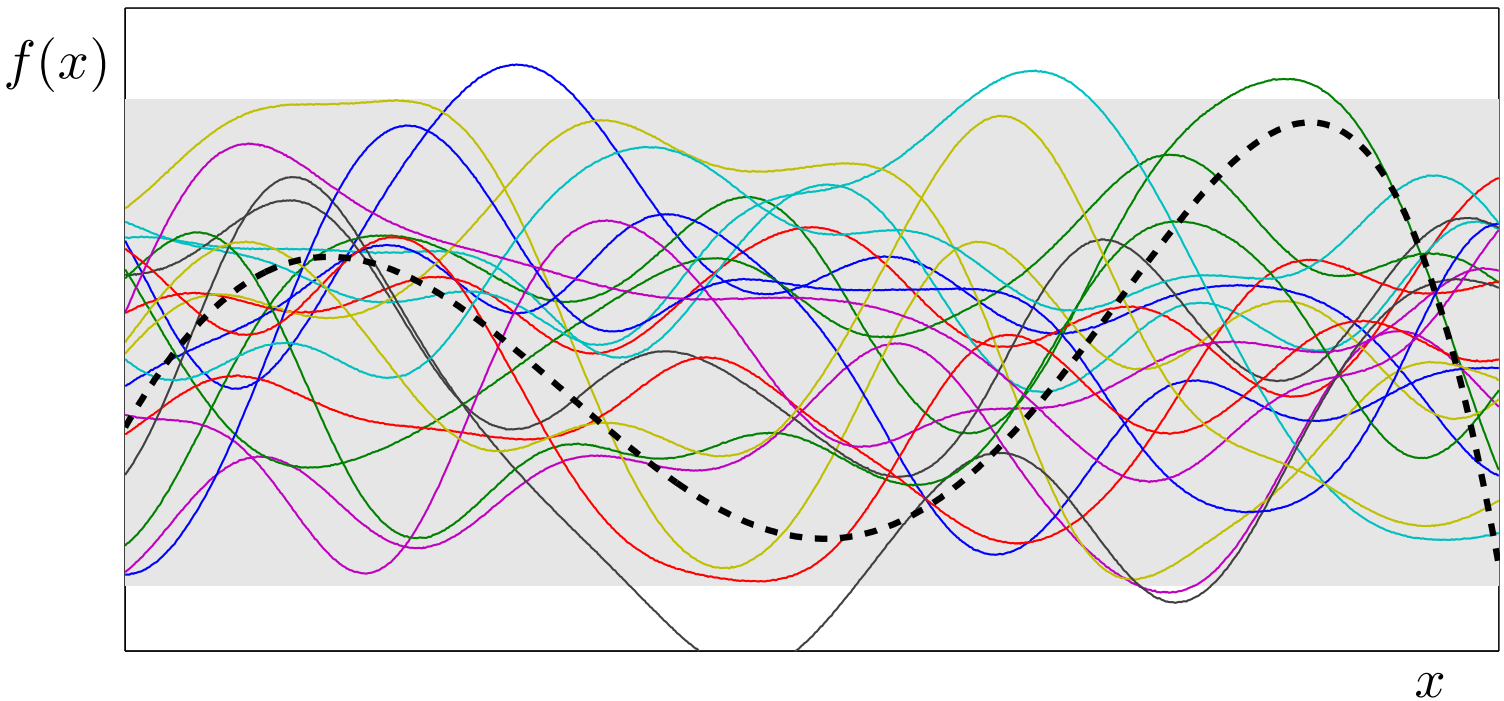
Prior $\mathcal{GP}$



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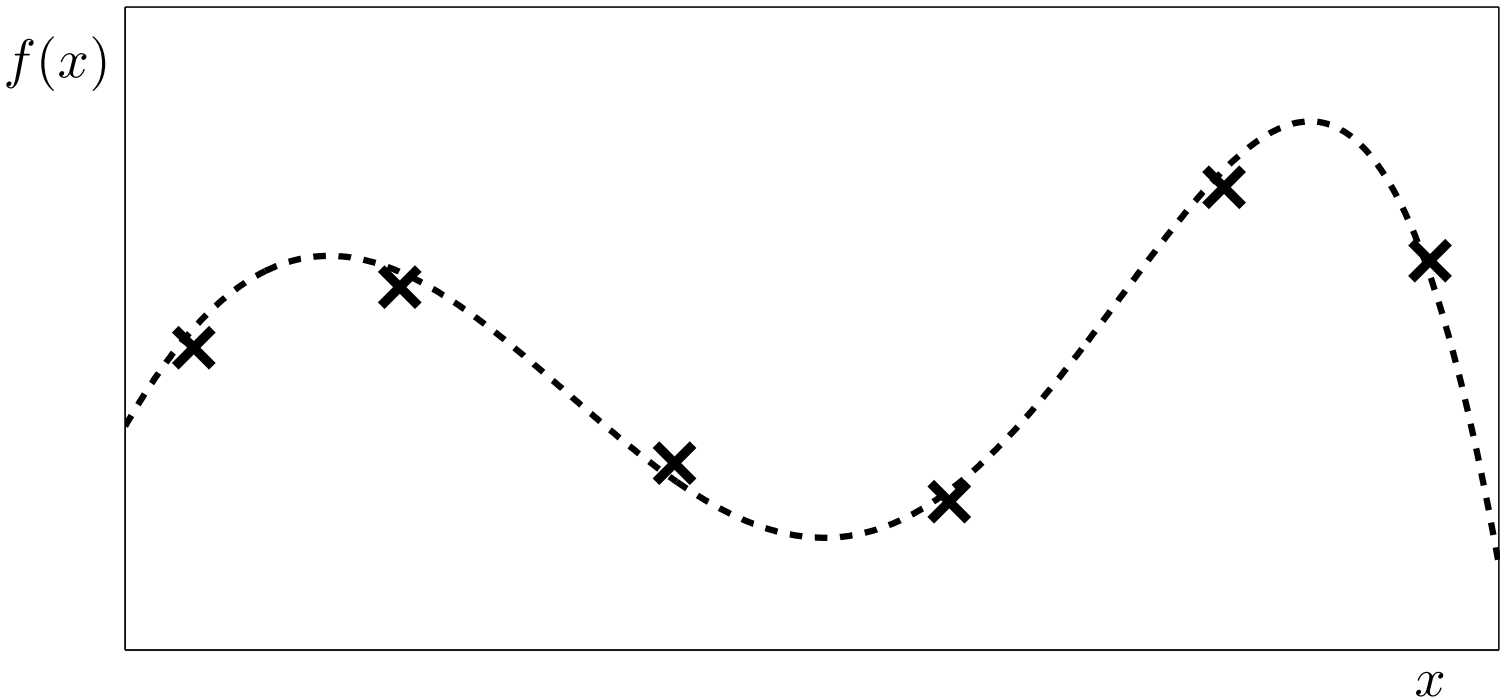
Observations



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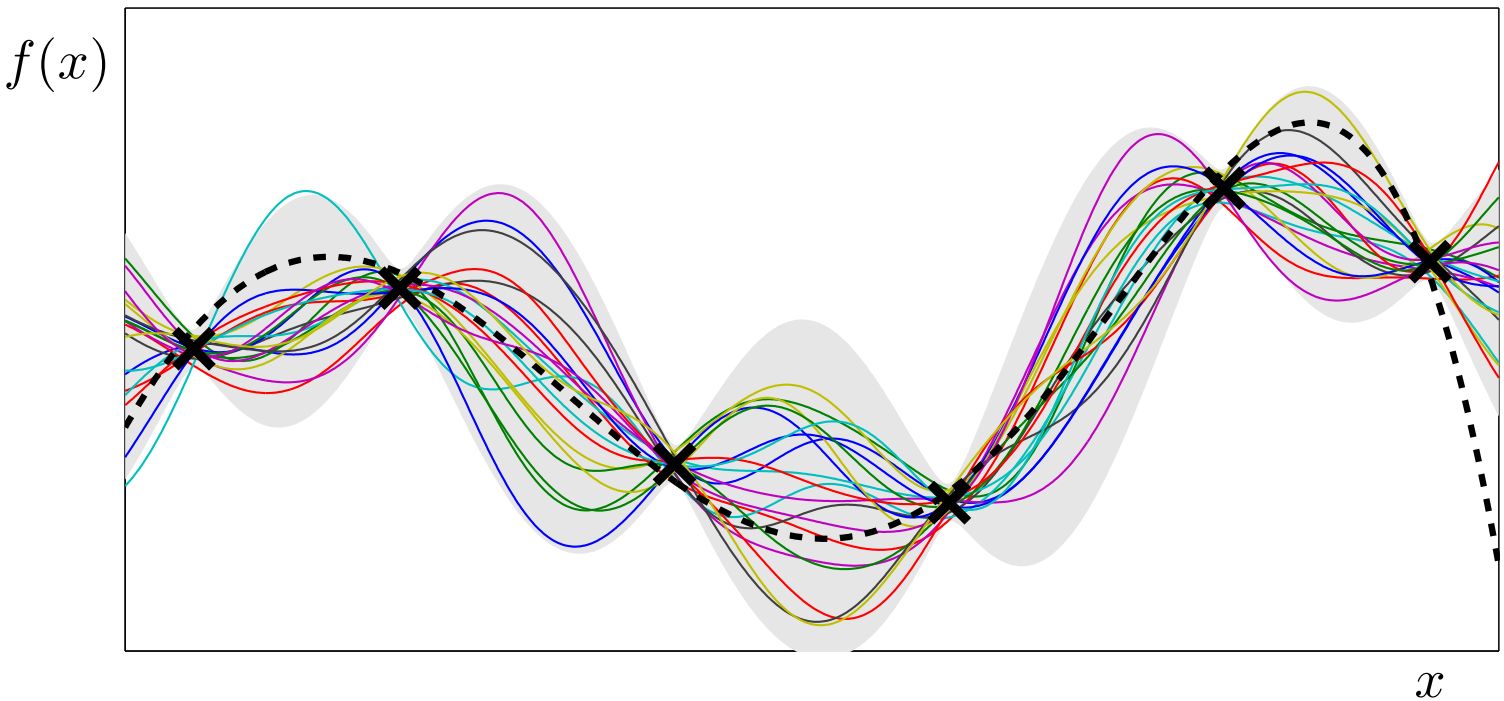
Posterior $\mathcal{GP}$ given observations



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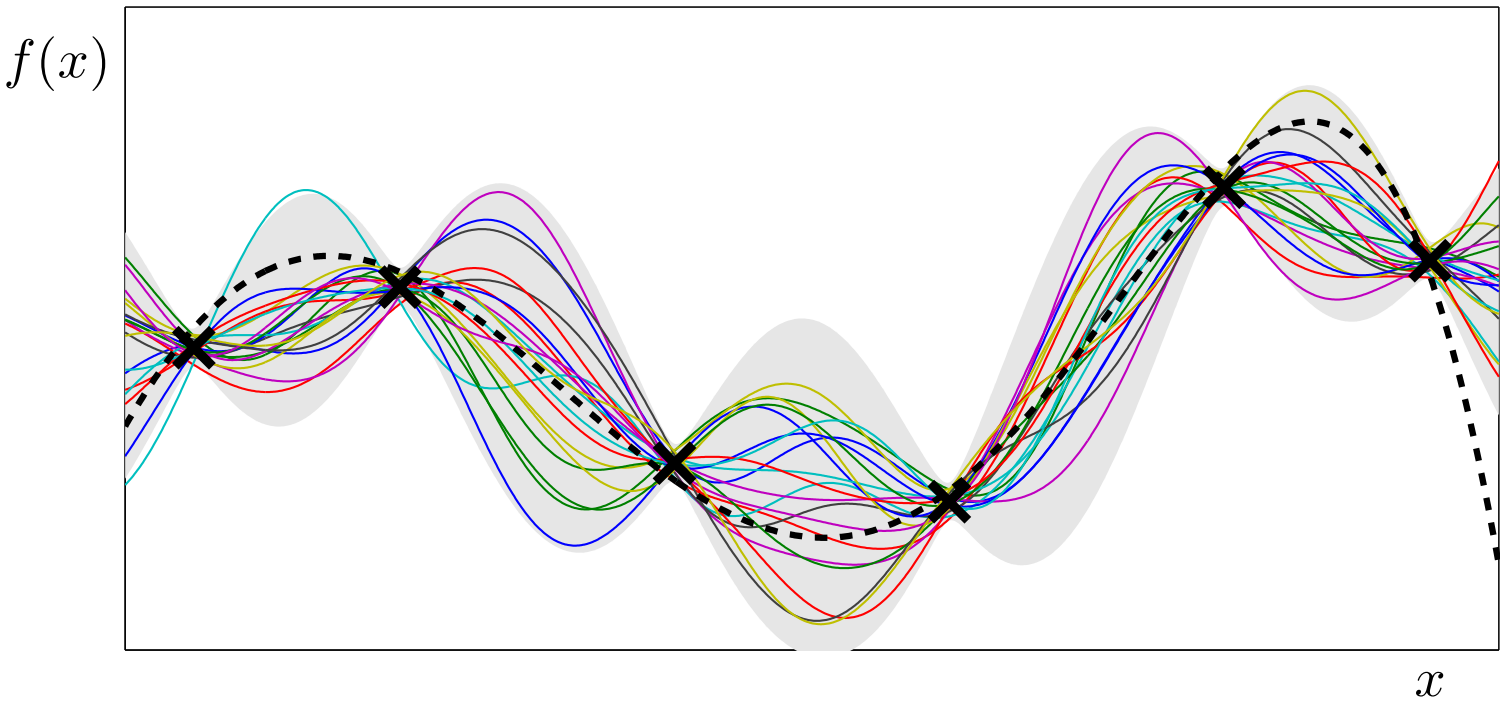


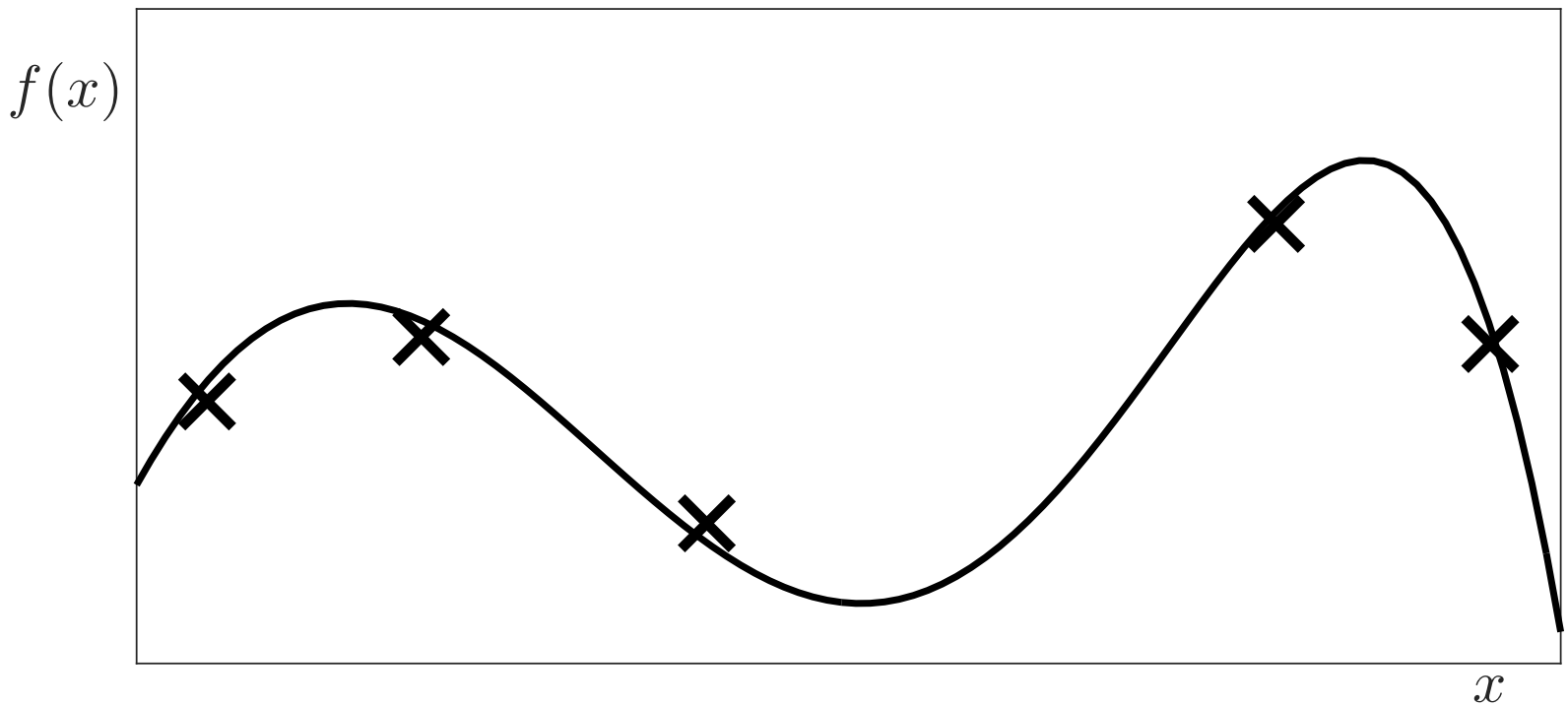
Completely characterised by mean function $\mu : \mathcal{X} \to \mathbb{R}$, and covariance kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
After t observations, $\quad f(x) \sim \mathcal{N}(\, \mu_t(x), \sigma_t^2(x)\,)$.

Algorithm 1: Upper Confidence Bounds in GP Bandits

Model $f \sim \mathcal{GP}(\mathbf{0}, \kappa)$.

Gaussian Process Upper Confidence Bound (GP-UCB)

(Srinivas et al. 2010)



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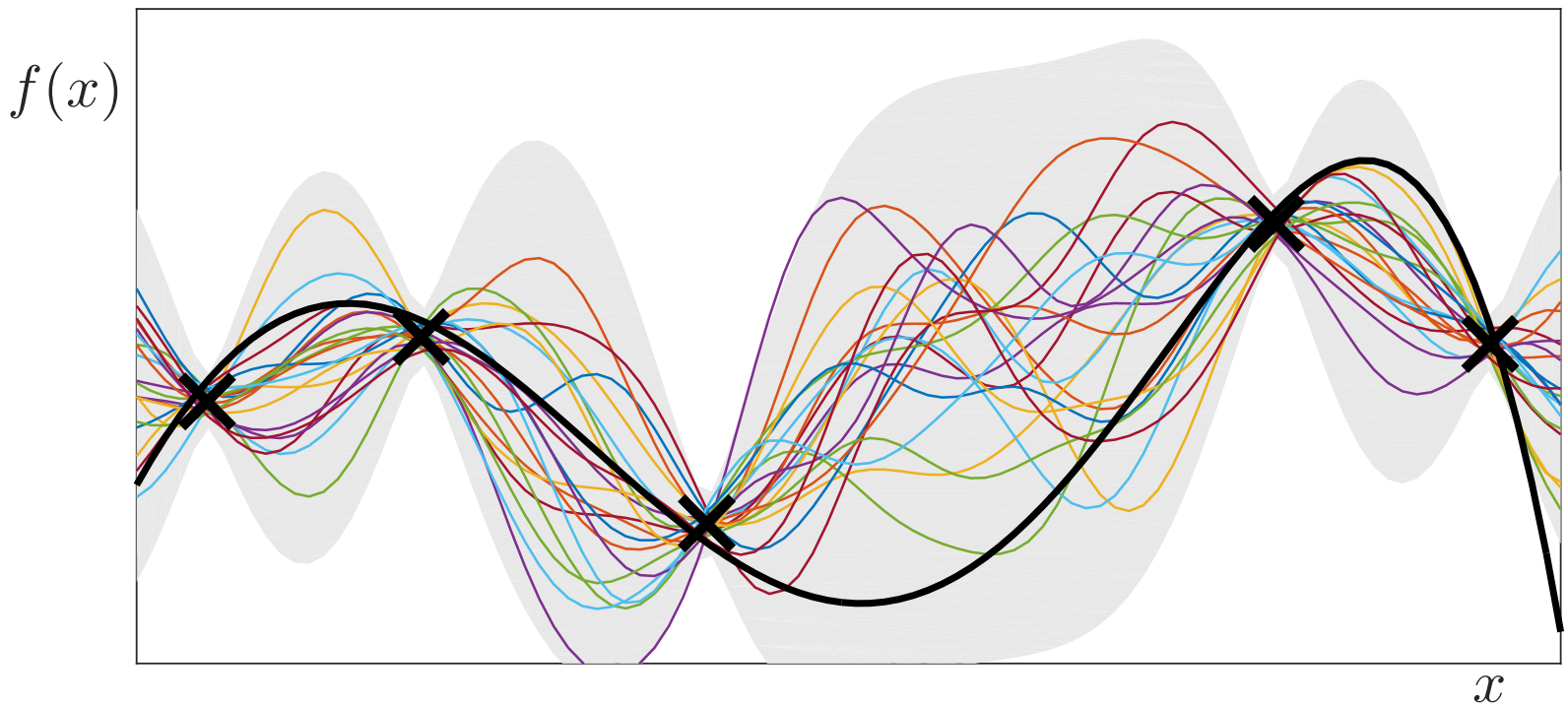

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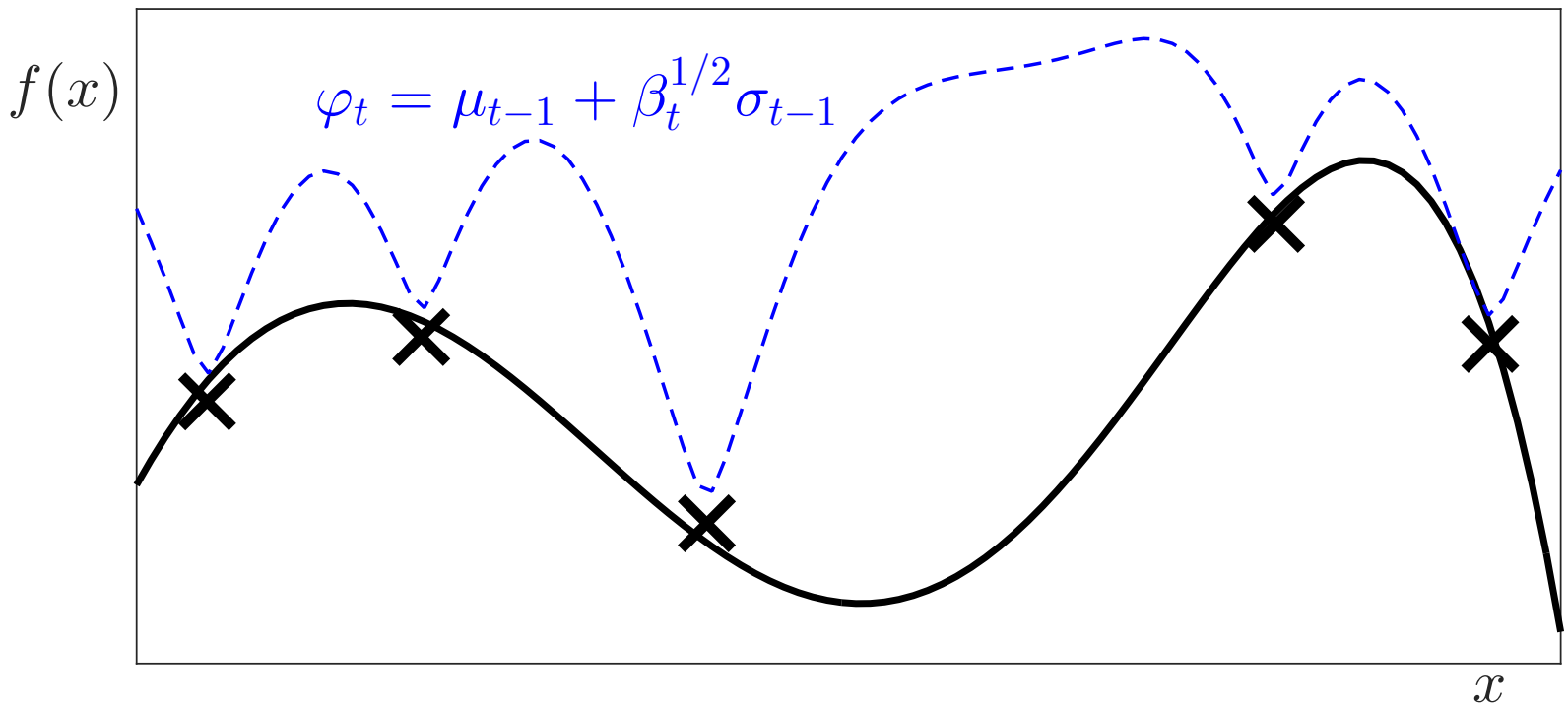

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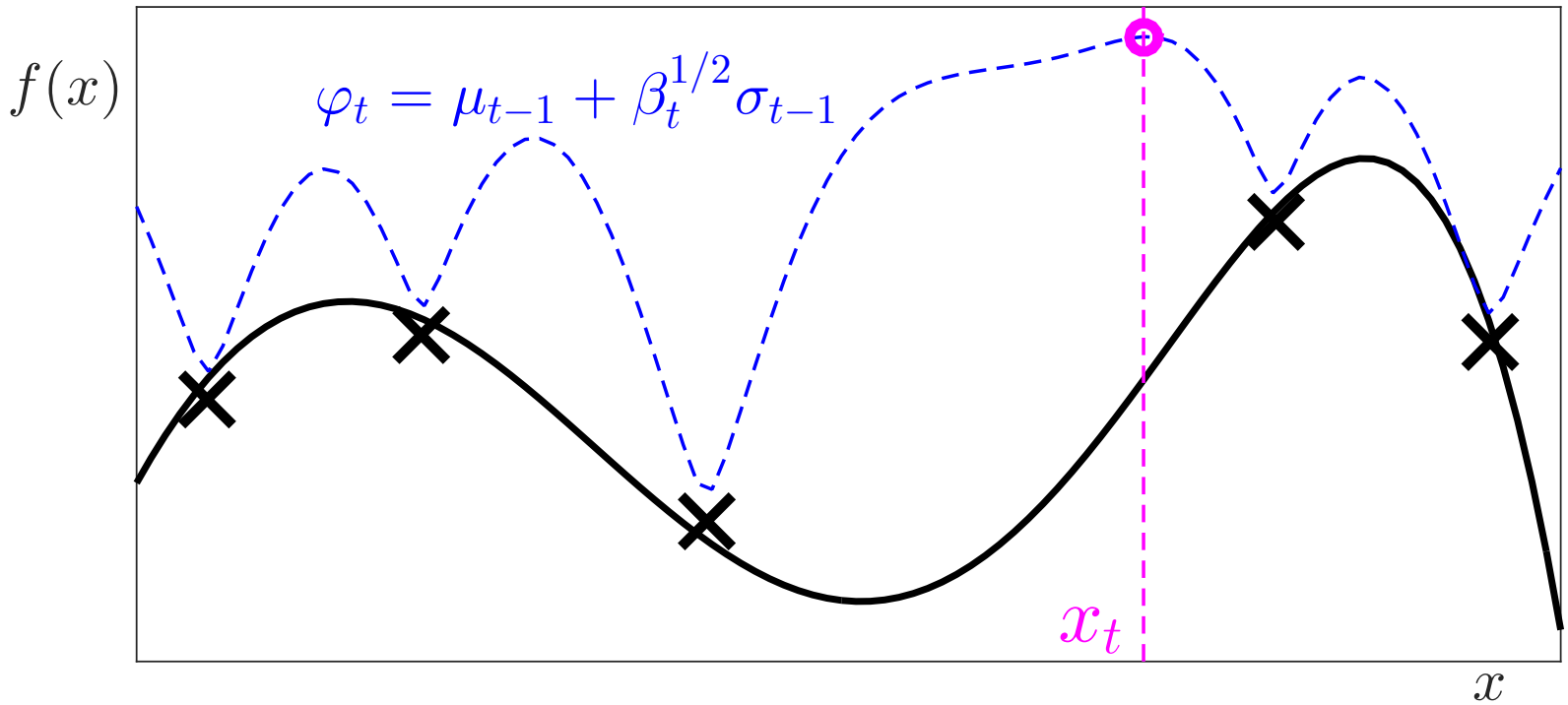

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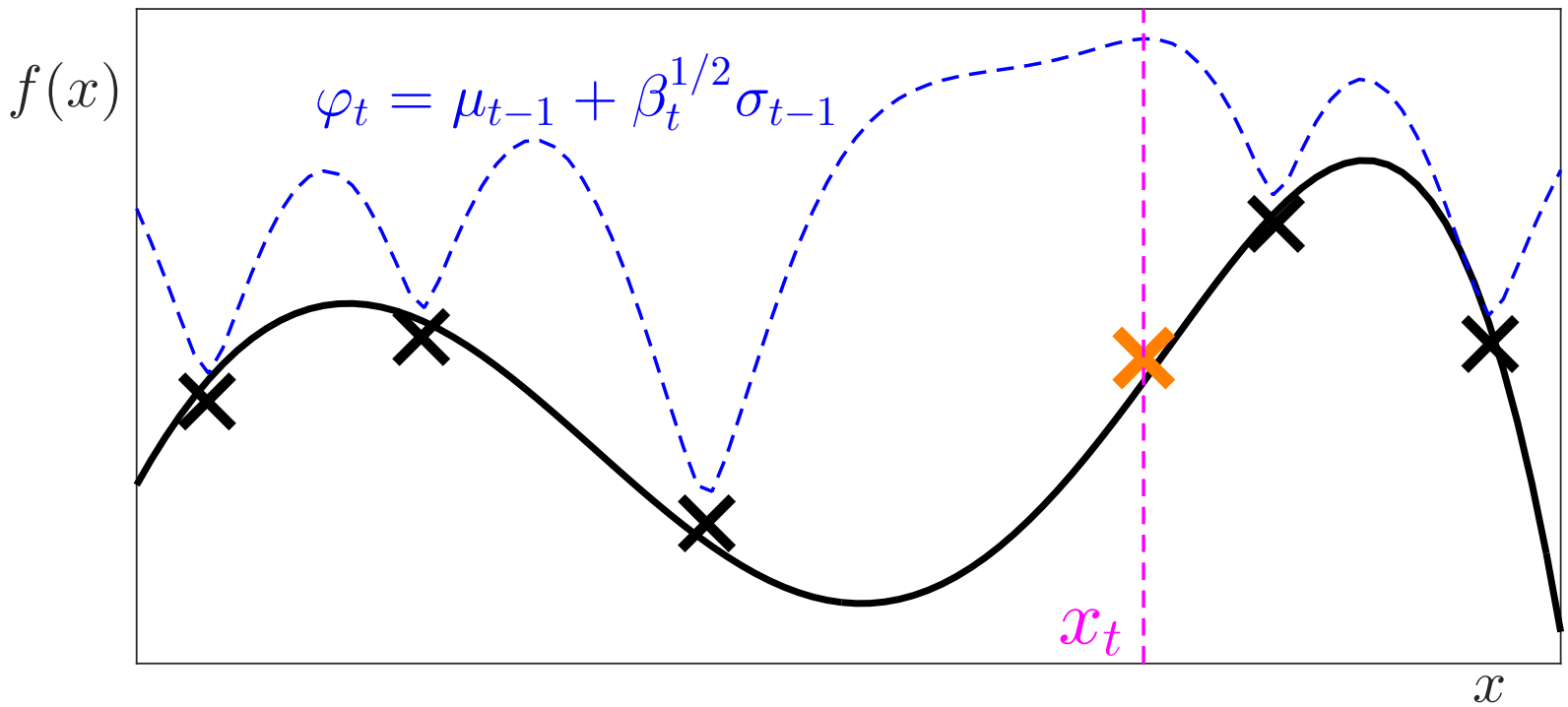

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GP-UCB

$$x_t = \operatorname*{argmax}_x \quad \mu_{t-1}(x) + \beta_t^{1/2} \sigma_{t-1}(x)$$

- μ_{t-1}: Exploitation
- σ_{t-1}: Exploration
- β_t controls the tradeoff. $\beta_t \asymp \log t$.

GP-UCB

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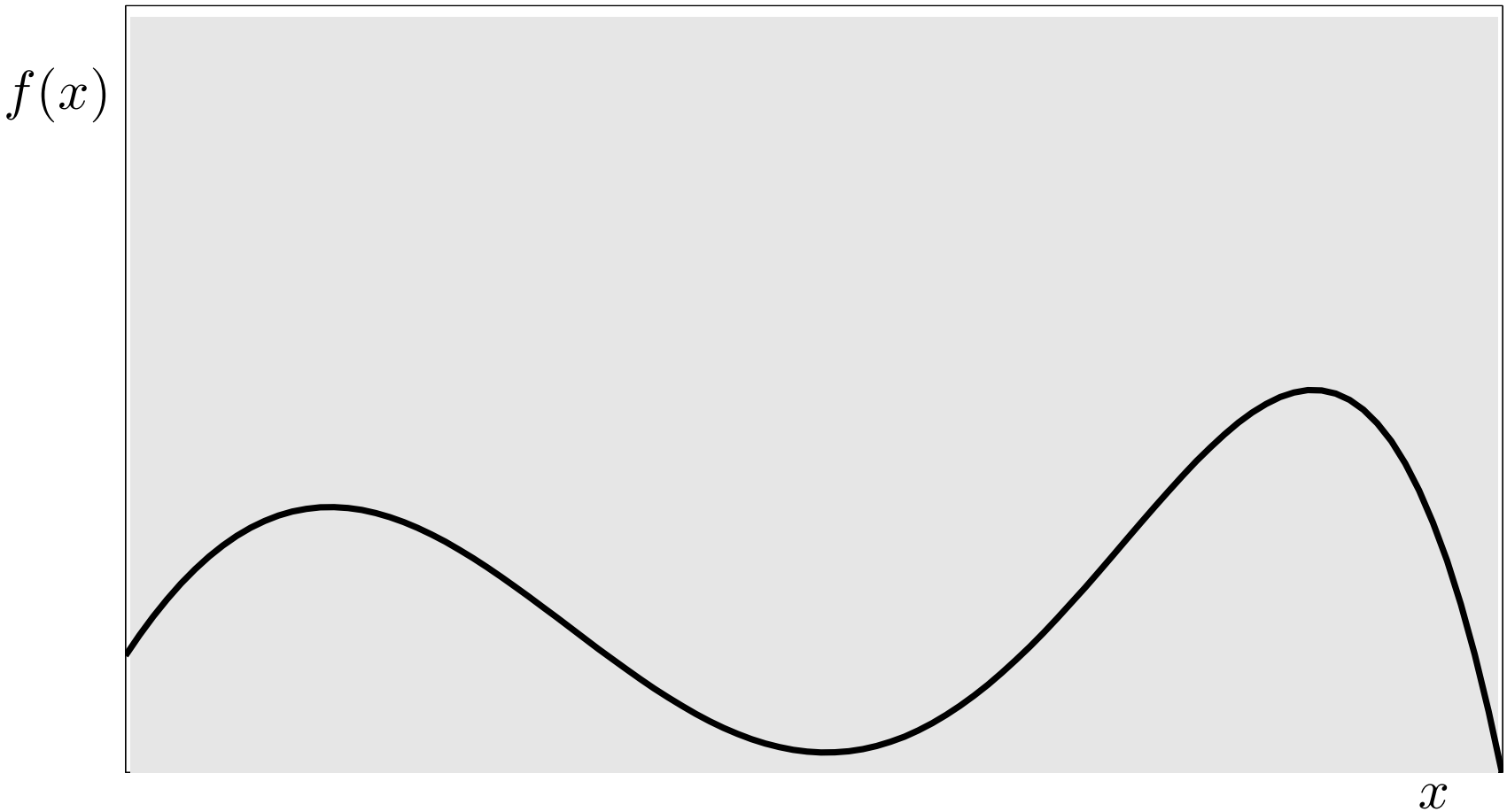

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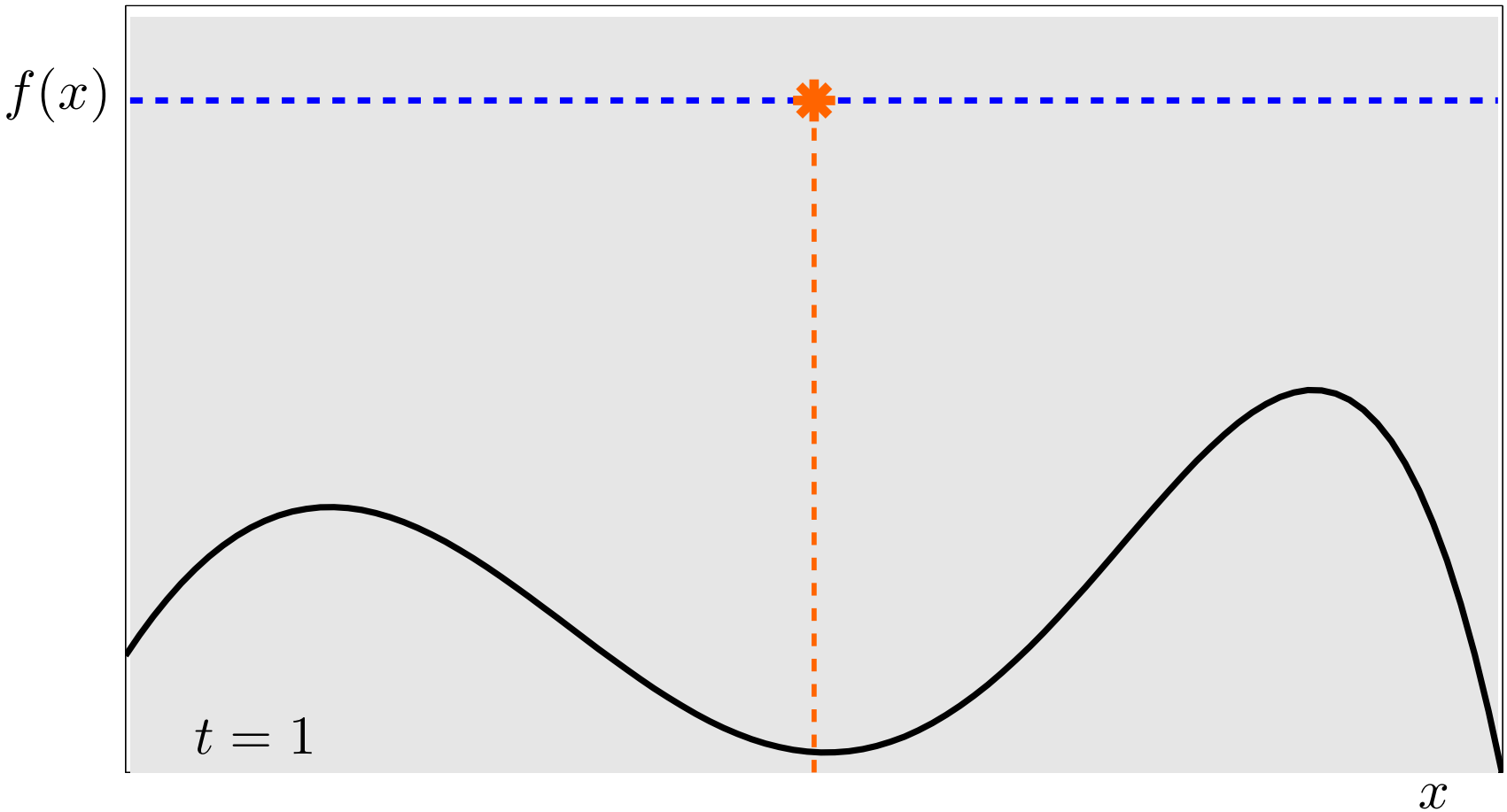

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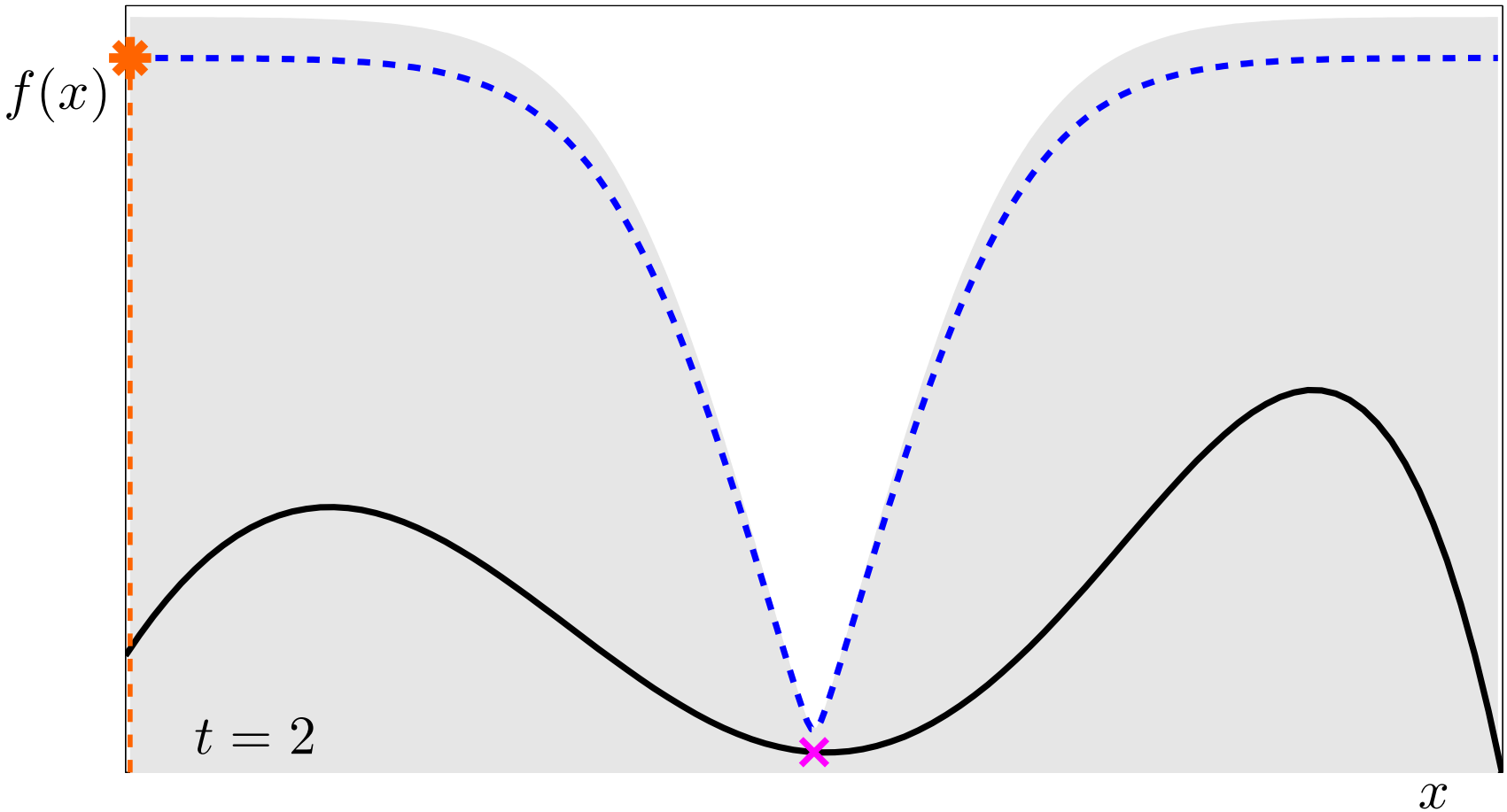

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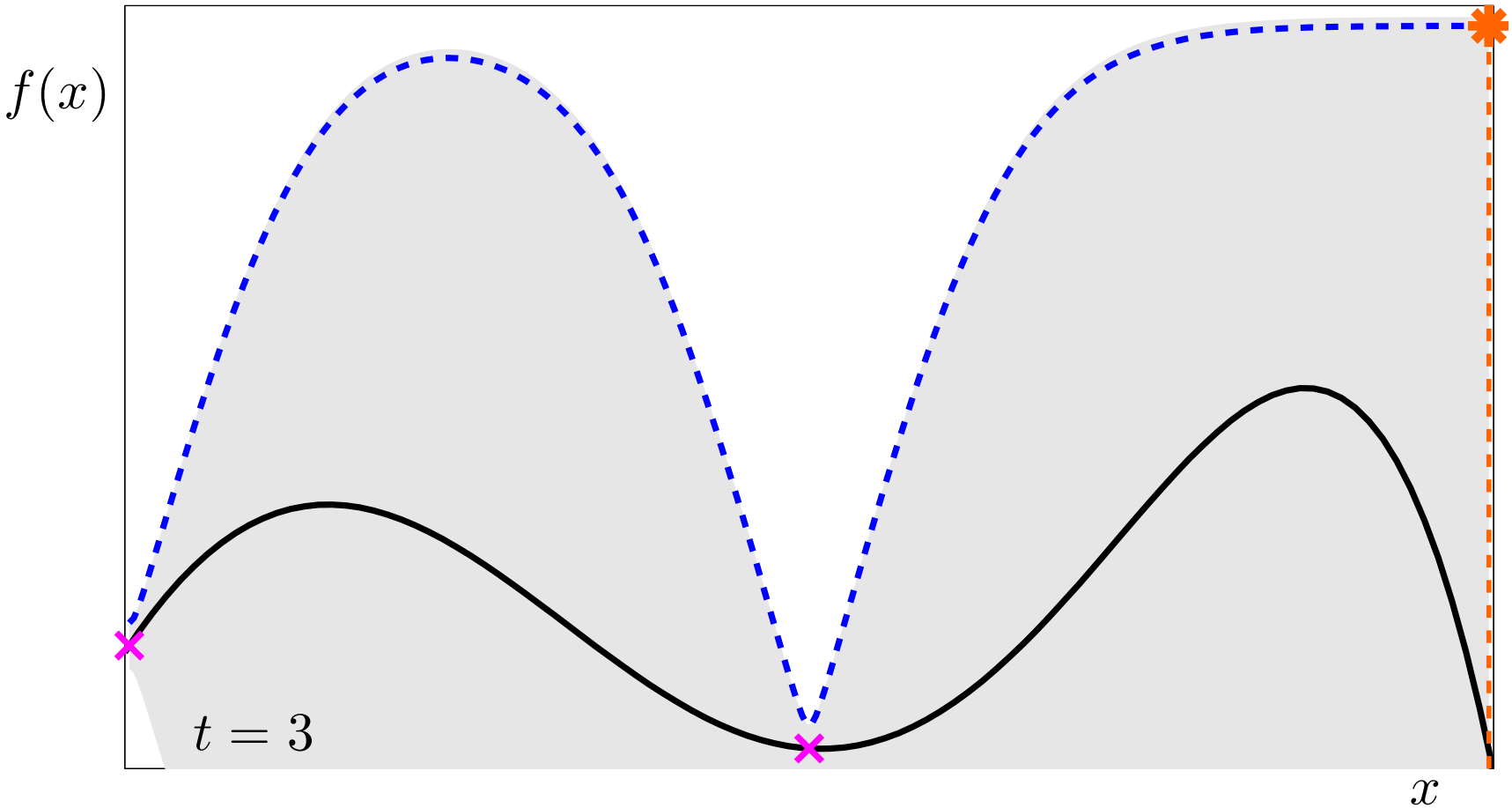

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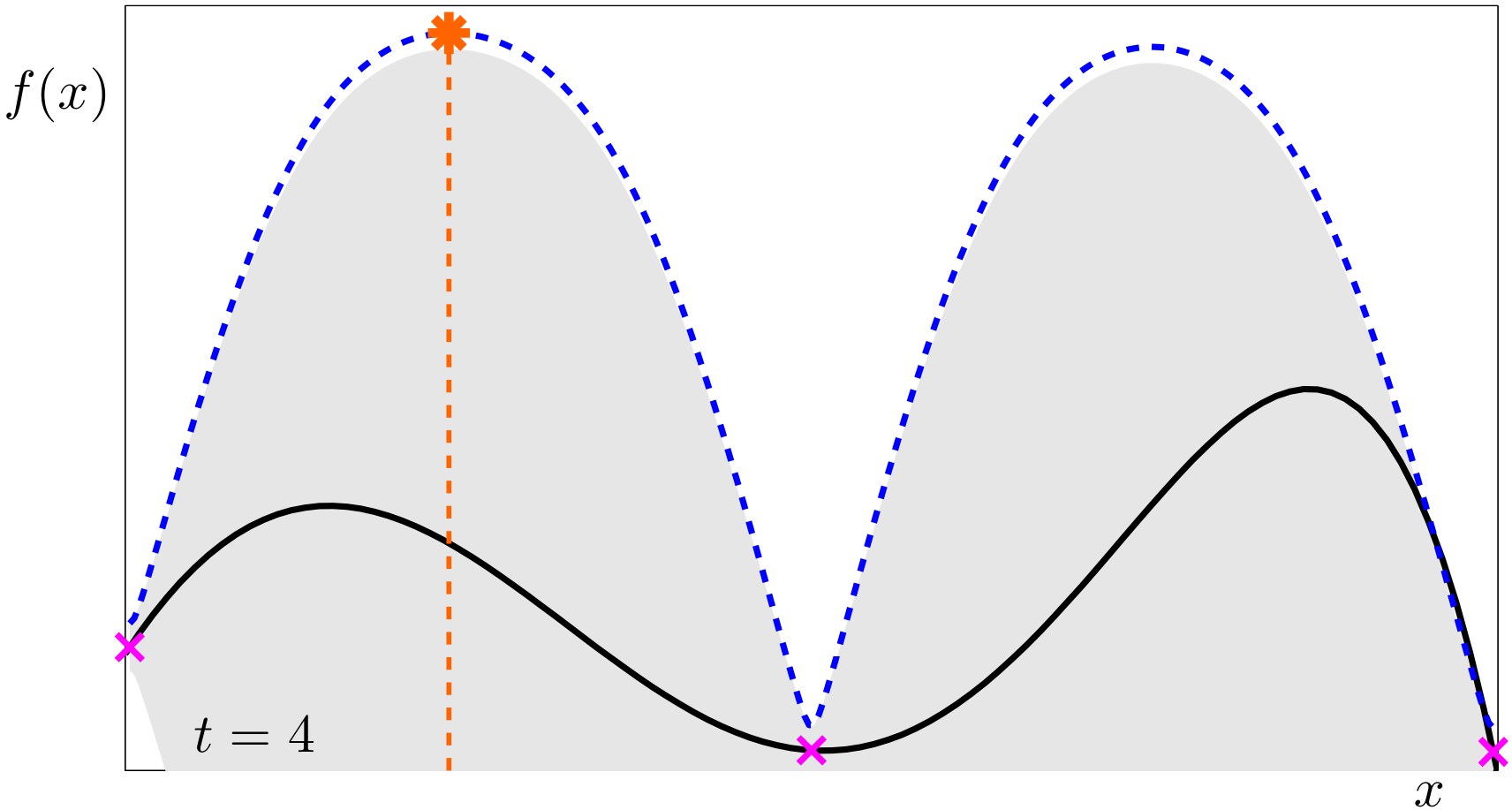

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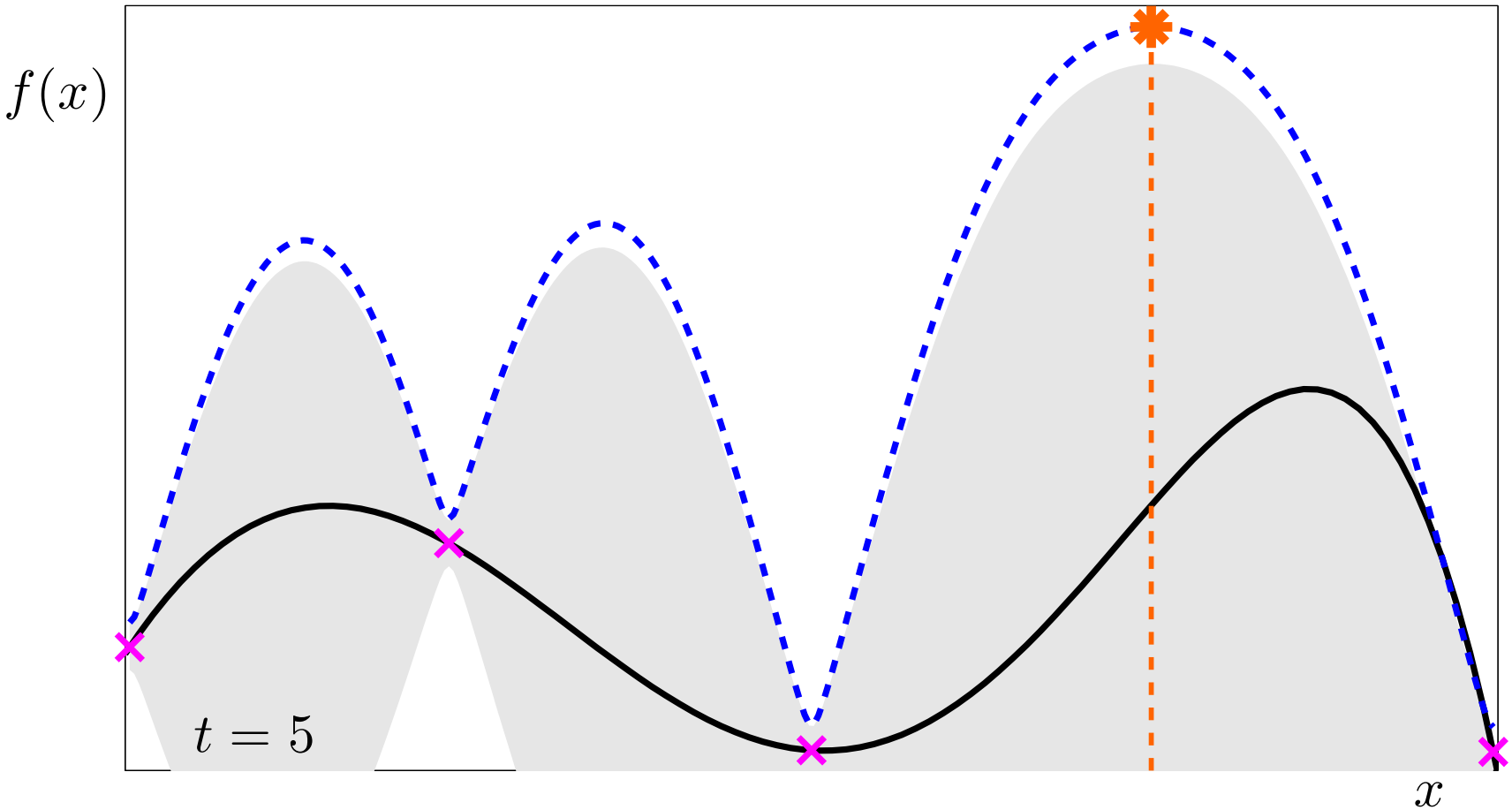

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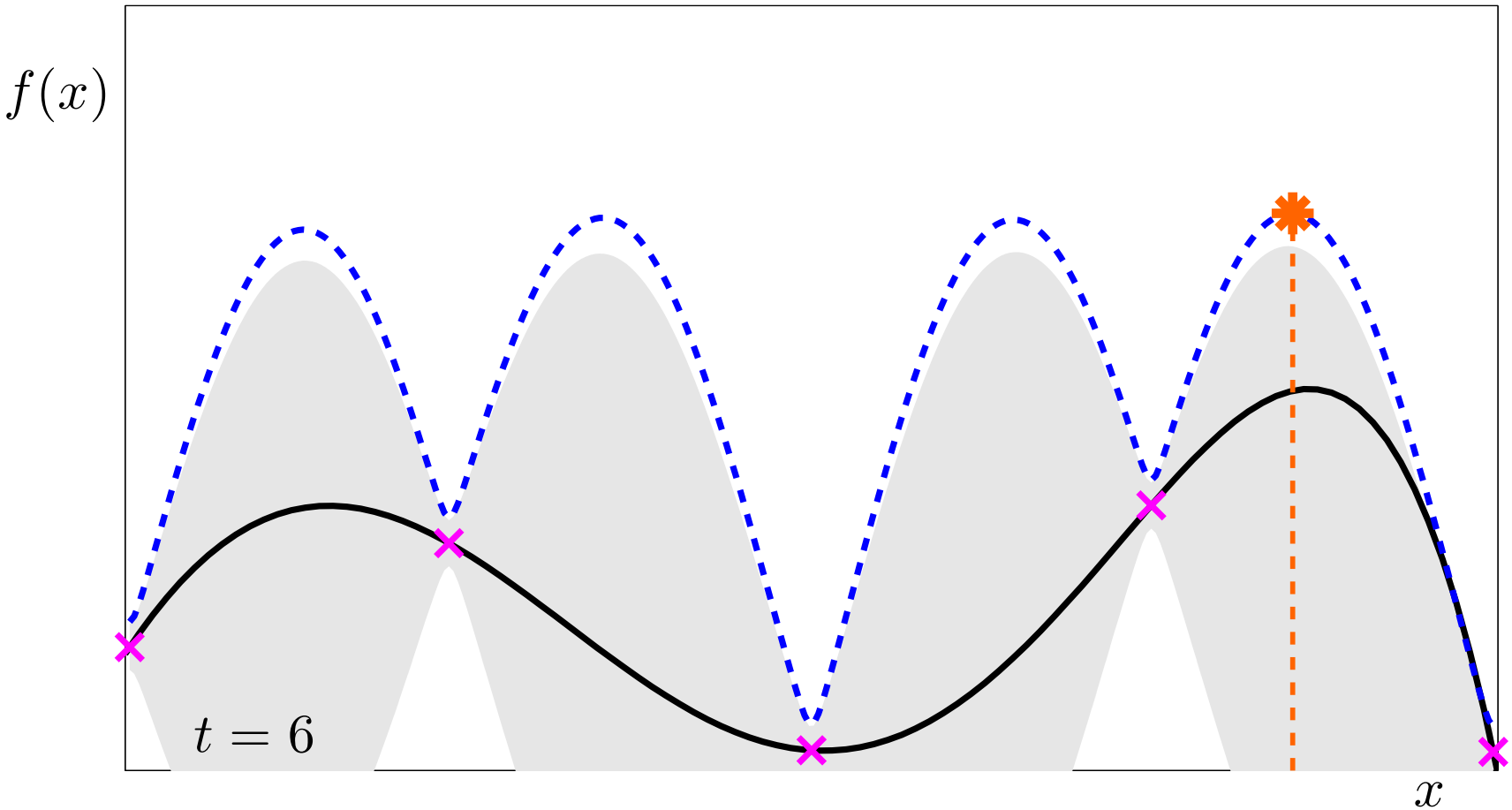

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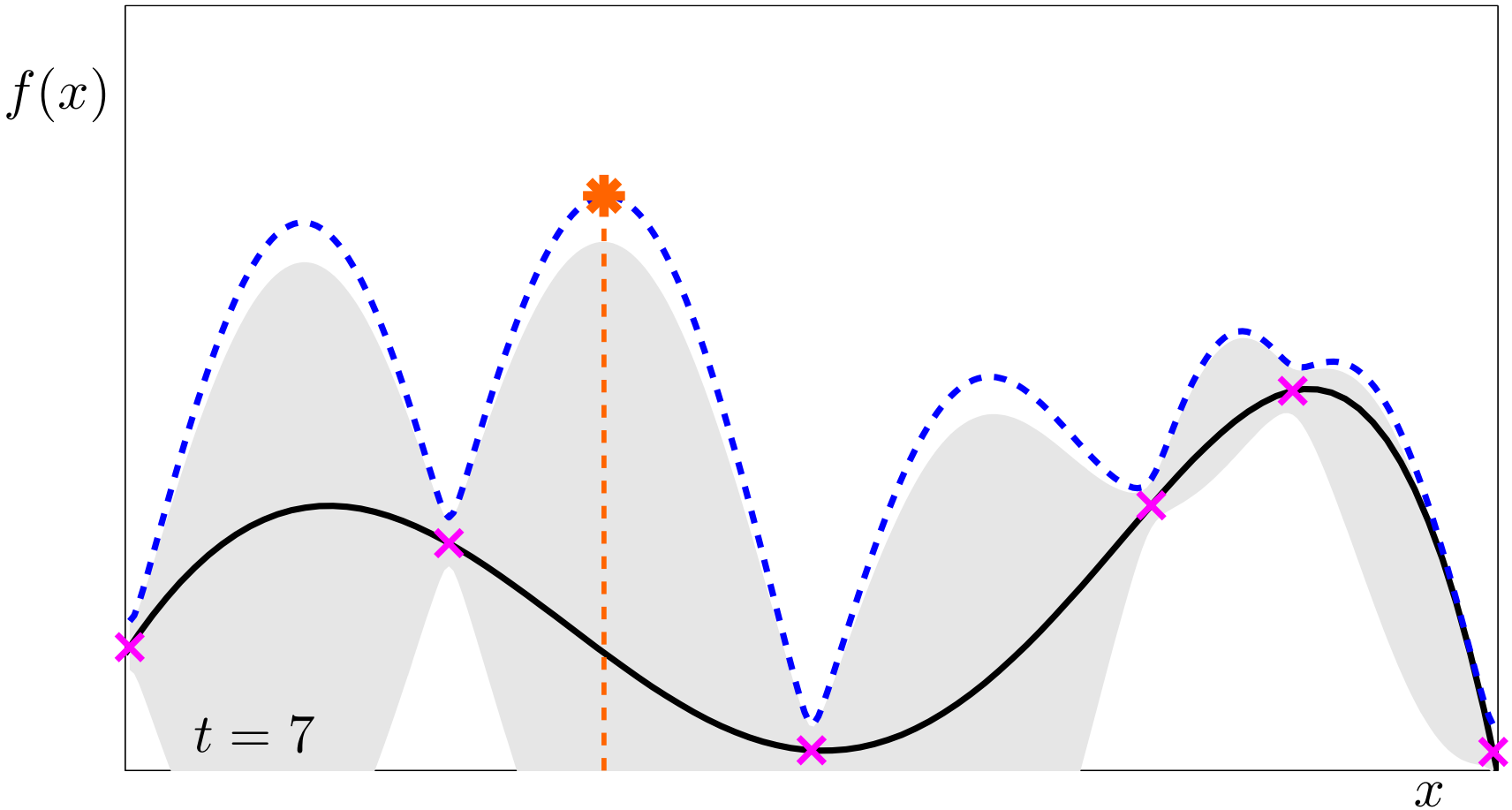

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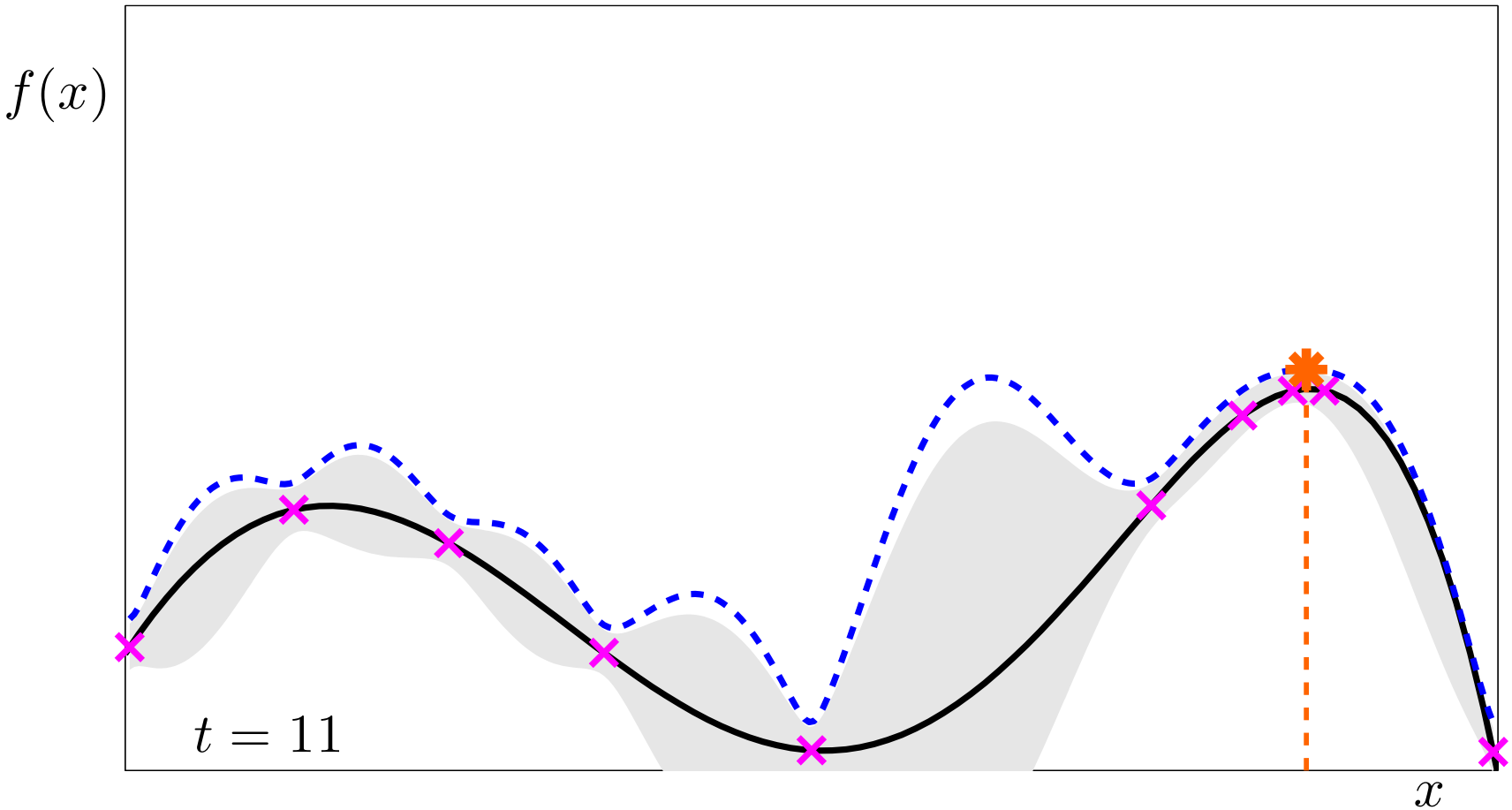

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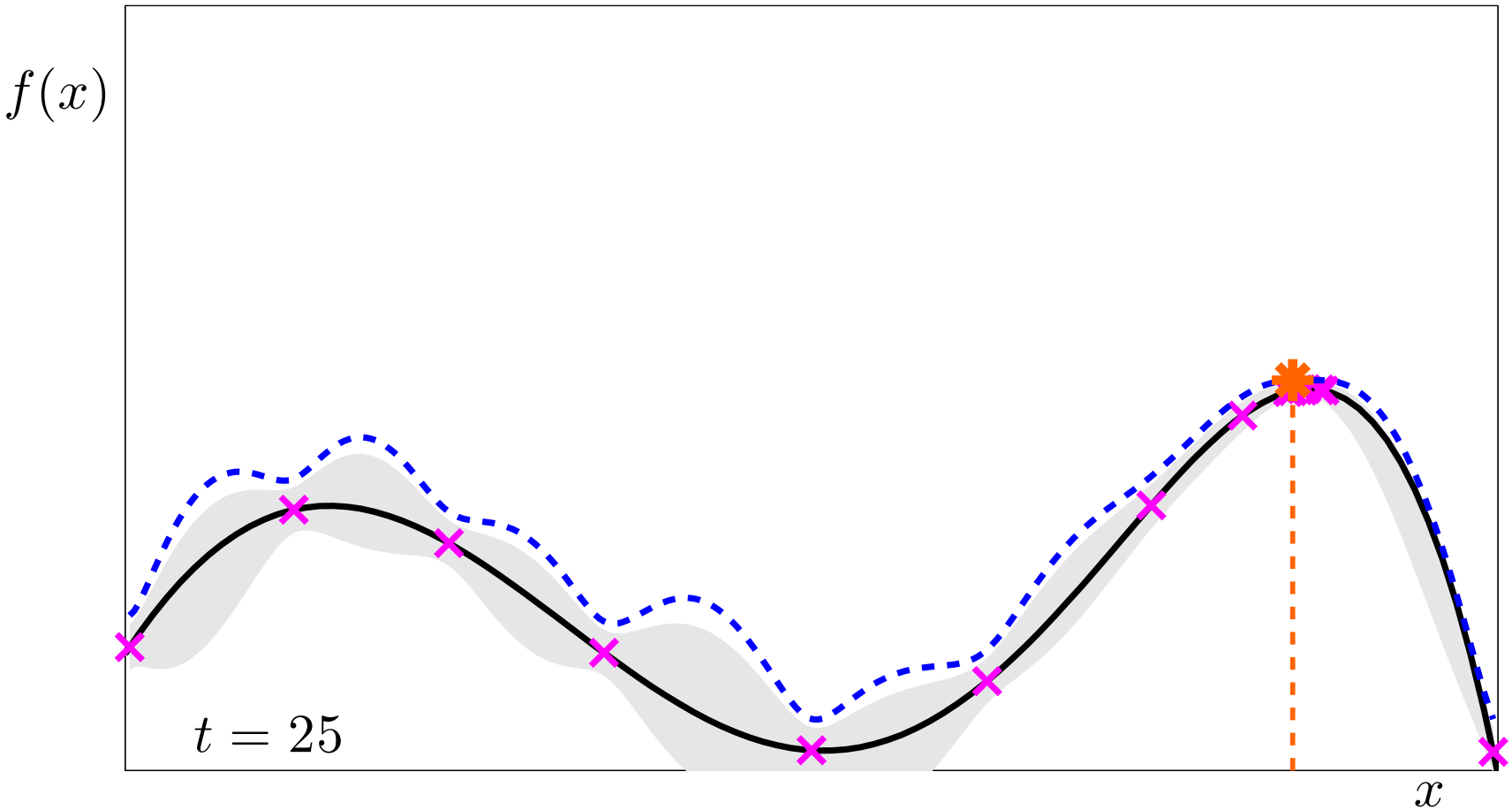
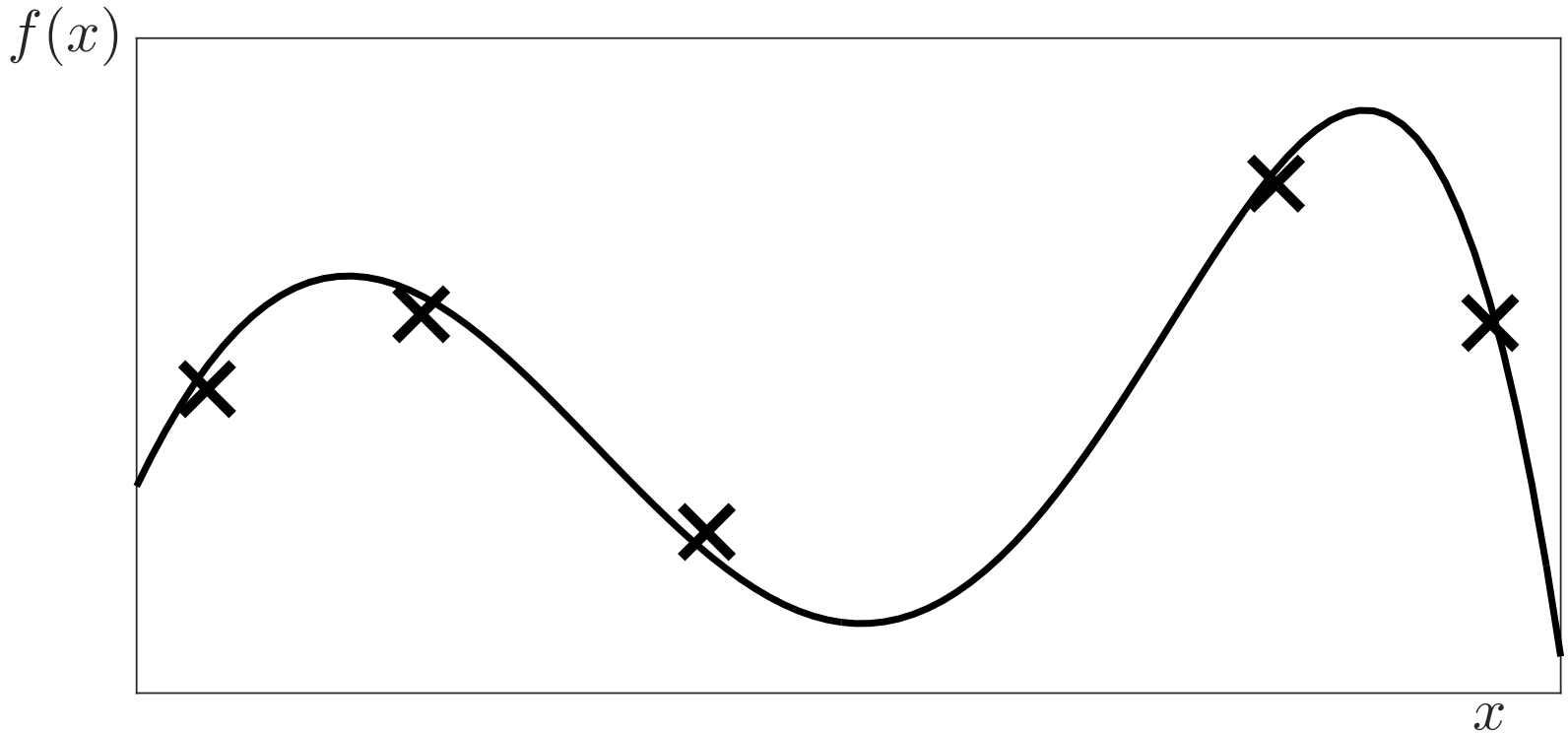


Algorithm 2: Thompson Sampling in GP Bandits

Model $f \sim \mathcal{GP}(\mathbf{0}, \kappa)$.

Thompson Sampling (TS) (Thompson, 1933).



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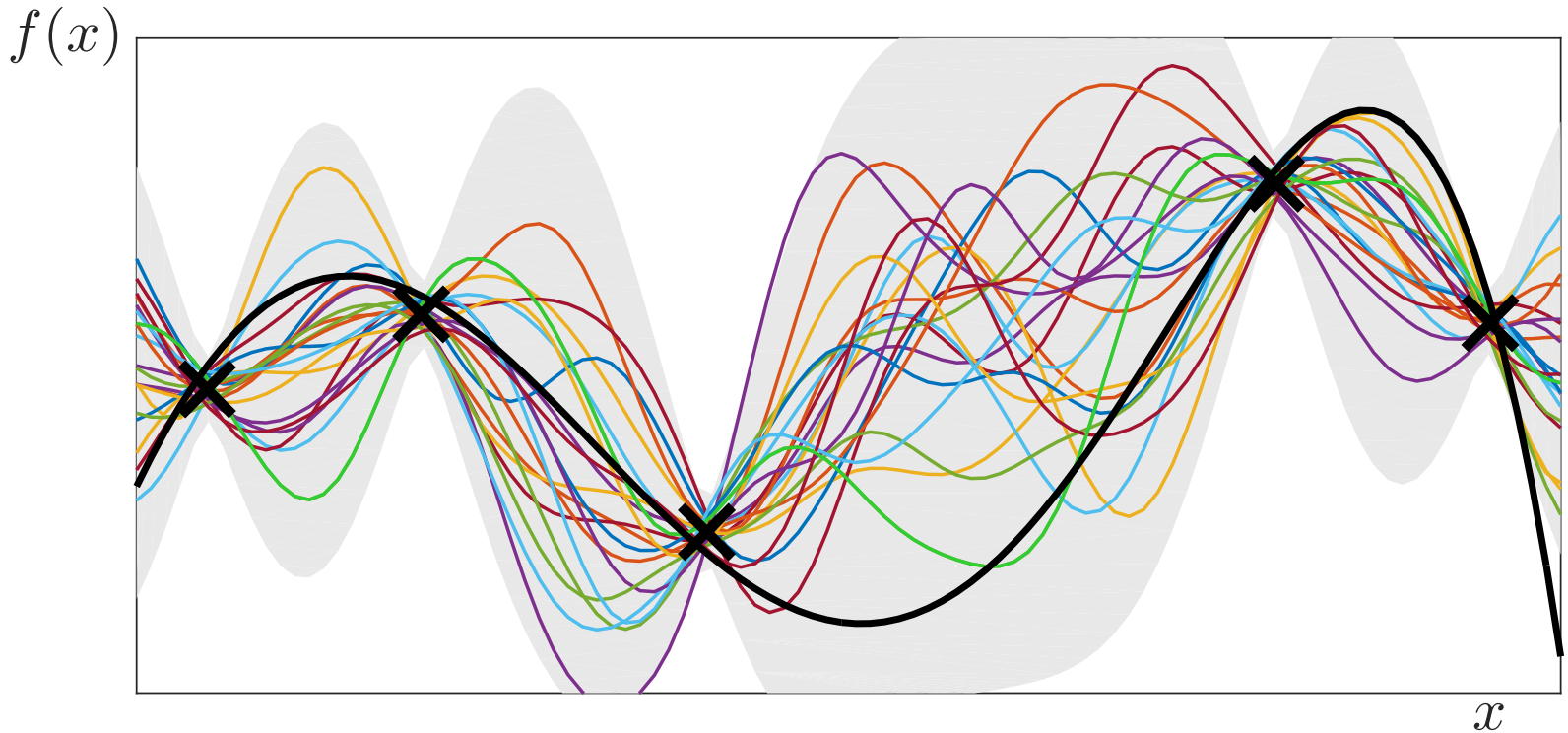

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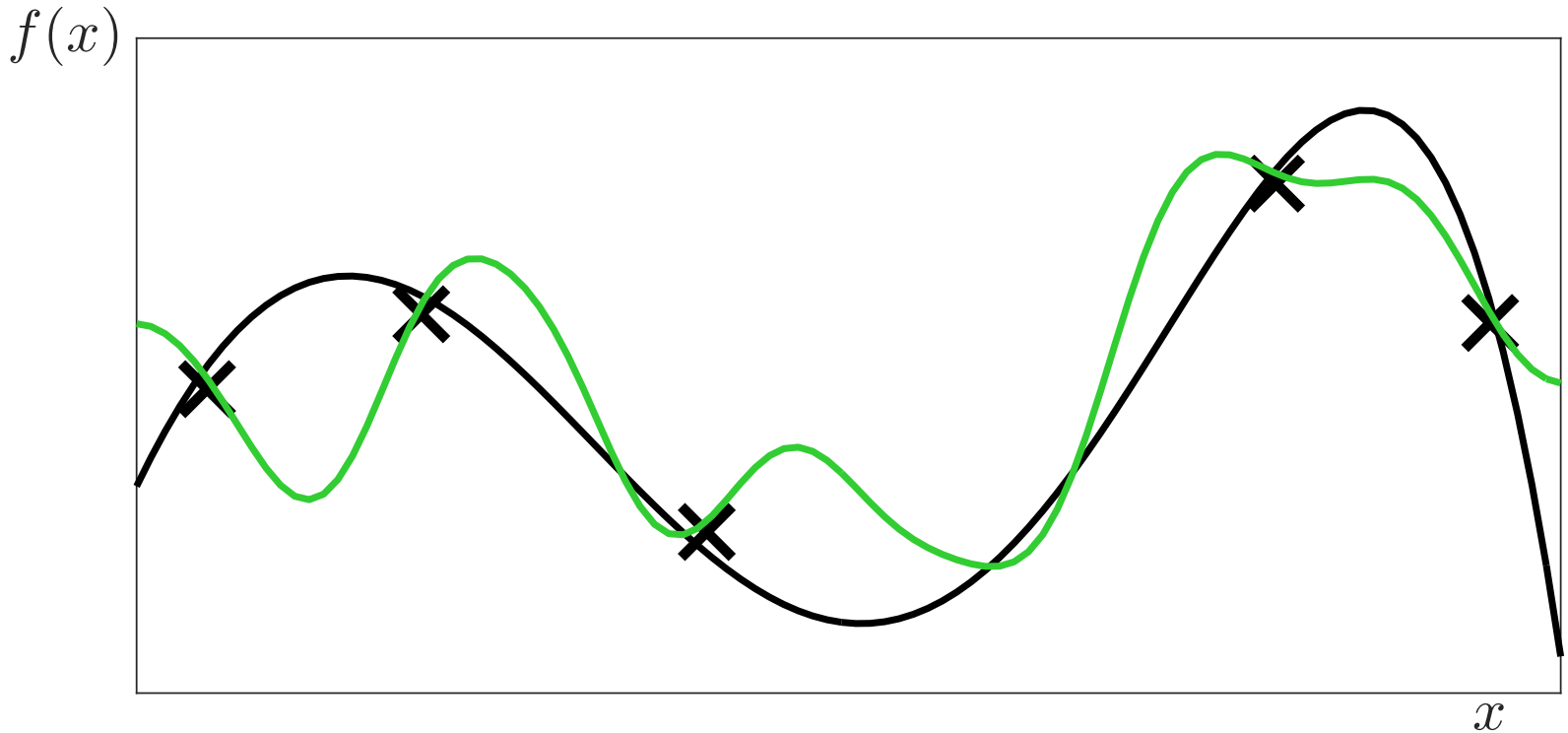

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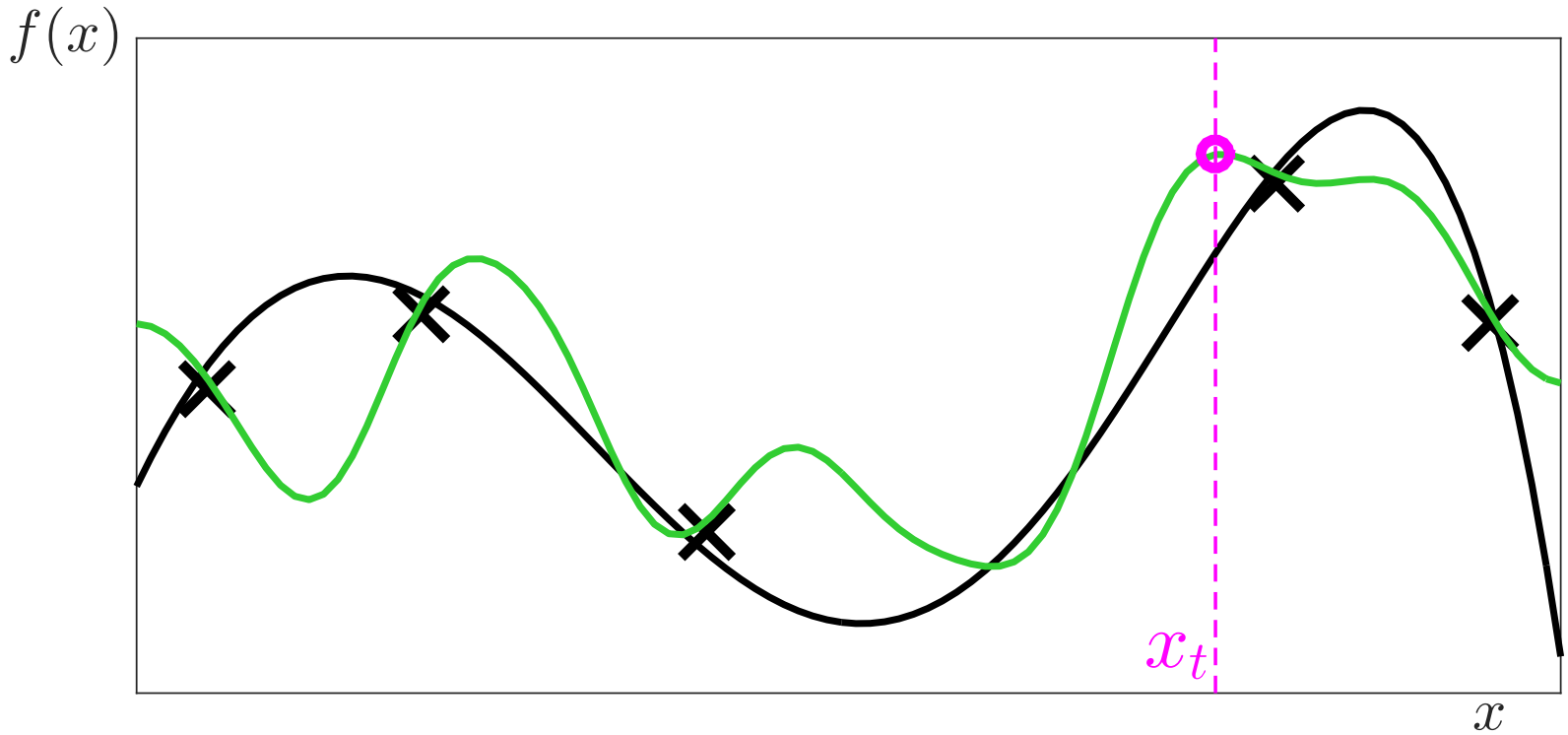

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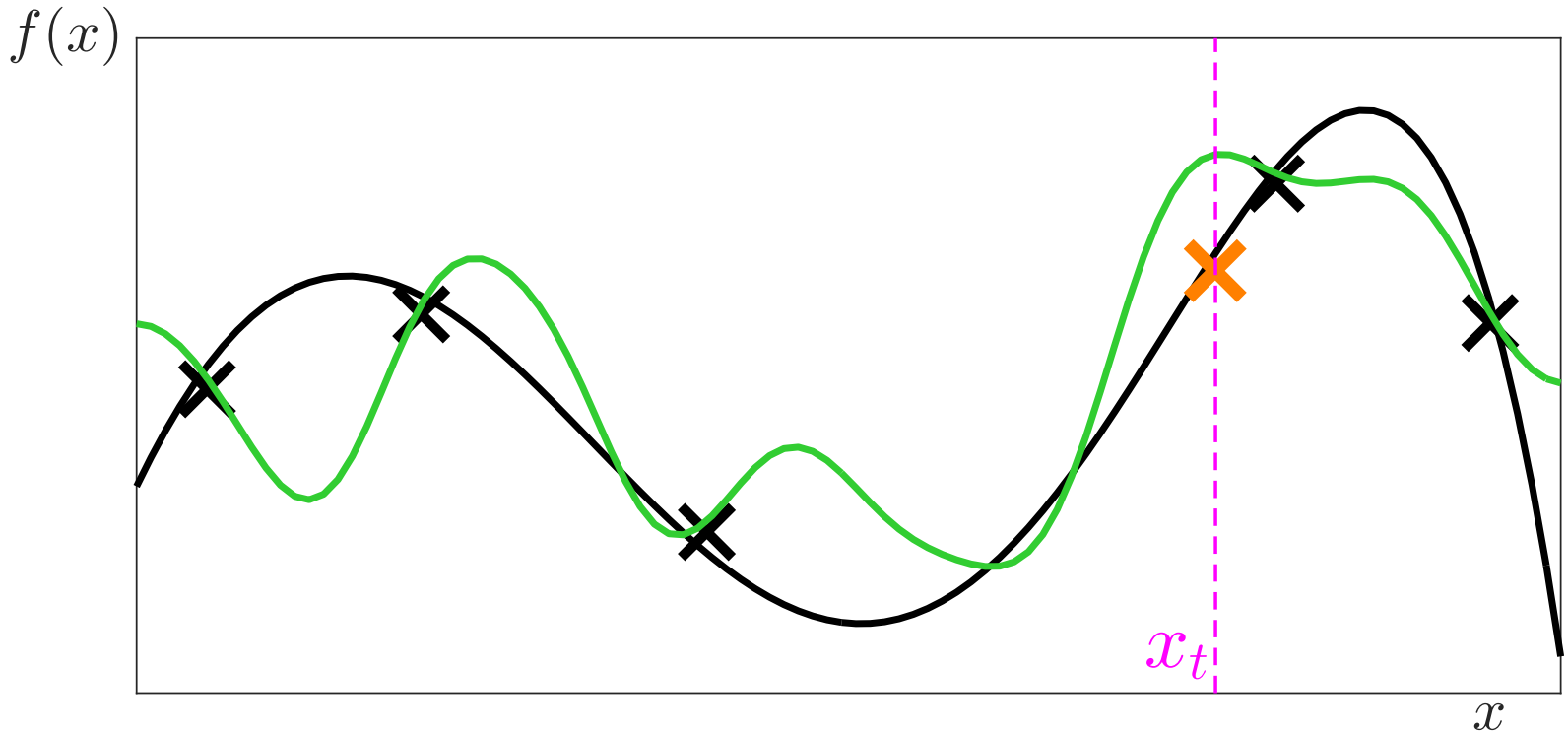

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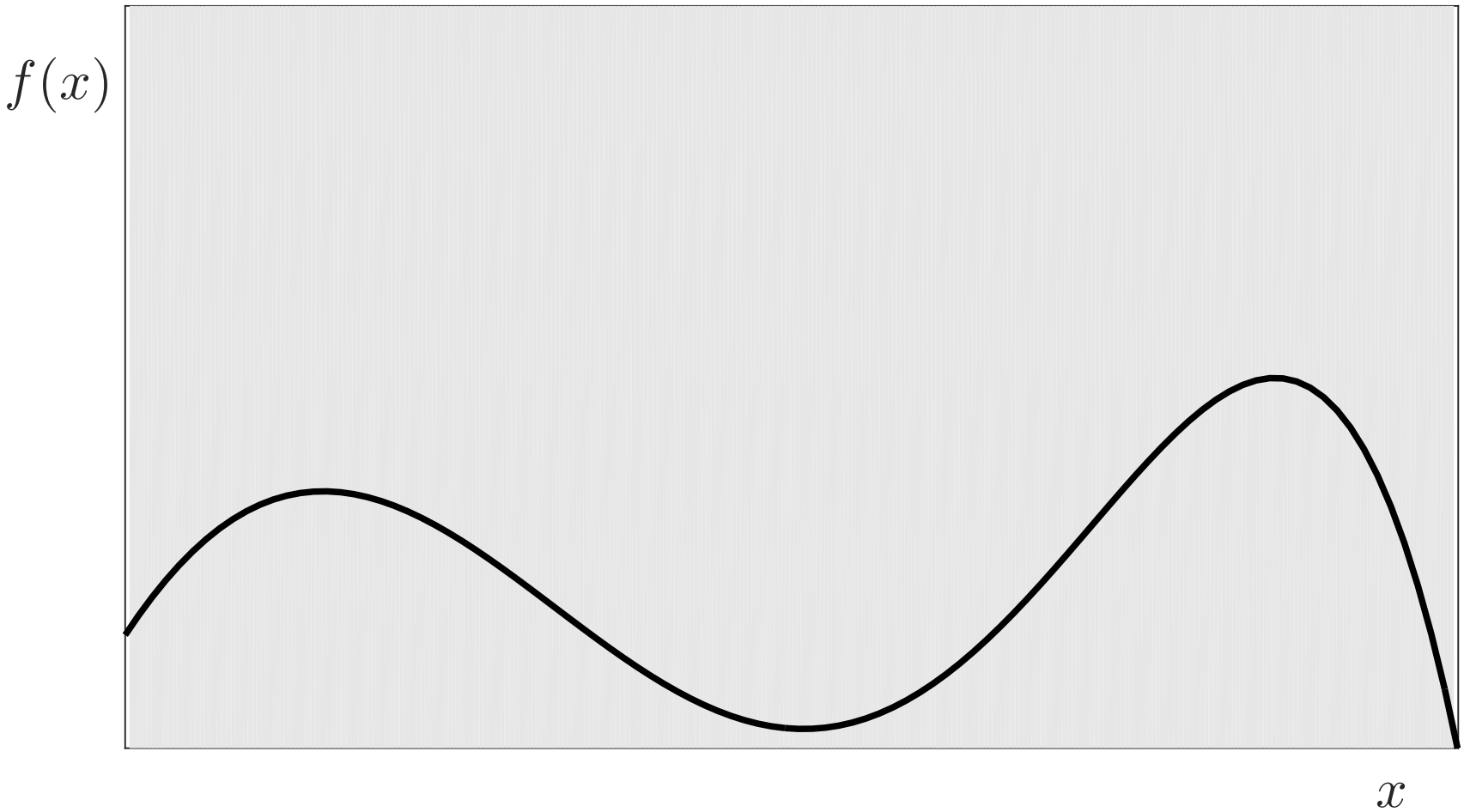

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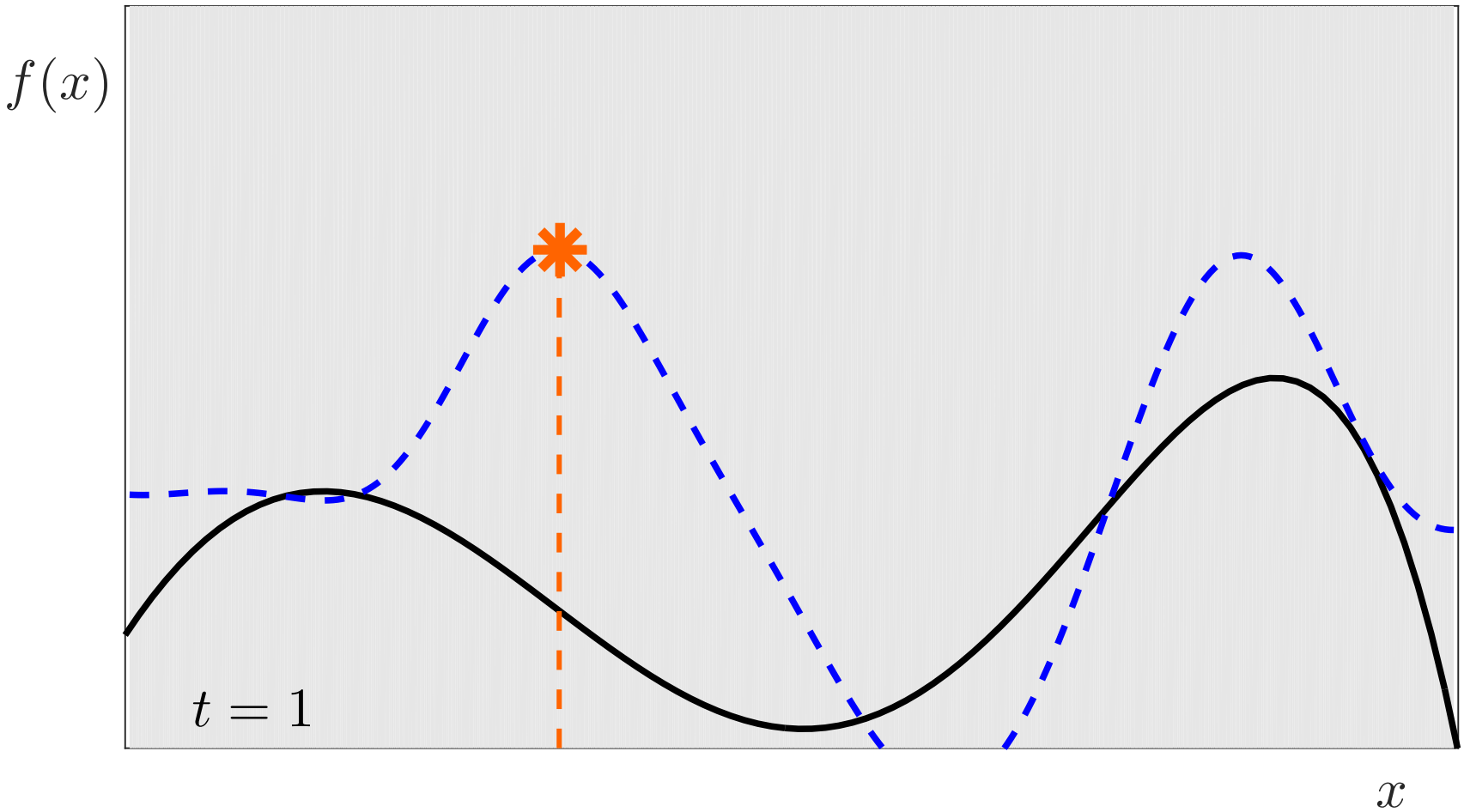

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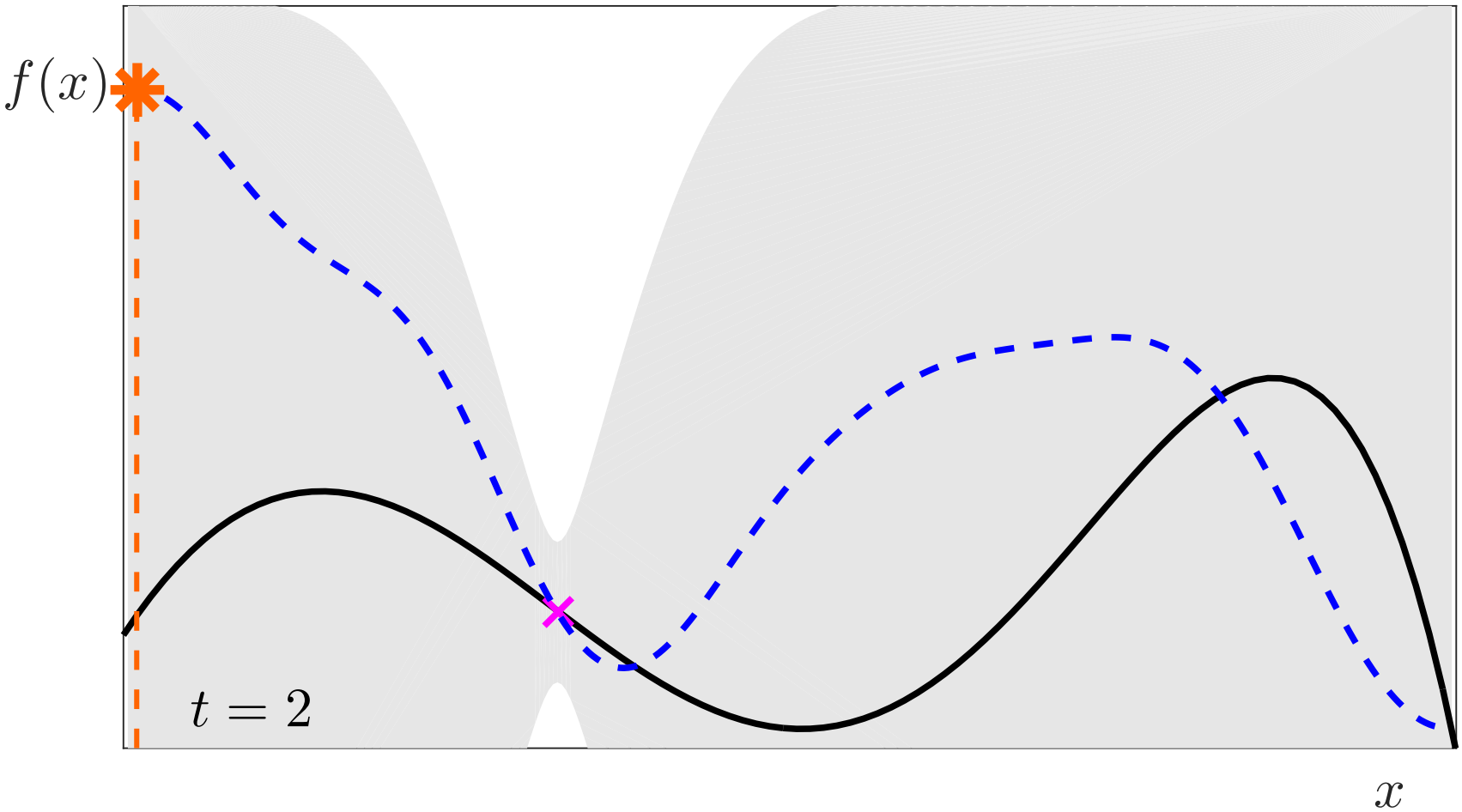

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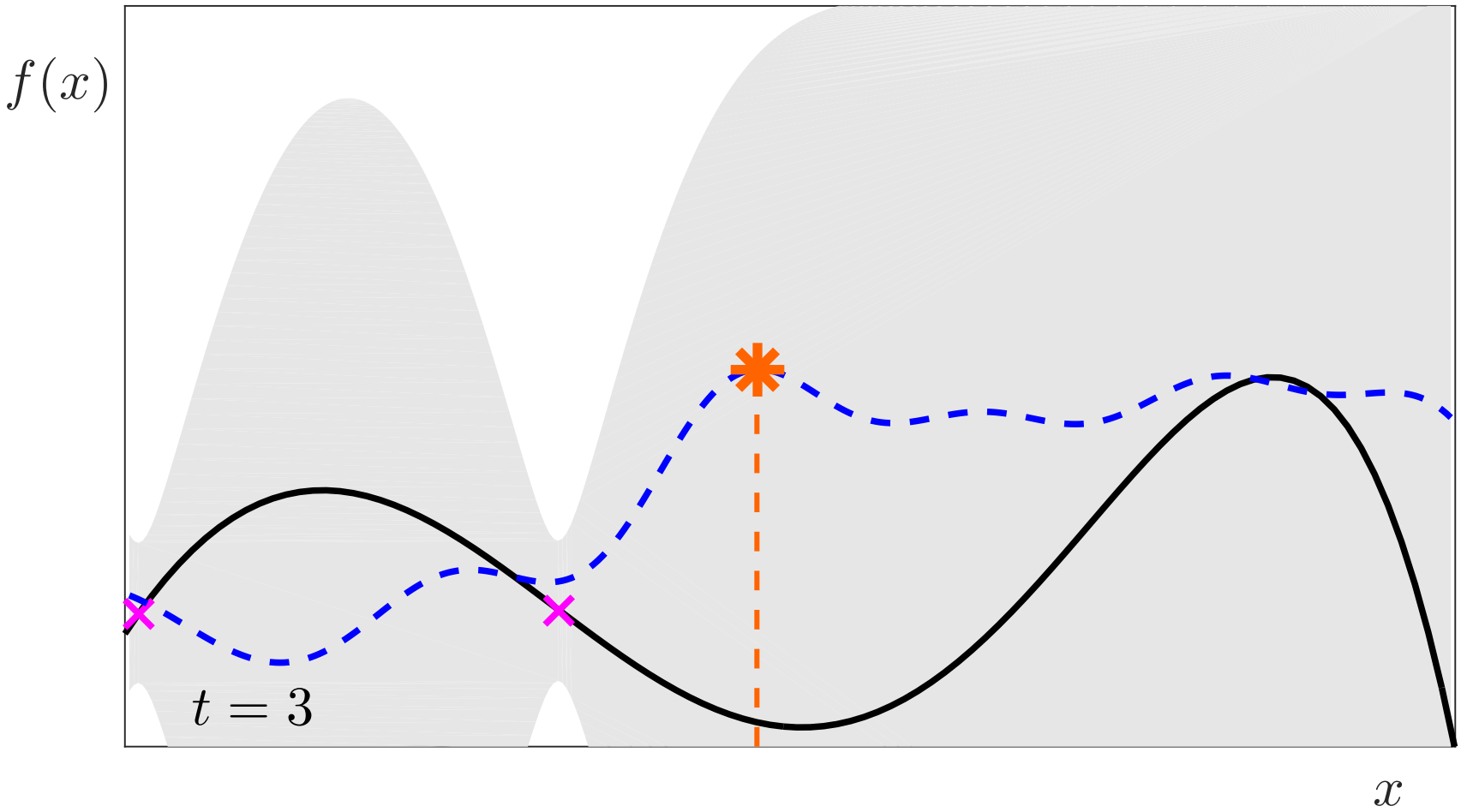

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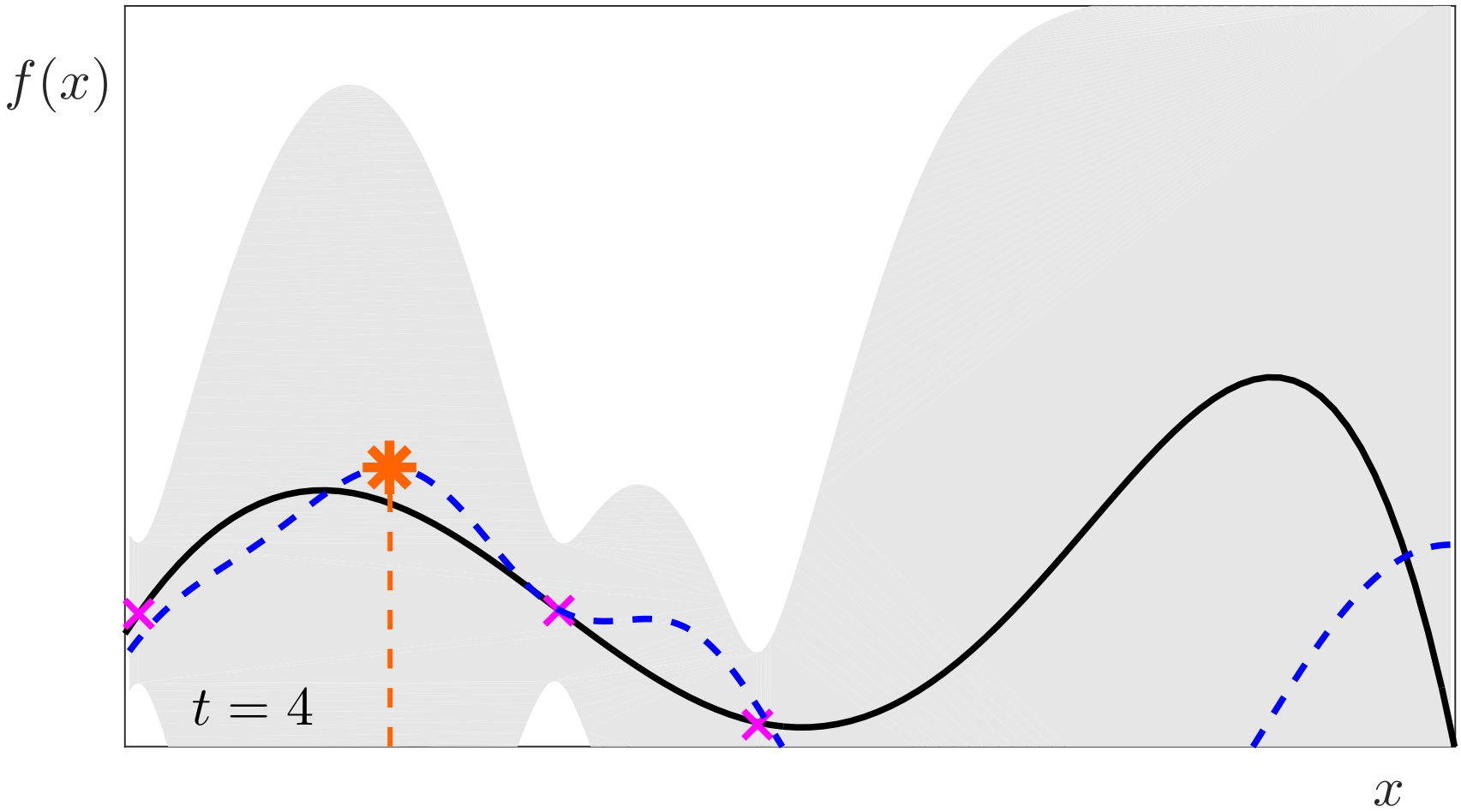

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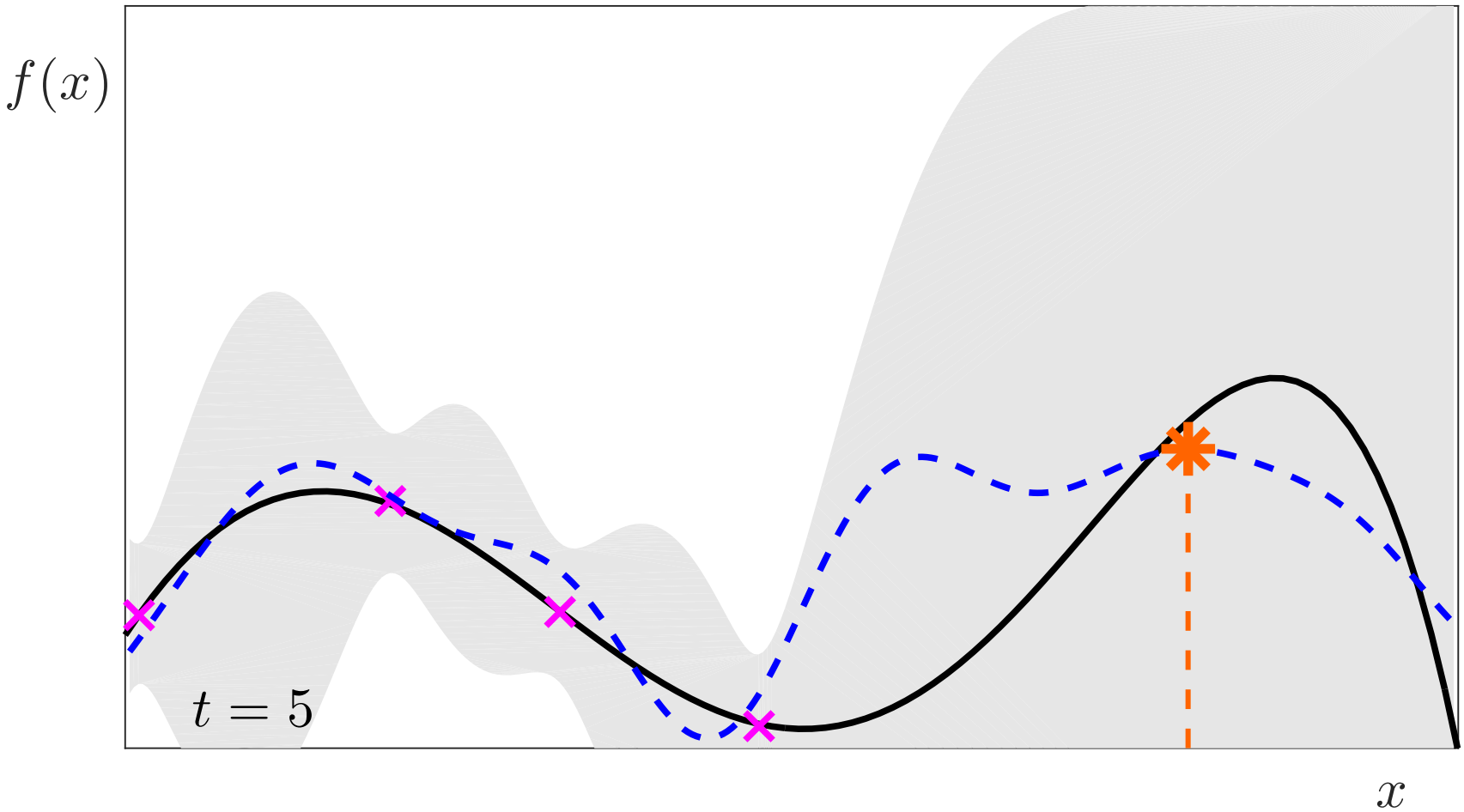

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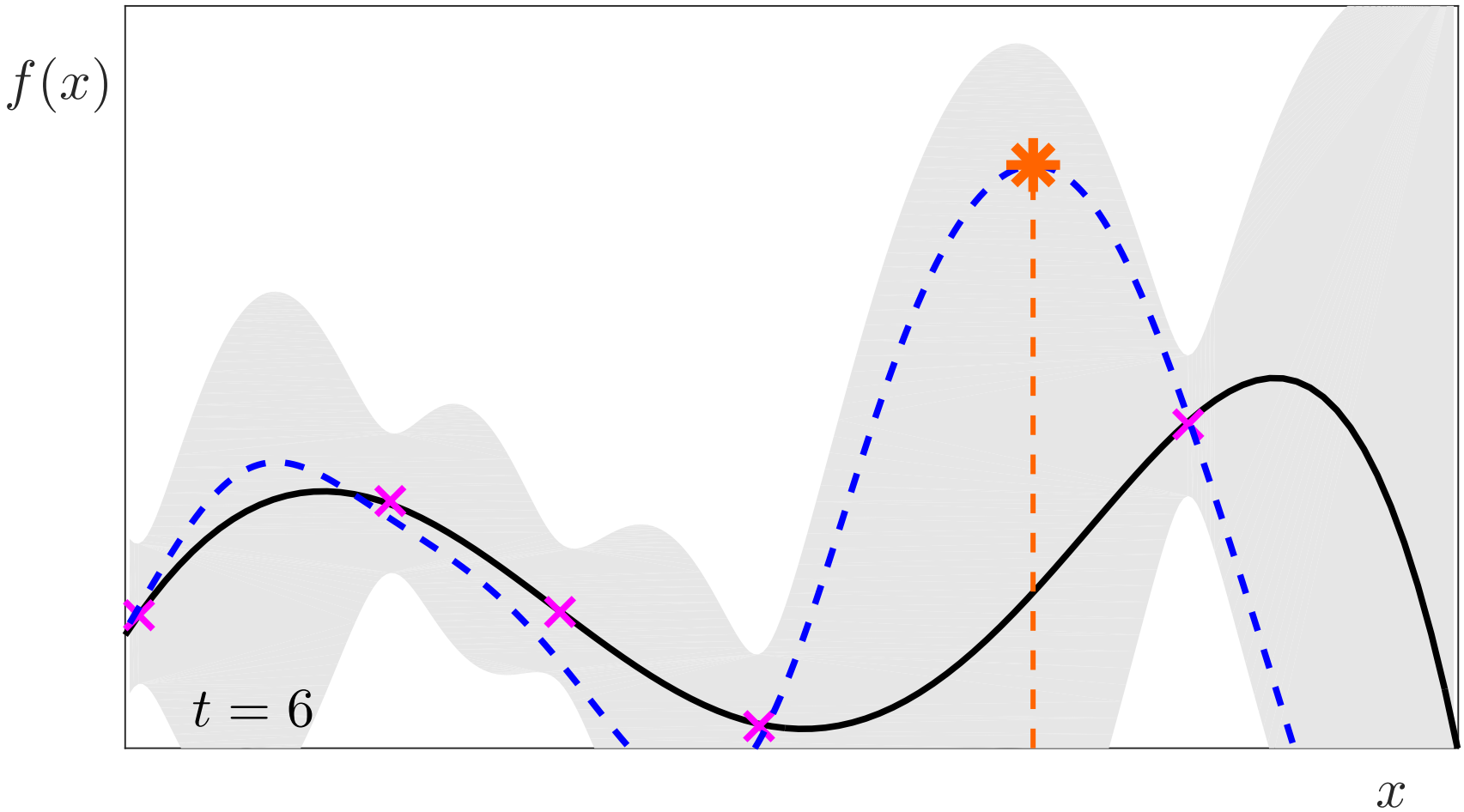

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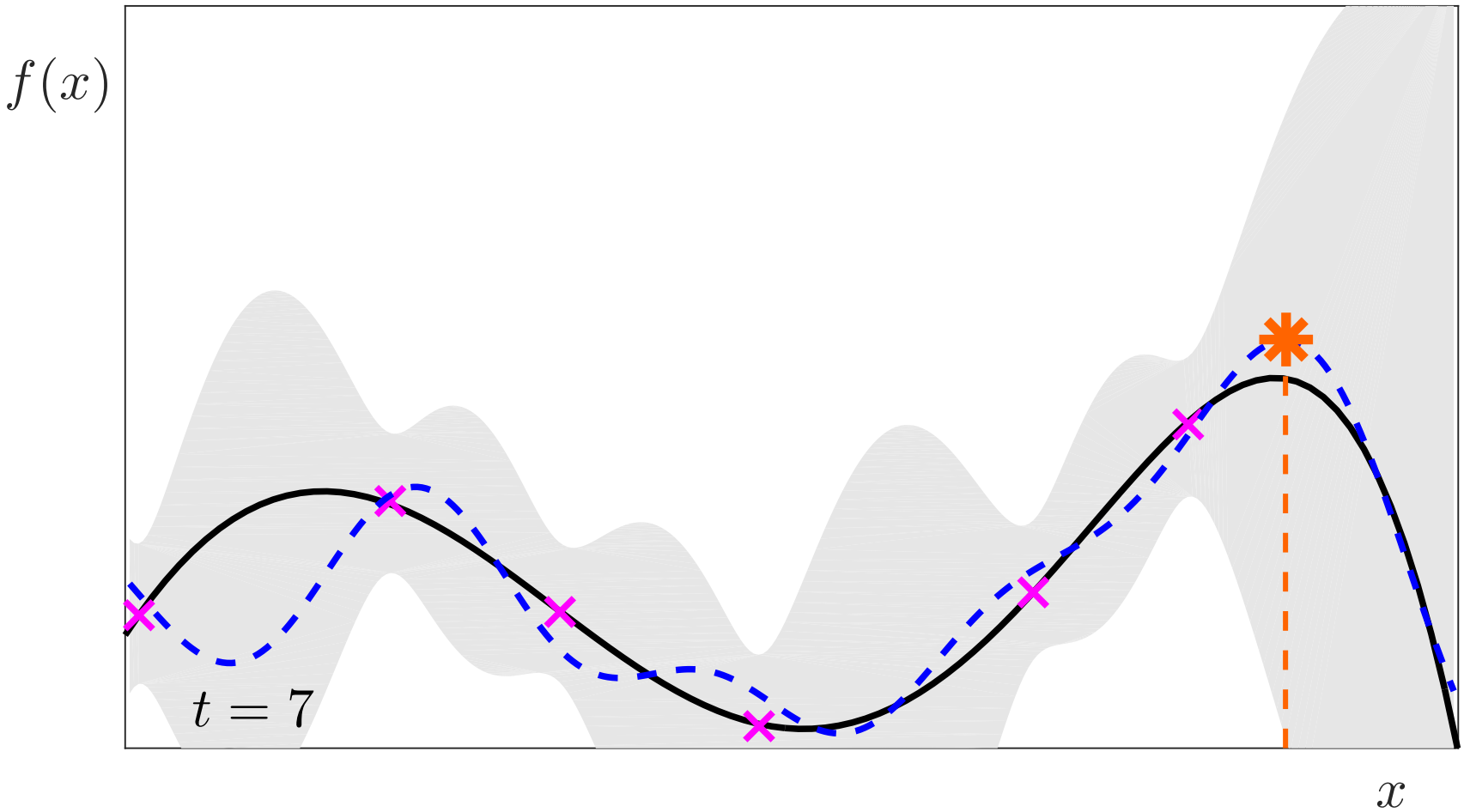

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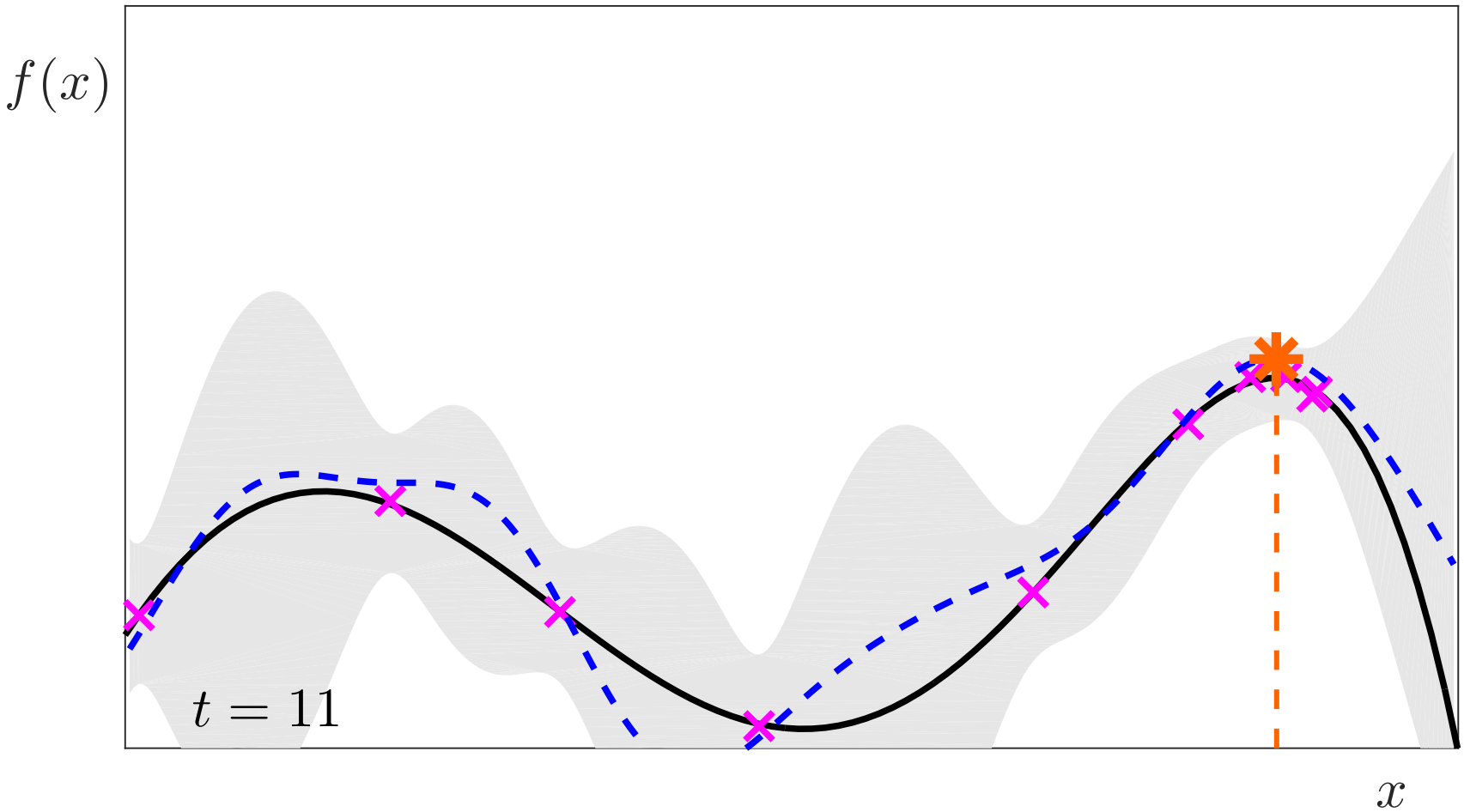

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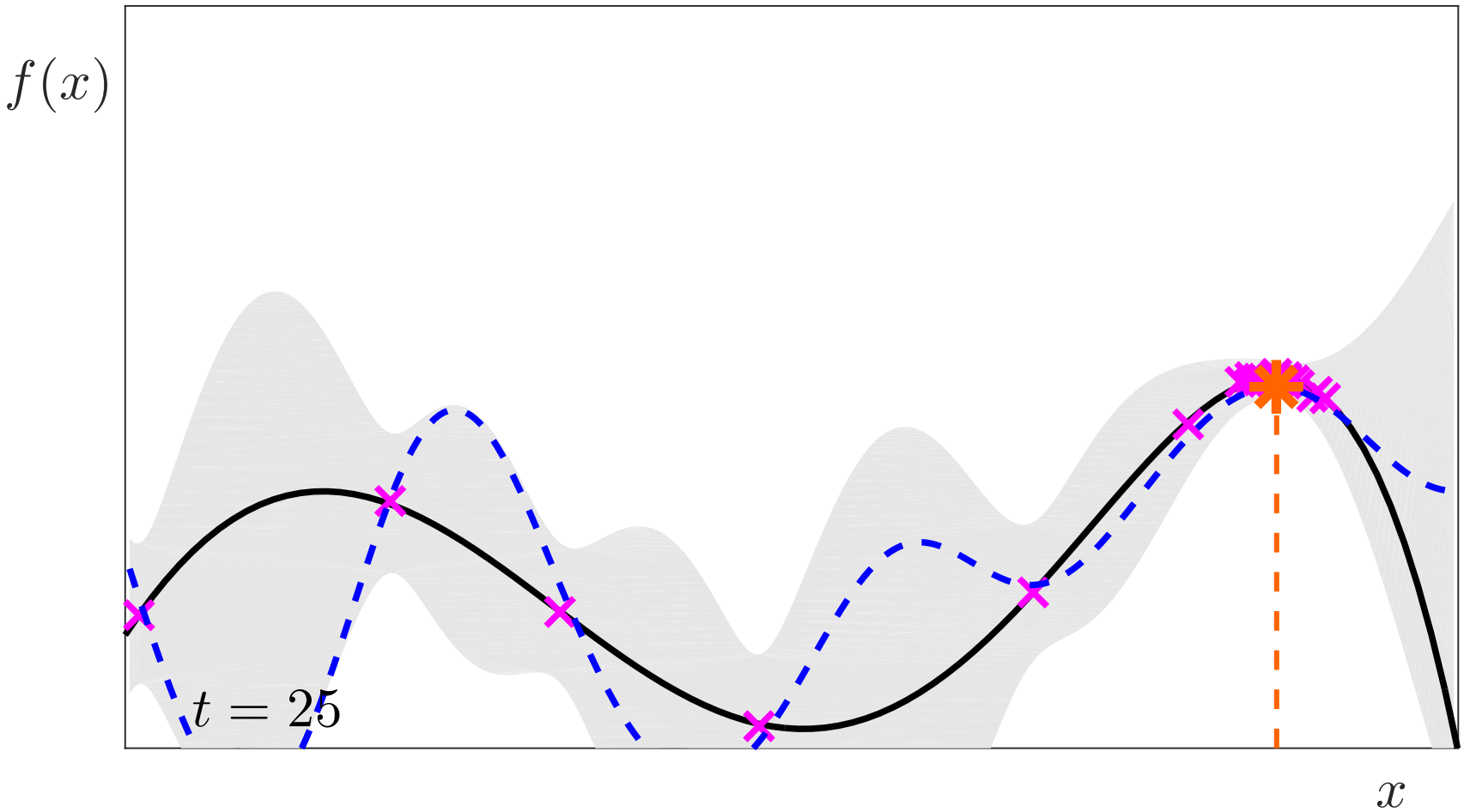

Bandits in the Bayesian Paradigm

Theory: Both UCB and TS will eventually find the optimum under appropriate smoothness assumptions of f. That is,

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- Expected improvement (Jones et al. 1998)
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Other Bayesian models for f:

- Neural networks (Snoek et al. 2015)
- Random Forests (Hutter 2009)

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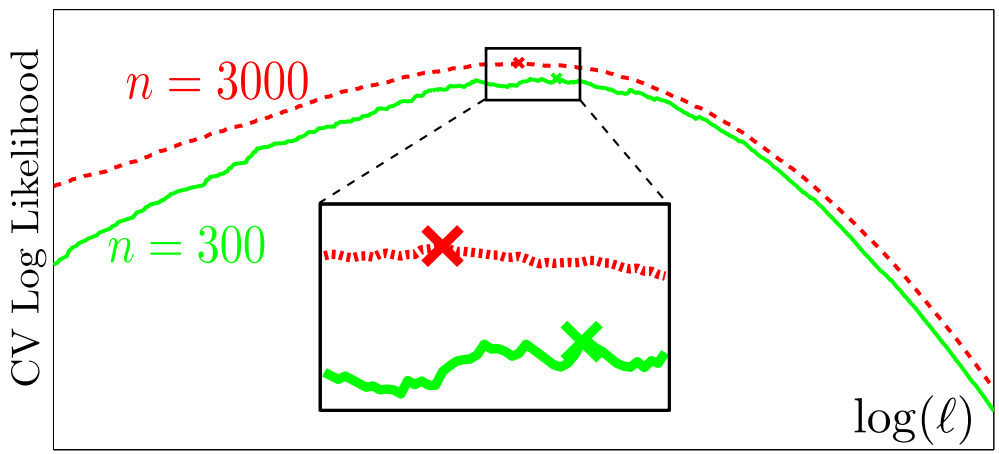
(N.B: Part II is a shameless plug for my research.)

Part 2.1: Multi-fidelity Bandits

Motivating question:
What if we have cheap approximations to f?

1. Hyper-parameter tuning: Train & validate with a subset of the data, and/or early stopping before convergence.

   E.g. Bandwidth (ℓ) selection in kernel density estimation.



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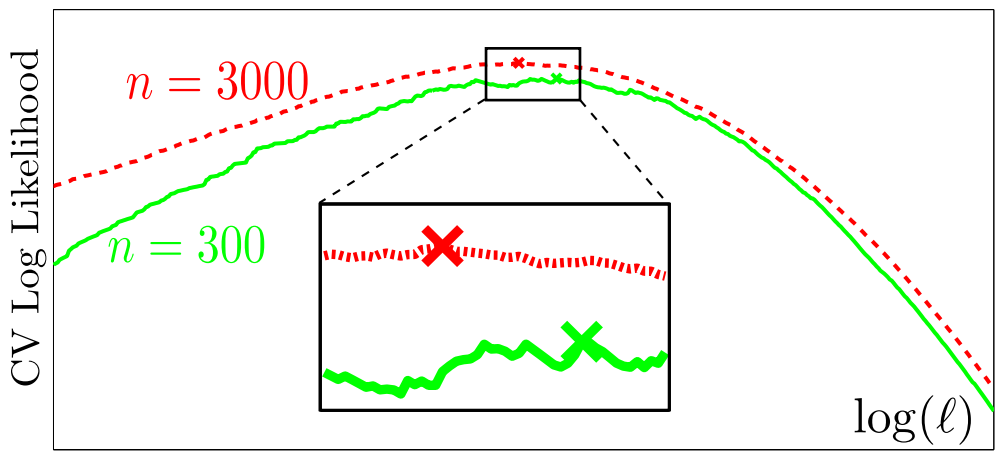

2. Computational astrophysics: cosmological simulations and numerical computations with less granularity.

3. Autonomous driving: simulation vs real world experiment.

Multi-fidelity Methods

For specific applications,

- Industrial design (Forrester et al. 2007)
- Hyper-parameter tuning (Agarwal et al. 2011, Klein et al. 2015, Li et al. 2016)
- Active learning (Zhang & Chaudhuri 2015)
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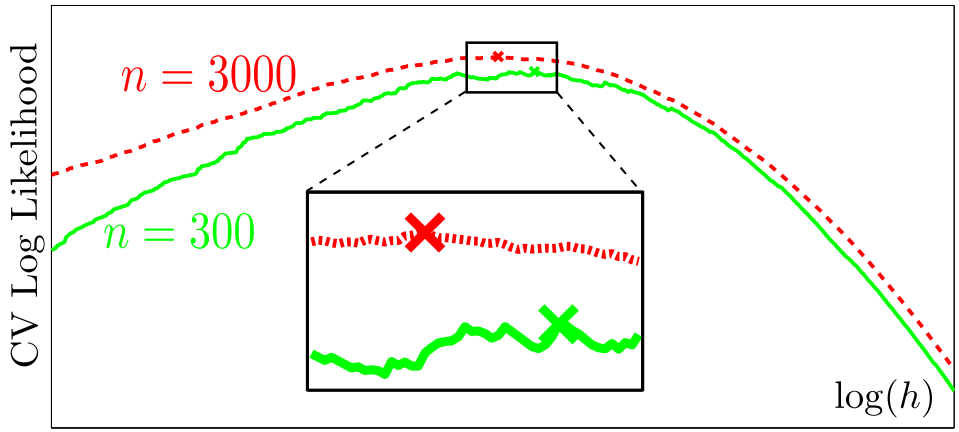
Multi-fidelity Bandits for Hyper-parameter tuning



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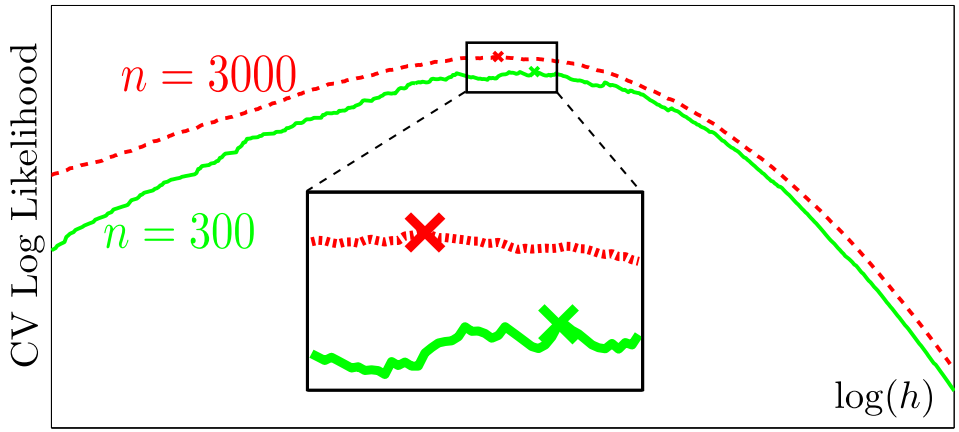

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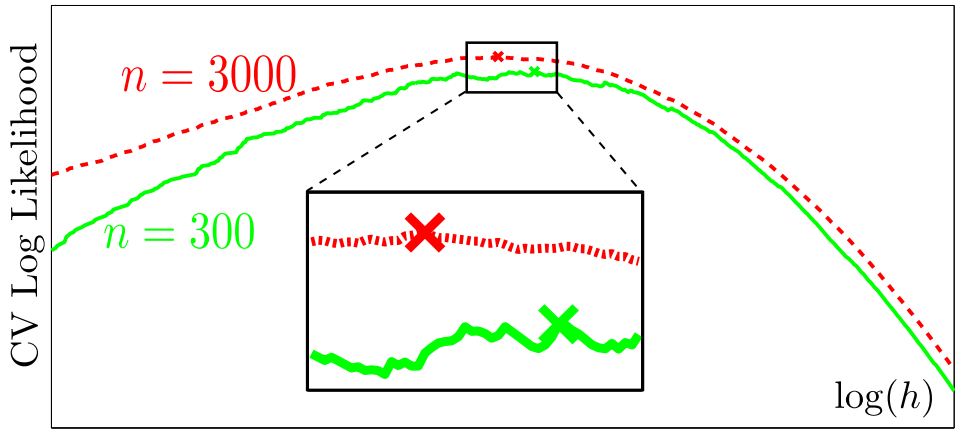

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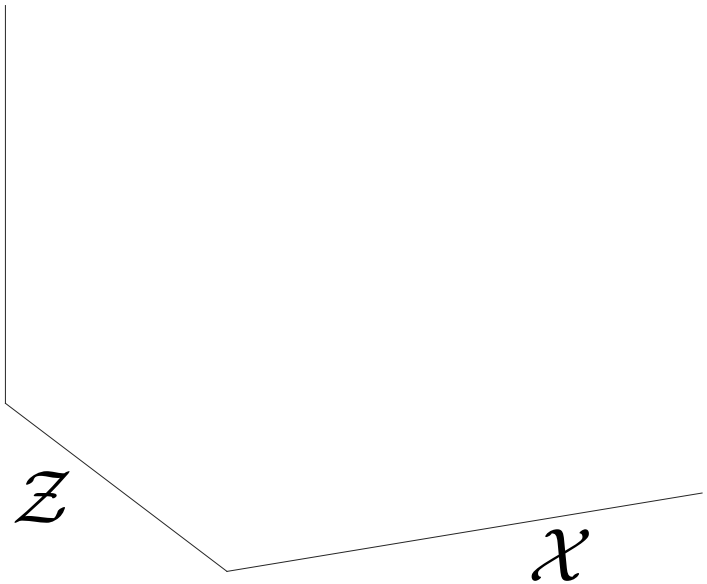
Approximations from a *continuous* 2D "fidelity space" (N, T).

Multi-fidelity Bandits

(Kandasamy et al. ICML 2017)



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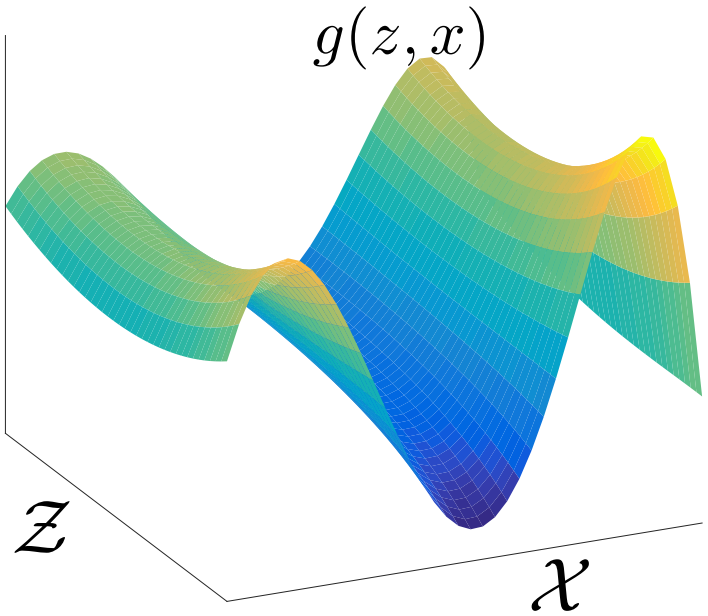

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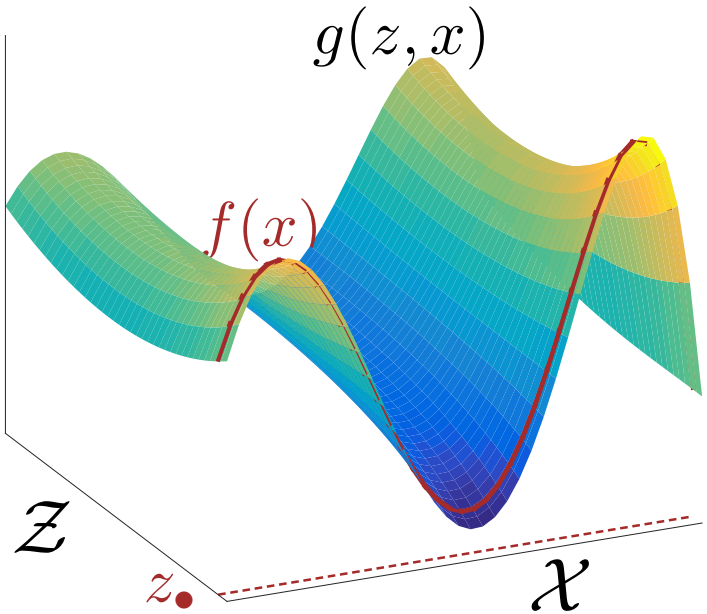

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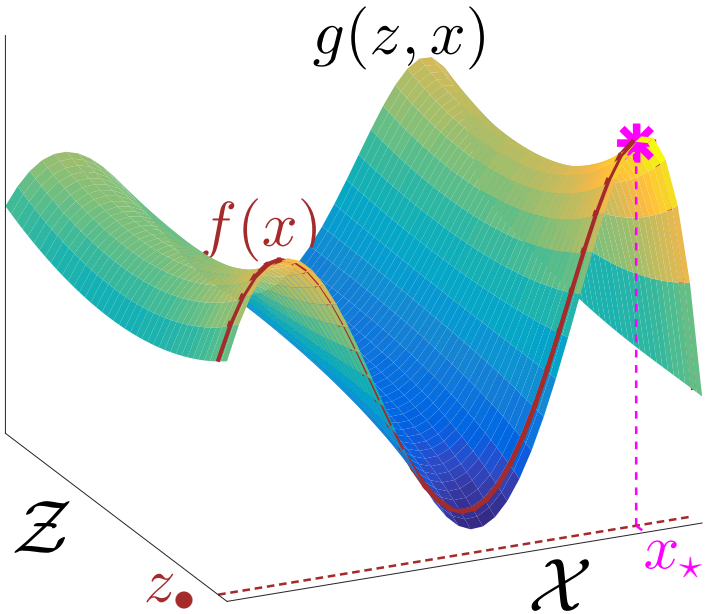

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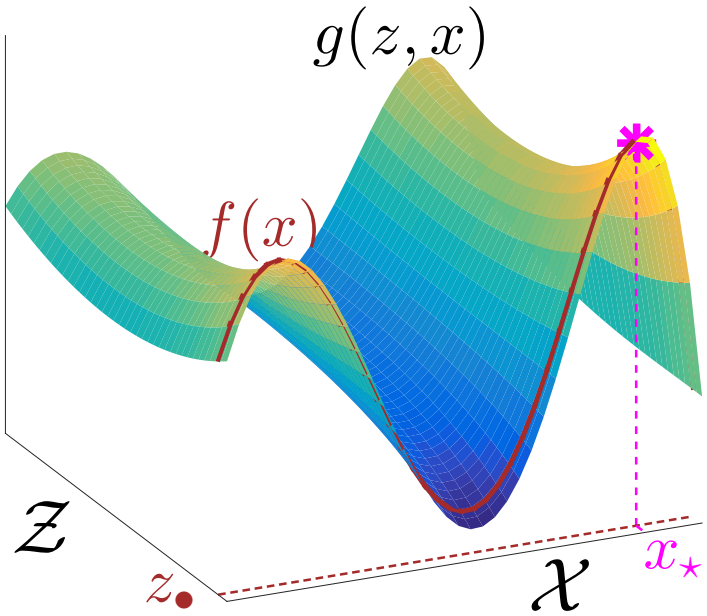

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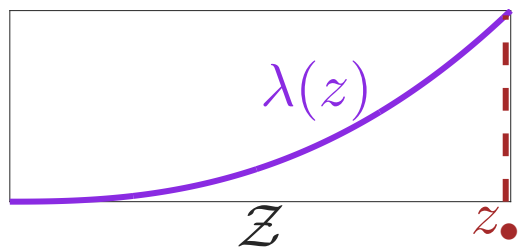
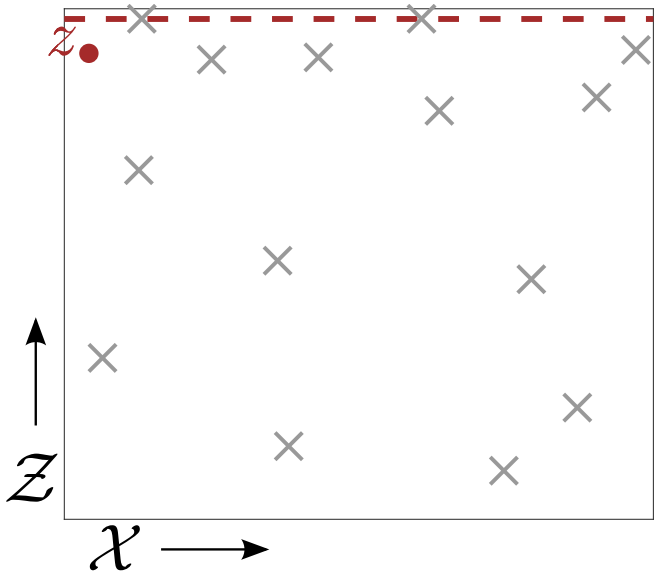
A cost function, $\lambda : \mathcal{Z} \to \mathbb{R}_+$.

$\lambda(z) = \lambda(N, T) = \mathcal{O}(N^2 T)$ (say).



Algorithm: BOCA (Kandasamy et al. ICML 2017)



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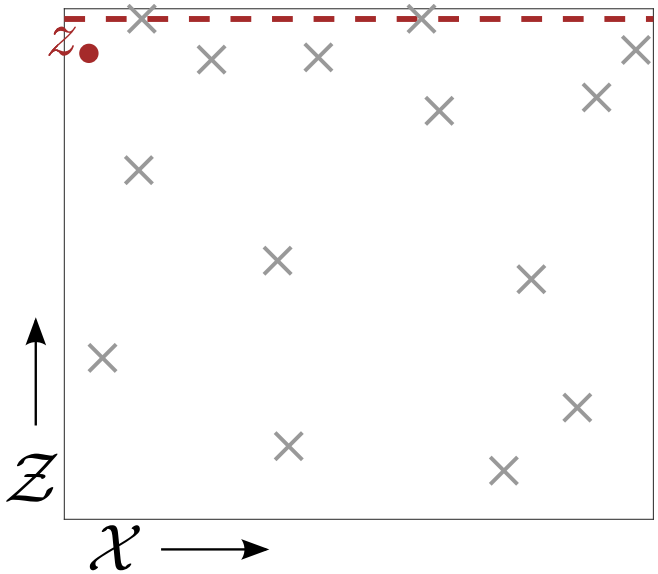

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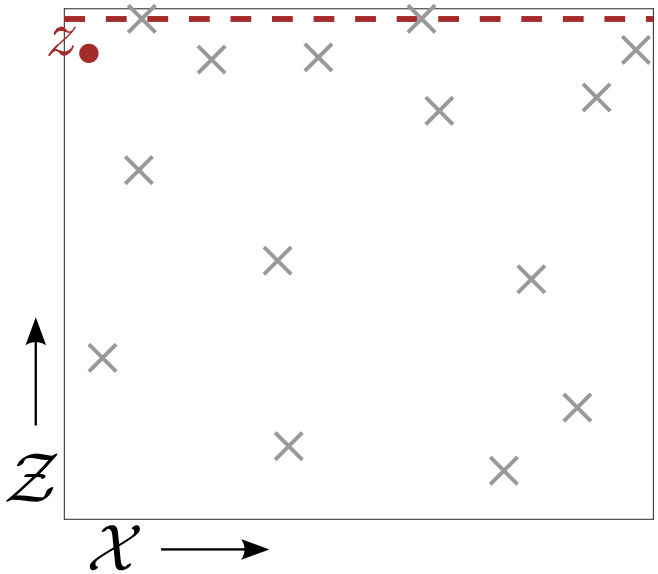

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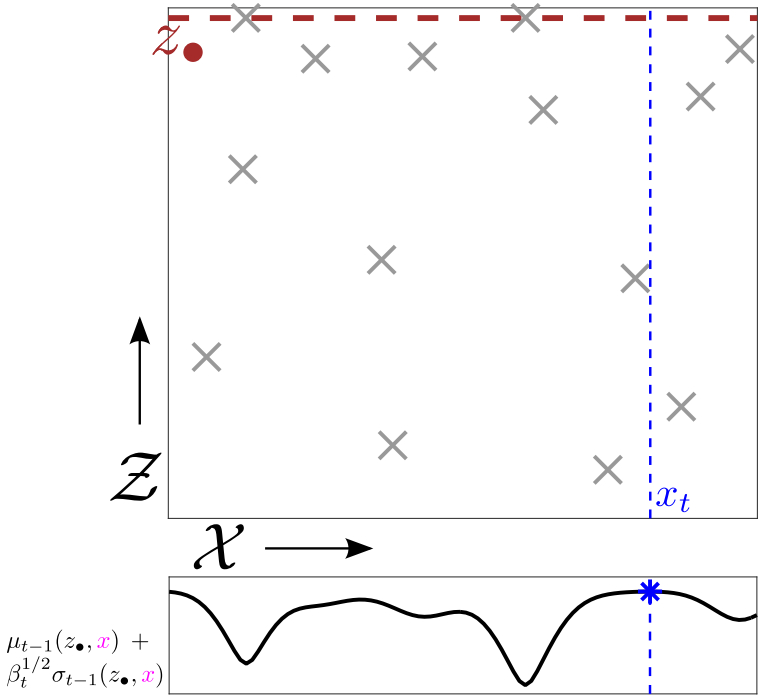

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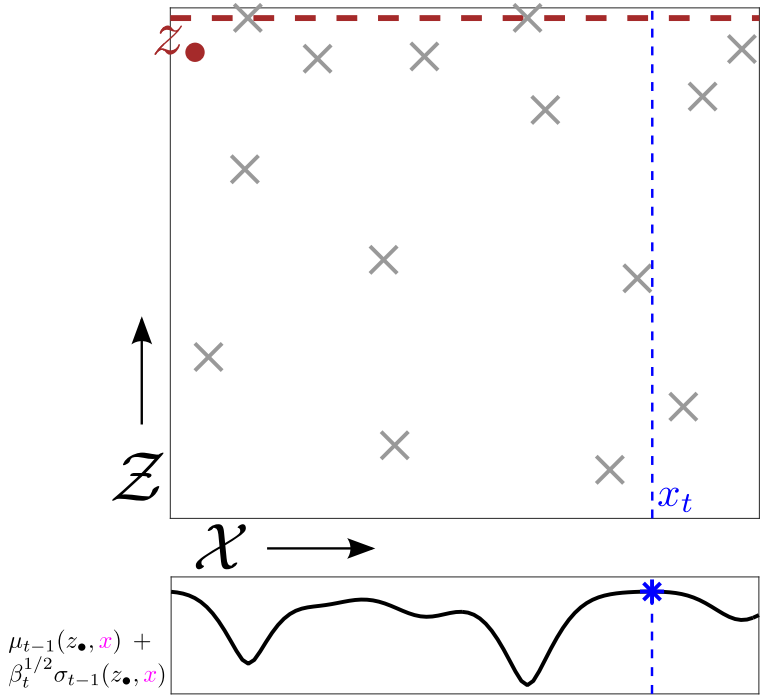

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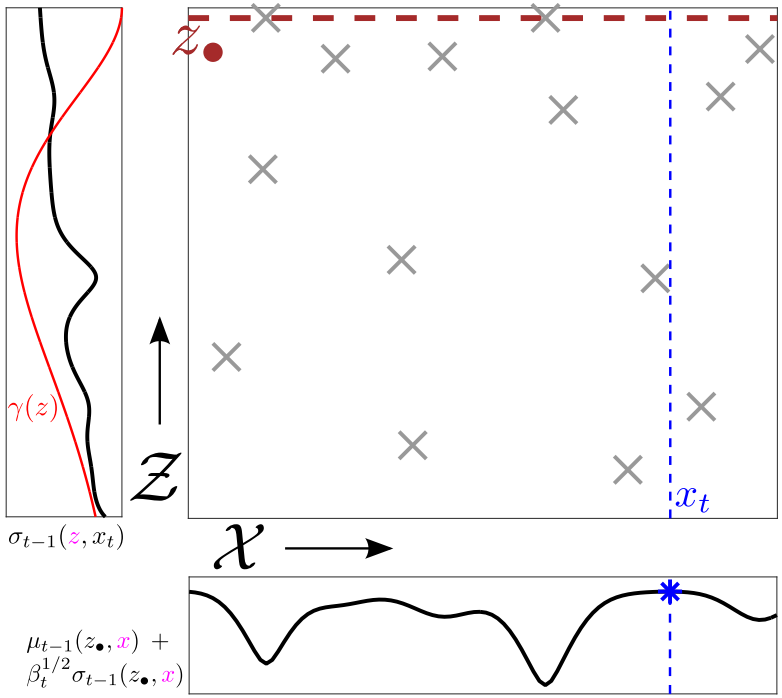

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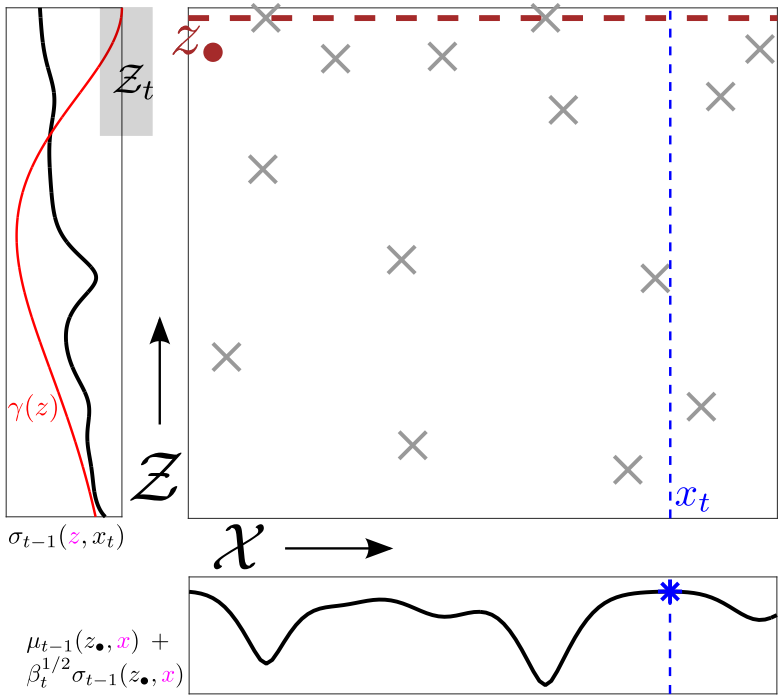

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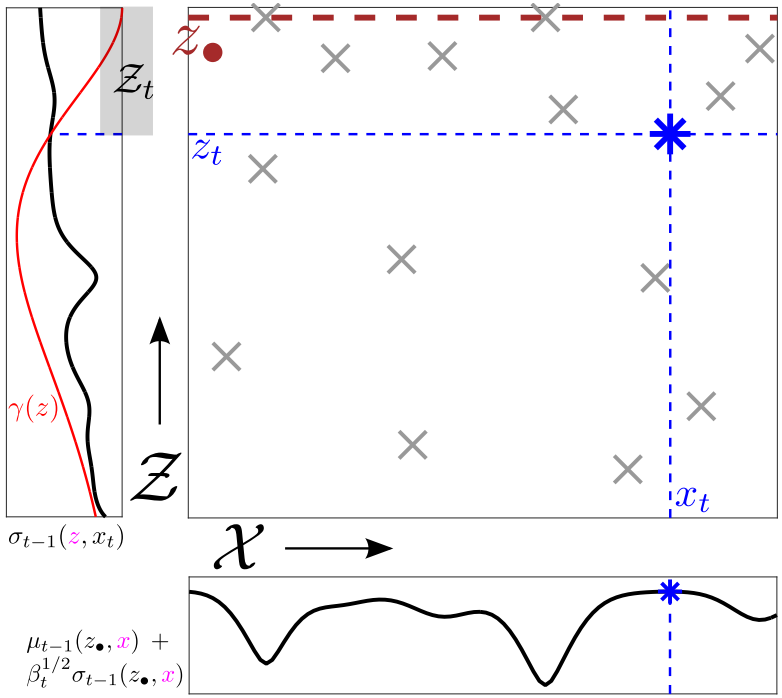

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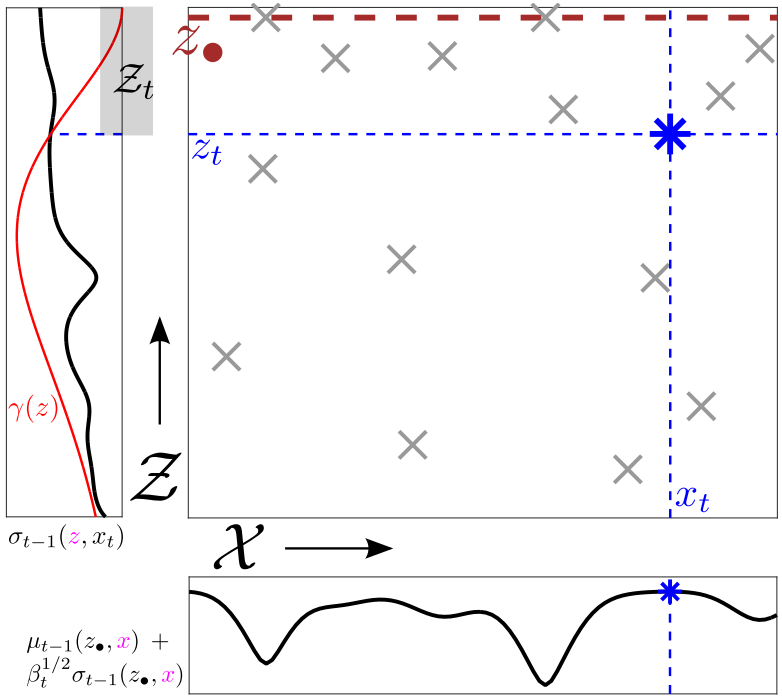

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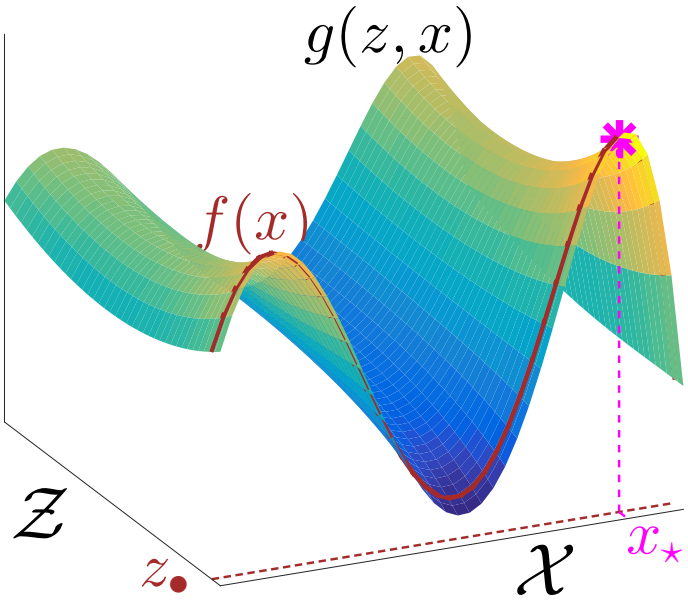
Theoretical Results for BOCA



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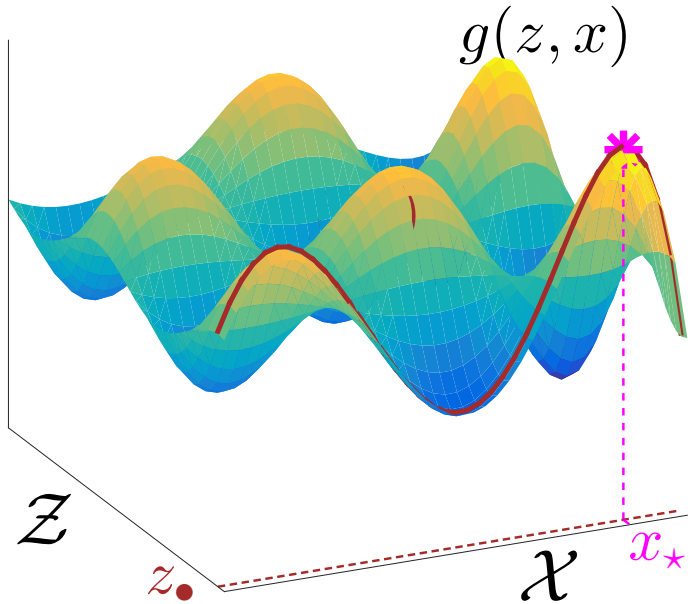

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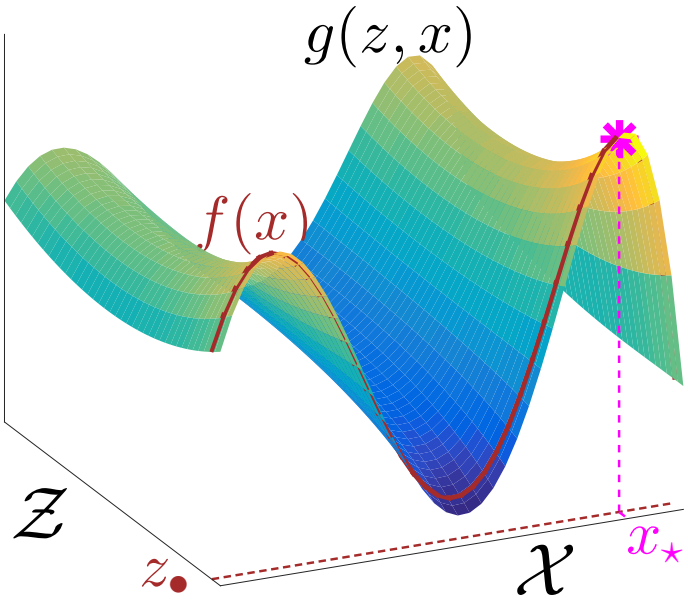

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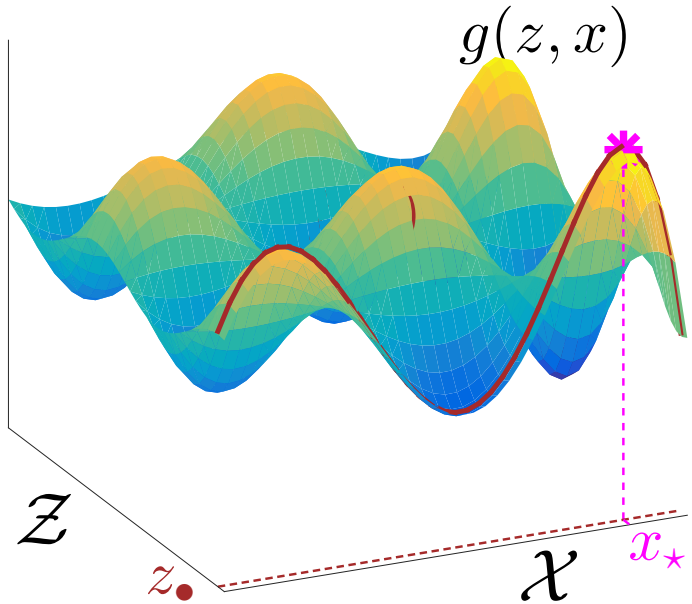
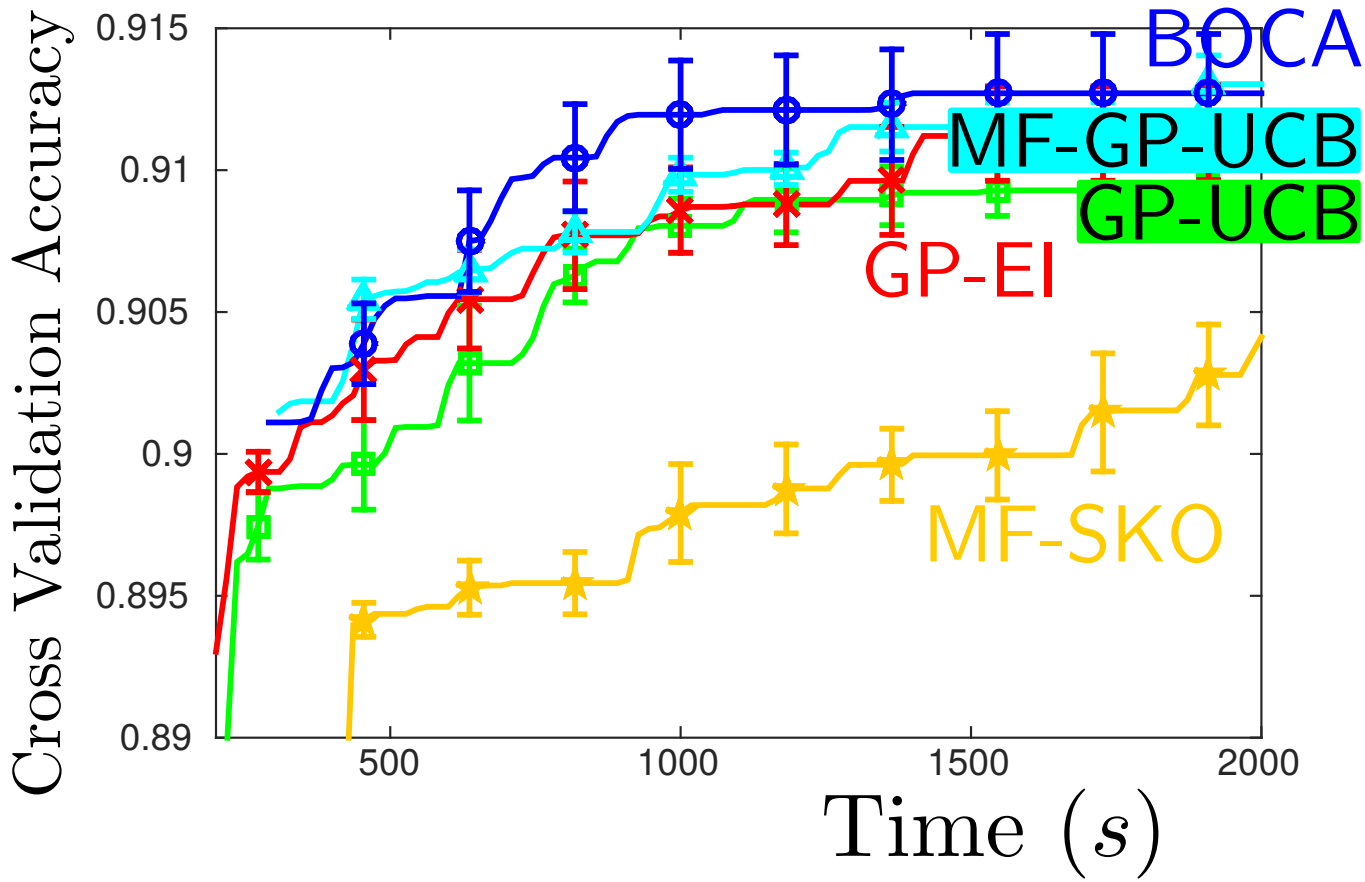


"bad"

Theorem: (Informal)
BOCA does better, i.e. achieves better Simple regret, than GP-UCB. The improvements are better in the "good" setting when compared to the "bad" setting.

Experiment: SVM with 20 News Groups

Tune two hyper-parameters for the SVM.
Dataset has $N_\bullet = 15K$ data and use $T_\bullet = 100$ iterations.
But can choose $N \in [5K, 15K]$ or $T \in [20, 100]$ (2D fidelity space).



Experiment: Cosmological inference on Type-1a supernovae data

Estimate Hubble constant, dark matter fraction & dark energy fraction by maximising likelihood on $N_\bullet = 192$ data.
Requires numerical integration on a grid of size $G_\bullet = 10^6$.
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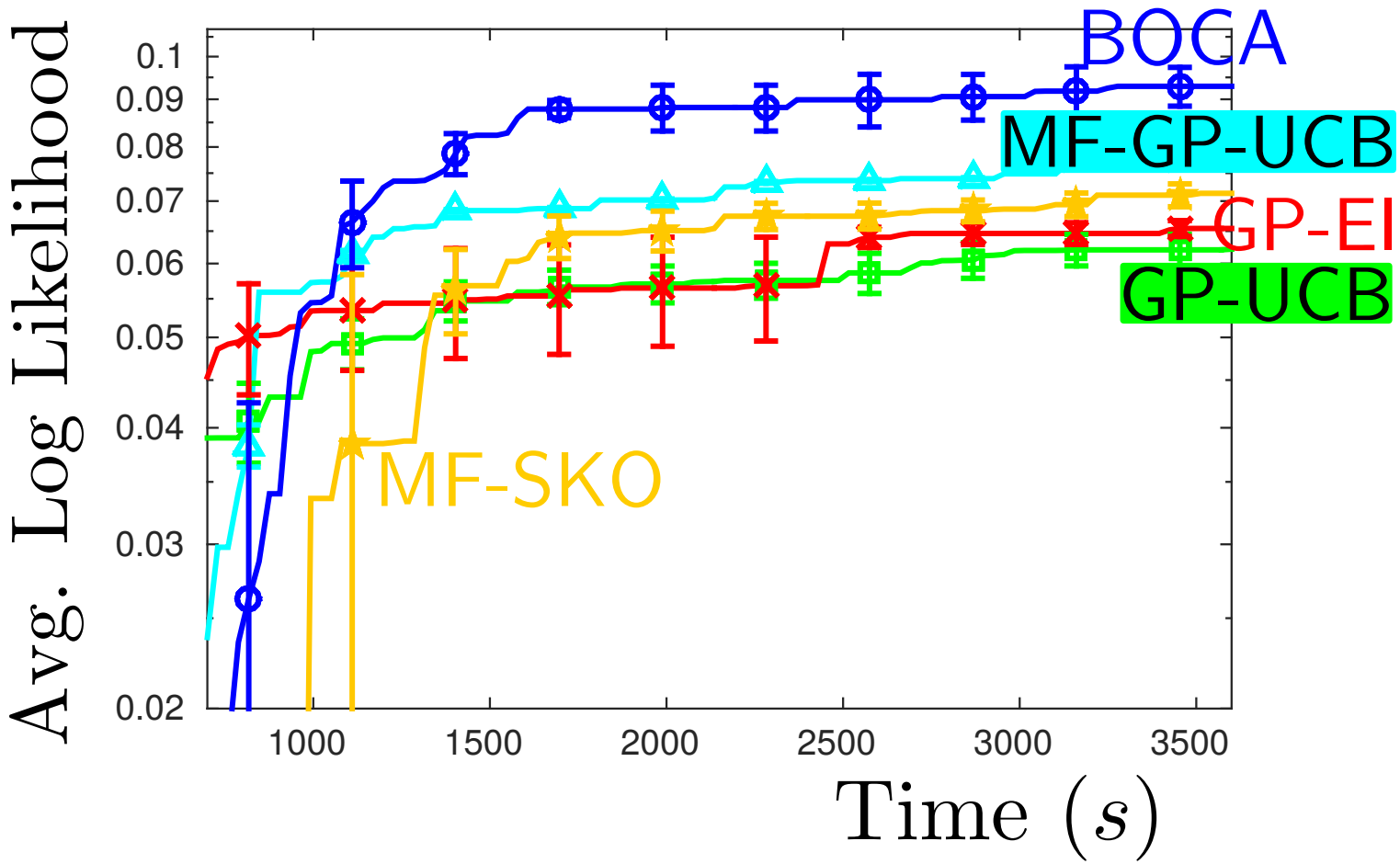

Hyper-band: A multi-fidelity method with incremental resource allocation (Li et al. 2016)

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Successive Halving (with finite $\mathcal{X}$):

1. Allocate a small resource R to each $x \in \mathcal{X}$.
   e.g. Train all hyper-parameters for 100 iterations.
2. Drop half of the x's that are performing worst.
3. Repeat steps 1 & 2 until one arm is left.

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Does not fall within the GP/Bayesian framework.

Hyper-band (cont'd)

When compared to Bayesian methods,

- **Pro:** Incremental resource allocation (do not need to retrain all models from the beginning).
- **Con:** Cannot use correlation between arms (e.g. if x_1 has large CV accuracy, then x_2 close to x_1 is also likely to do well).

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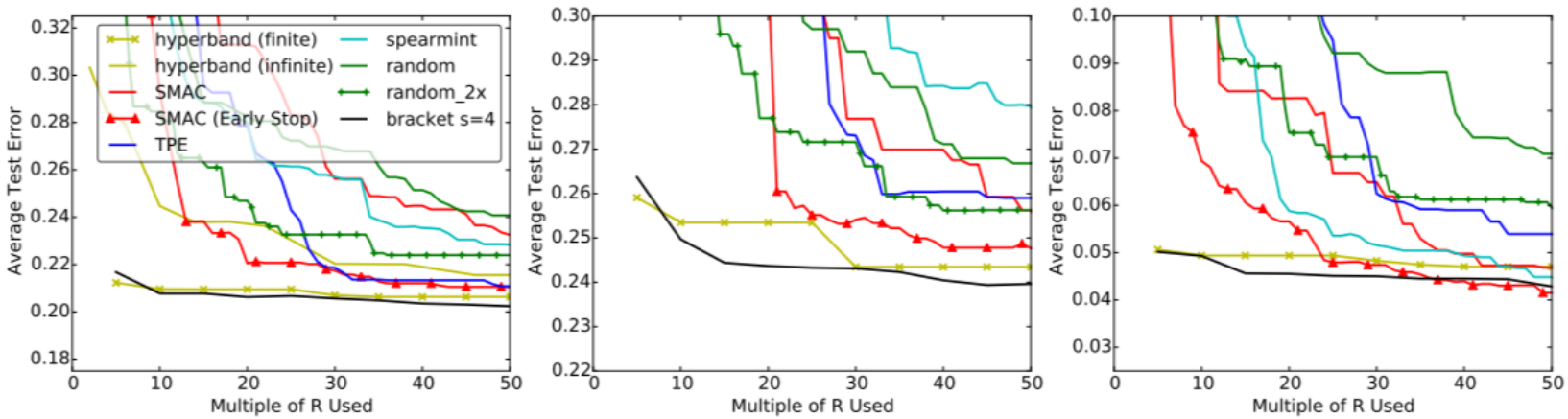
Experiments:



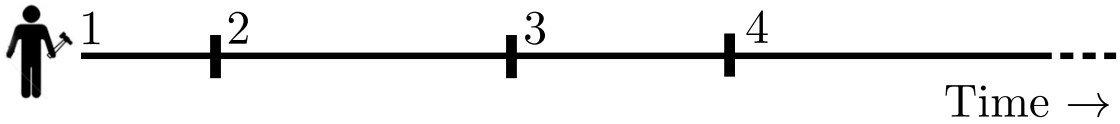
(a) CIFAR-10 (b) MRBI (c) SVHN

Outline

- Part I: Bandits in the Bayesian Paradigm
  1. Gaussian processes
  2. Algorithms: Upper Confidence Bound (UCB) & Thompson Sampling (TS)
- Part II: Scaling up Bandits
  1. Multi-fidelity bandit: cheap approximations to an expensive experiment
  2. Parallelising function evaluations
  3. High dimensional input spaces

Part 2.2: Parallelising arm pulls

Sequential evaluations with one worker



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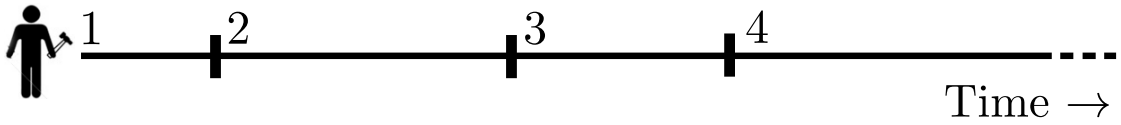

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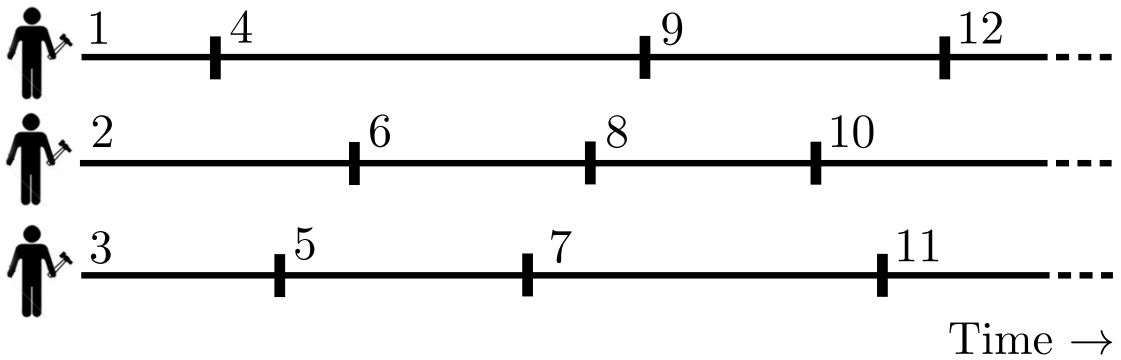

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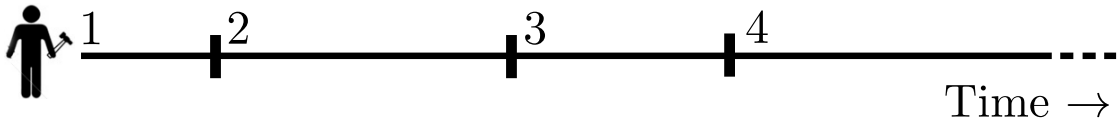

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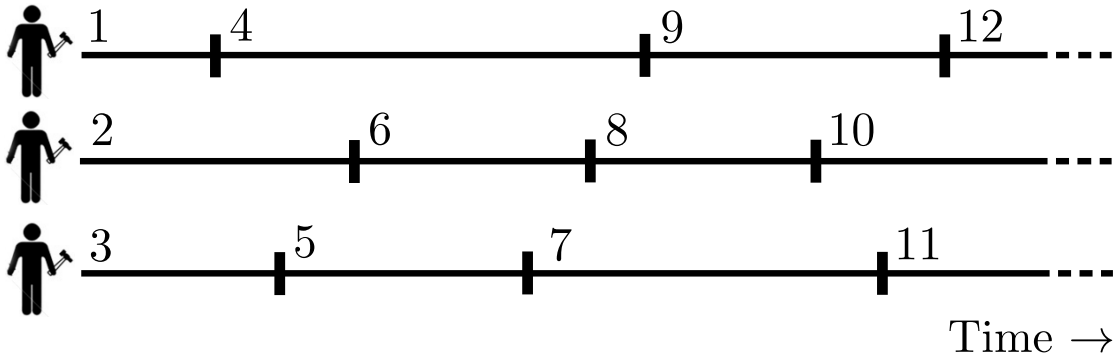
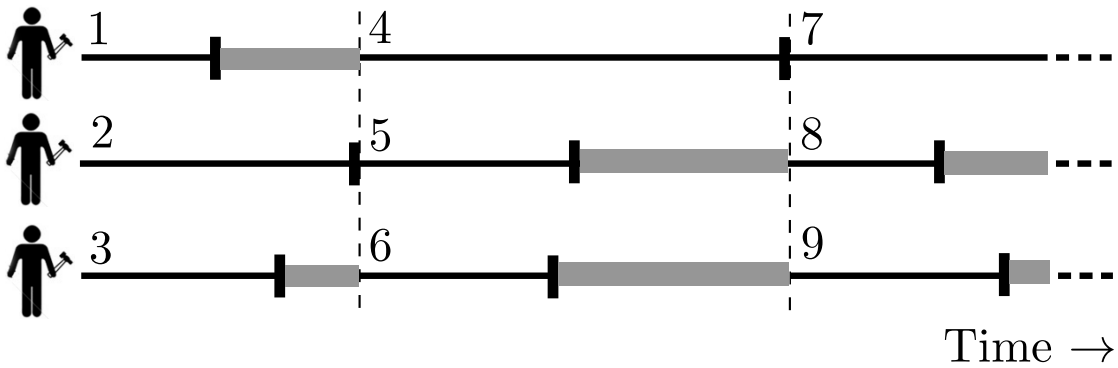


Parallel evaluations with M workers (Synchronous)



Why parallelisation?

- **Computational experiments:** infrastructure with 100-1000's CPUs or GPUs.

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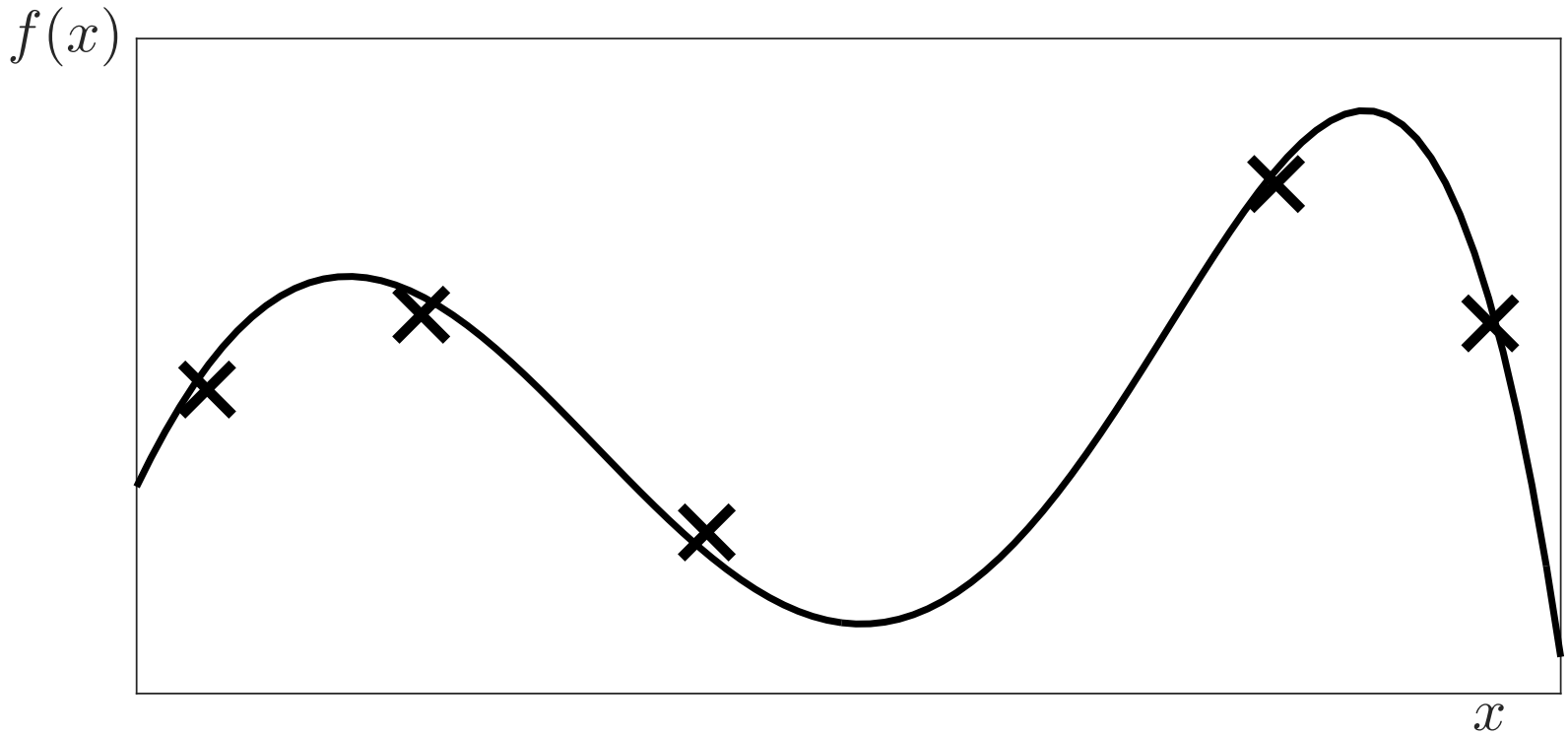
Prior work: (Ginsbourger et al. 2011, Janusevskis et al. 2012, Wang et al. 2016, González et al. 2015, Desautels et al. 2014, Contal et al. 2013, Shah and Ghahramani 2015, Kathuria et al. 2016, Wang et al. 2017, Wu and Frazier 2016, Hernandez-Lobato et al. 2017)

Shortcomings

- **Asynchronicity**
- **Theoretical guarantees**
- **Computationally & conceptually simple**

Review: Sequential Thompson Sampling in GP Bandits

Thompson Sampling (TS) (Thompson, 1933).



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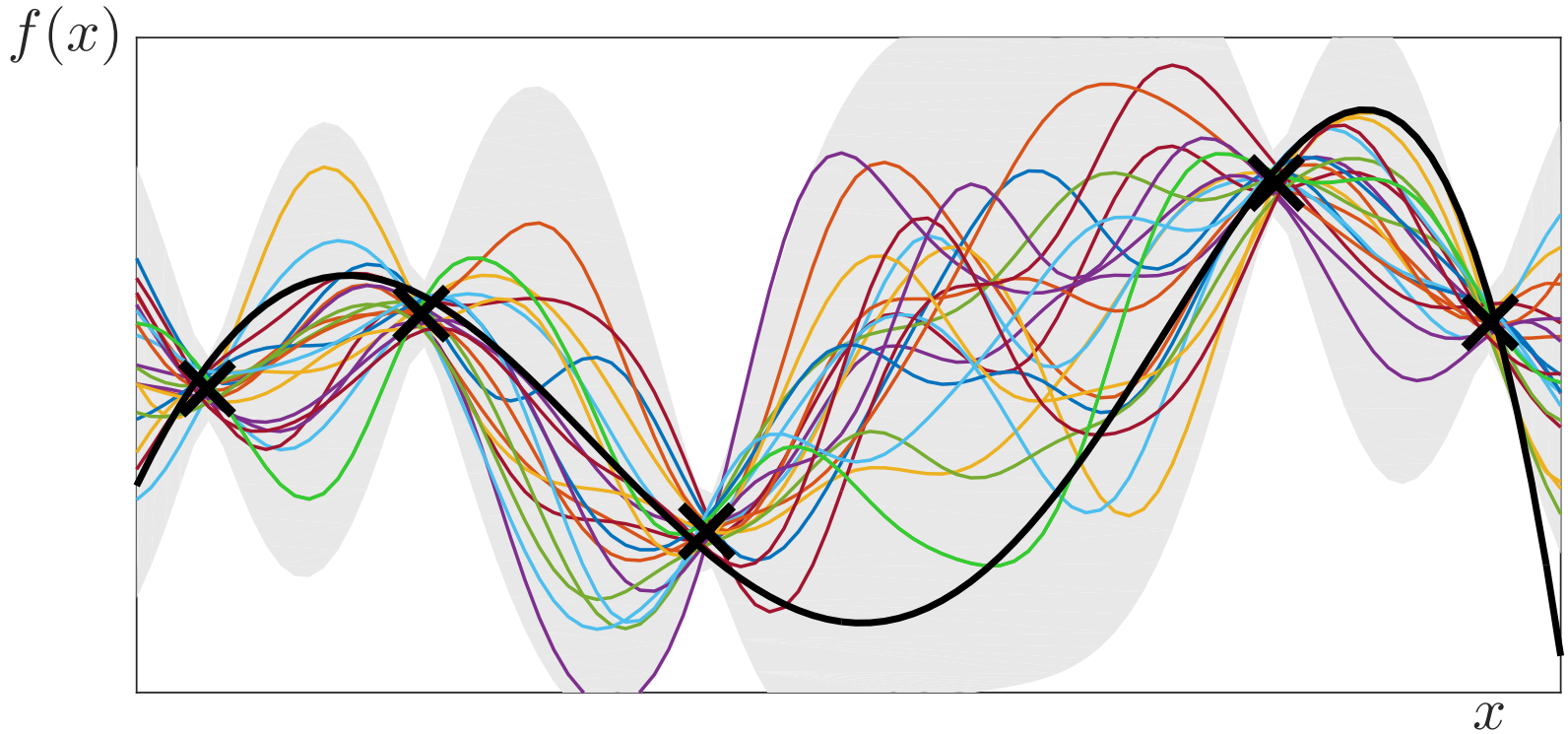

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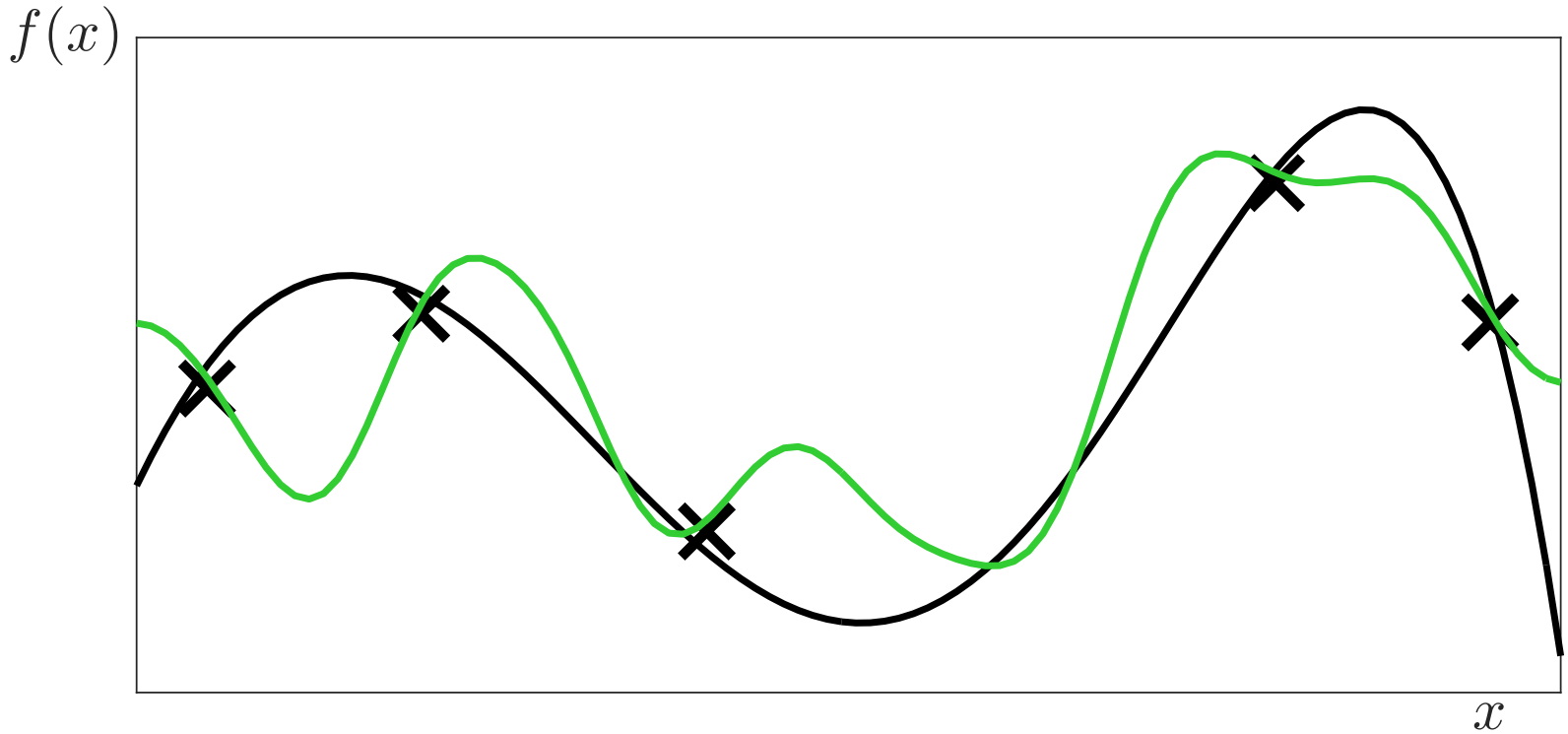

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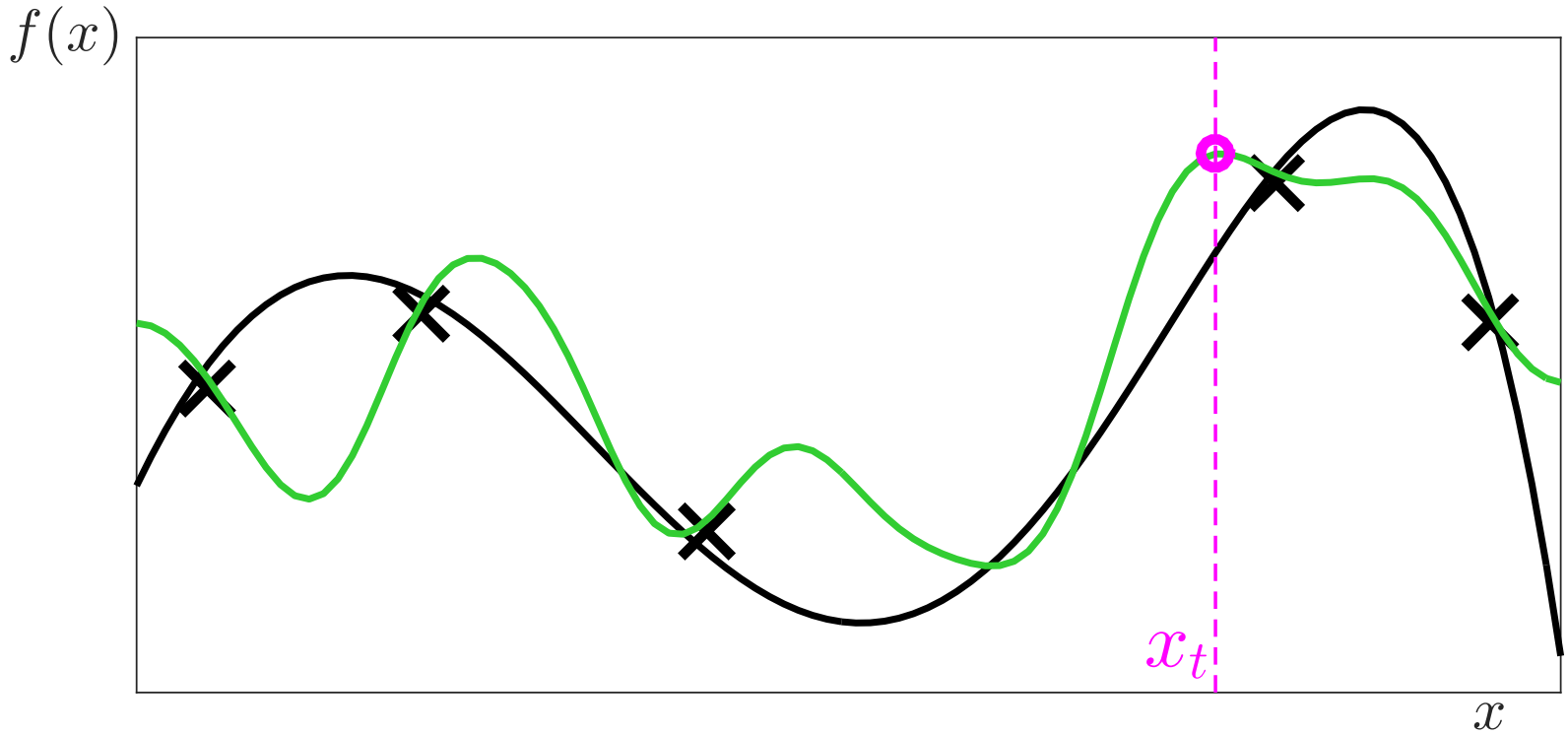

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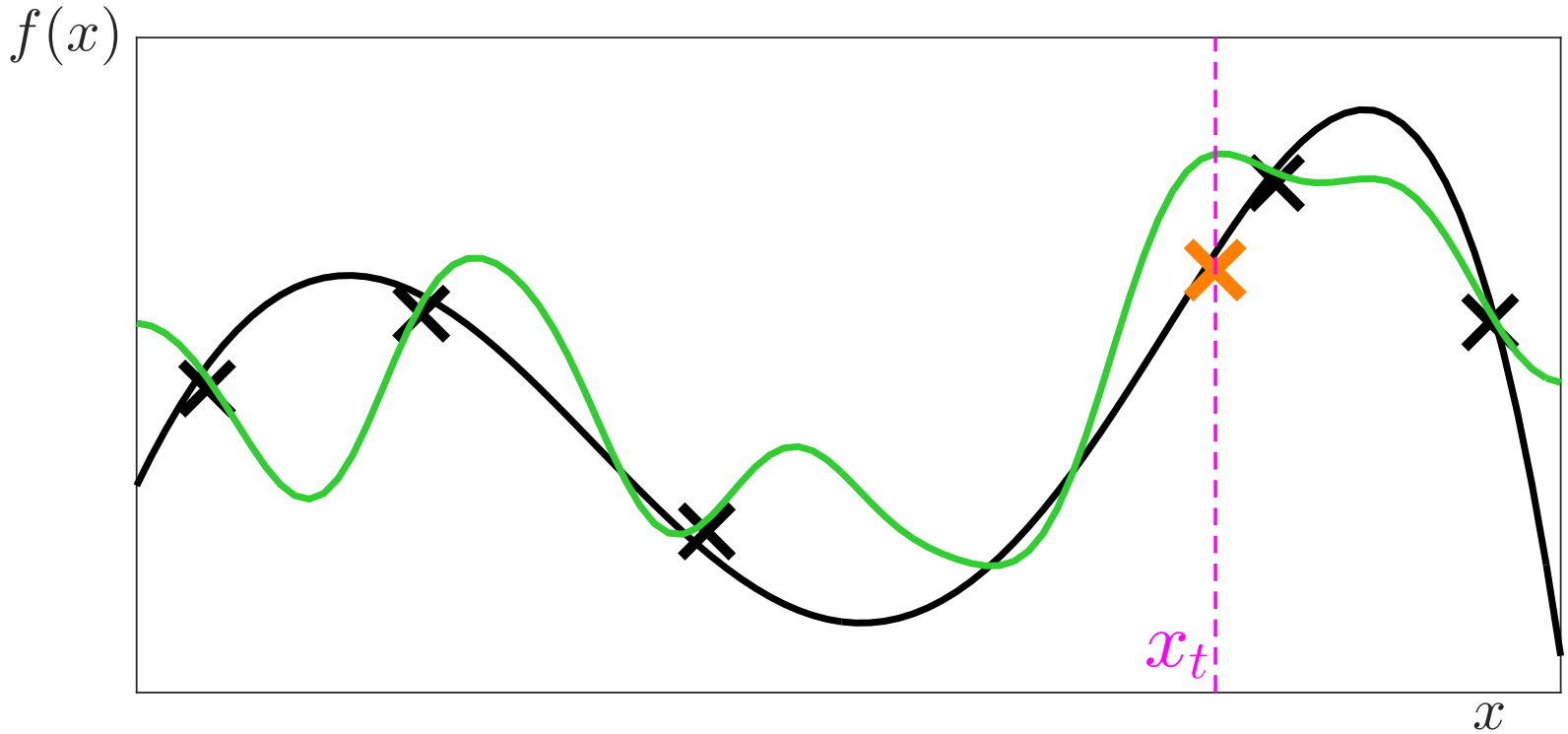

1) Construct posterior $\mathcal{GP}$. 2) Draw sample g from posterior.
3) Choose $x_t = \mathrm{argmax}_x\, g(x)$. 4) Evaluate f at x_t.

Parallelised Thompson Sampling (Kandasamy et al. Arxiv 2017)

Asynchronous: asyTS

At any given time,

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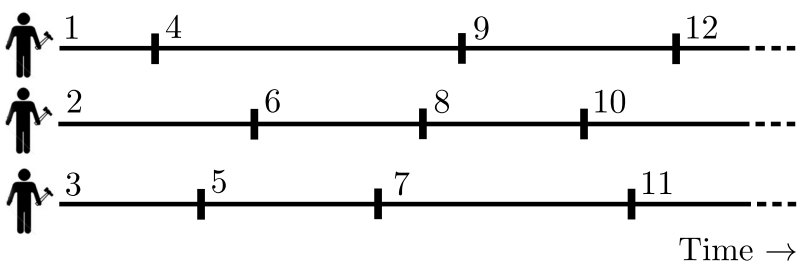

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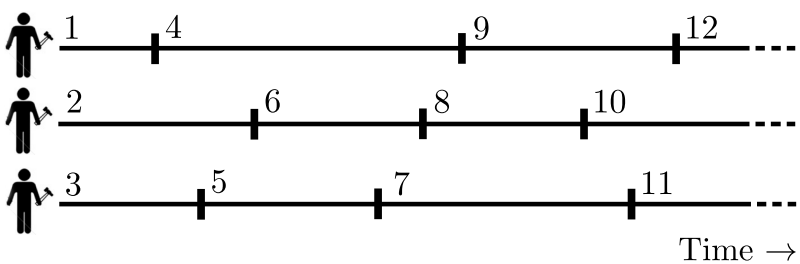

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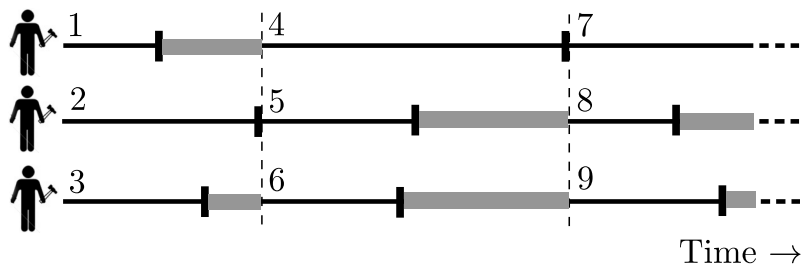

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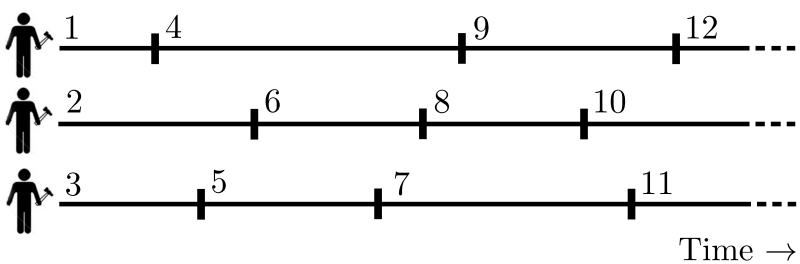

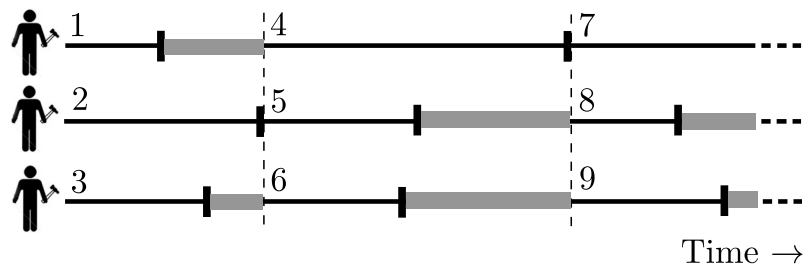

Variants in prior work: (Osband et al. 2016, Israelsen et al. 2016, Hernandez-Lobato et al. 2017)

Theoretical Results for TS: number of evaluations

Sequential TS, SE Kernel (Russo & van Roy 2014)

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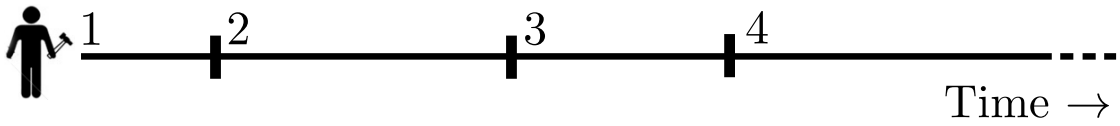

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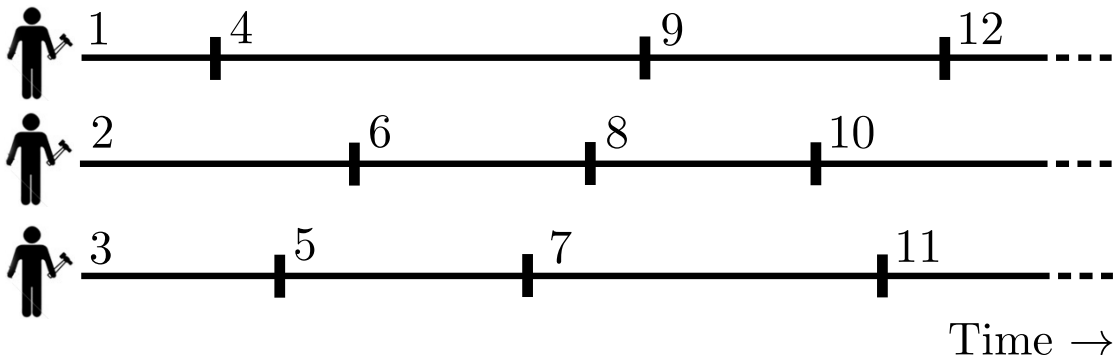

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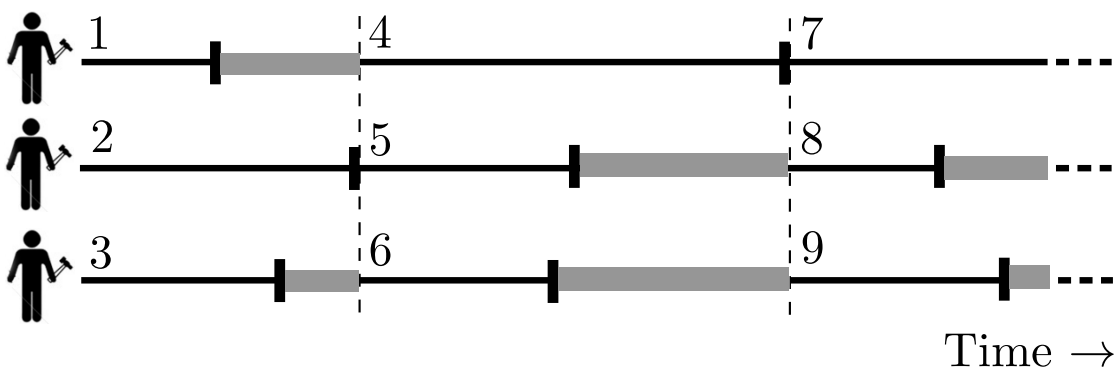

Theoretical Results: Simple regret with time

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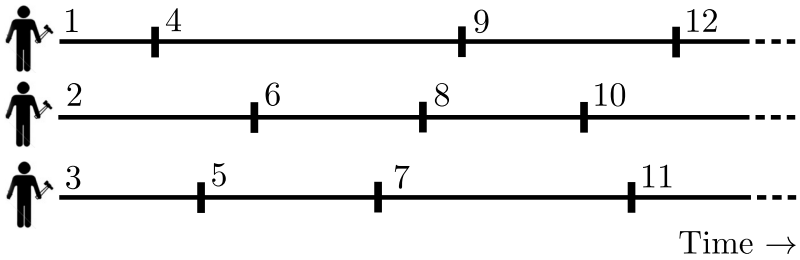

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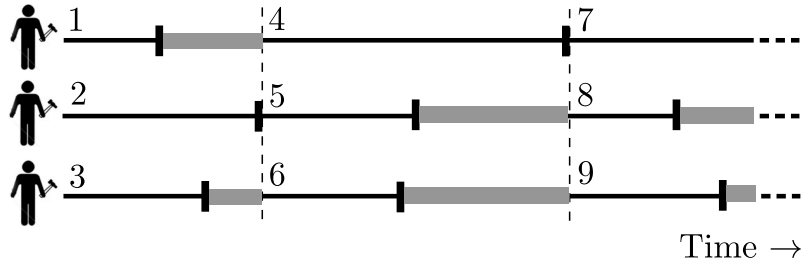

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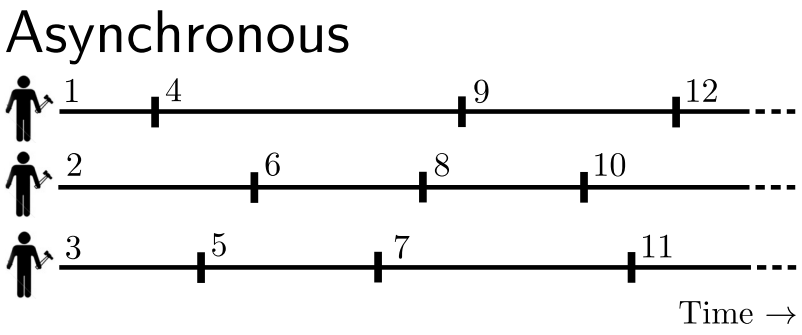

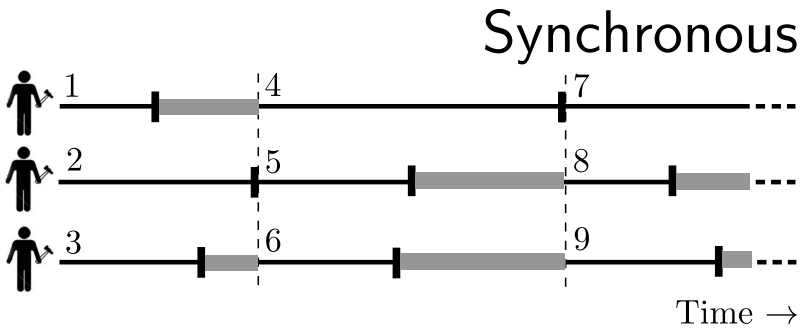

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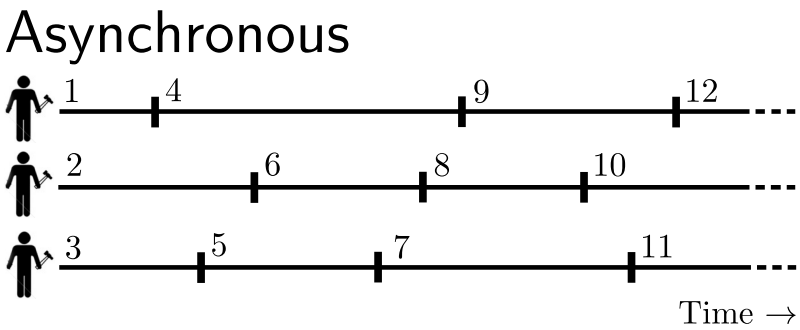

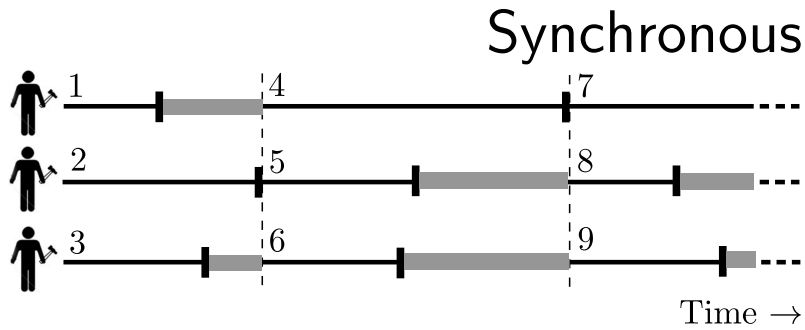

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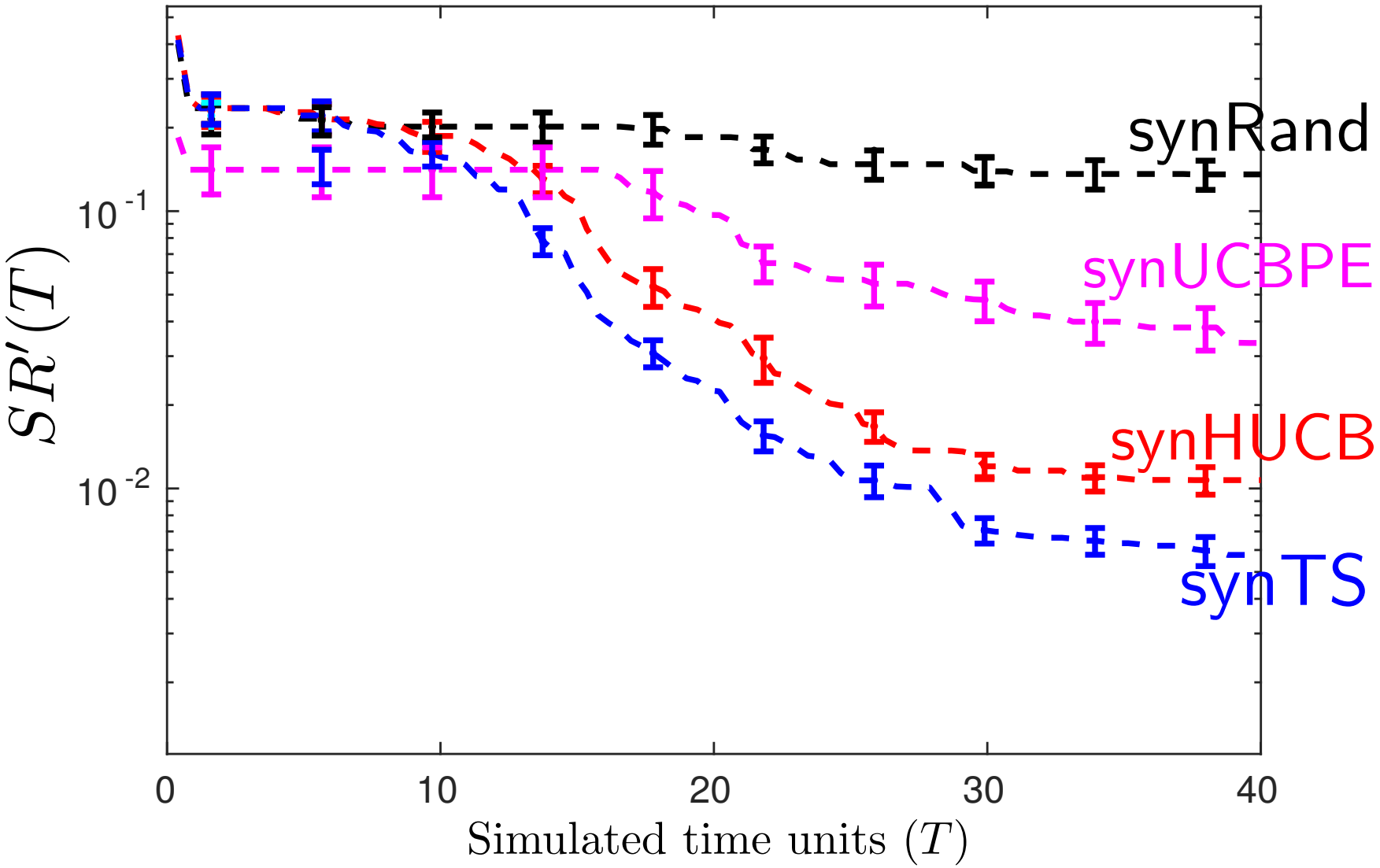
- Sub-gaussian tail decay: $\sqrt{\log(M)}$ factor
- Sub-exponential tail decay: $\log(M)$ factor

Experiment: Branin-2D $M = 4$

Evaluation time sampled from a uniform distribution



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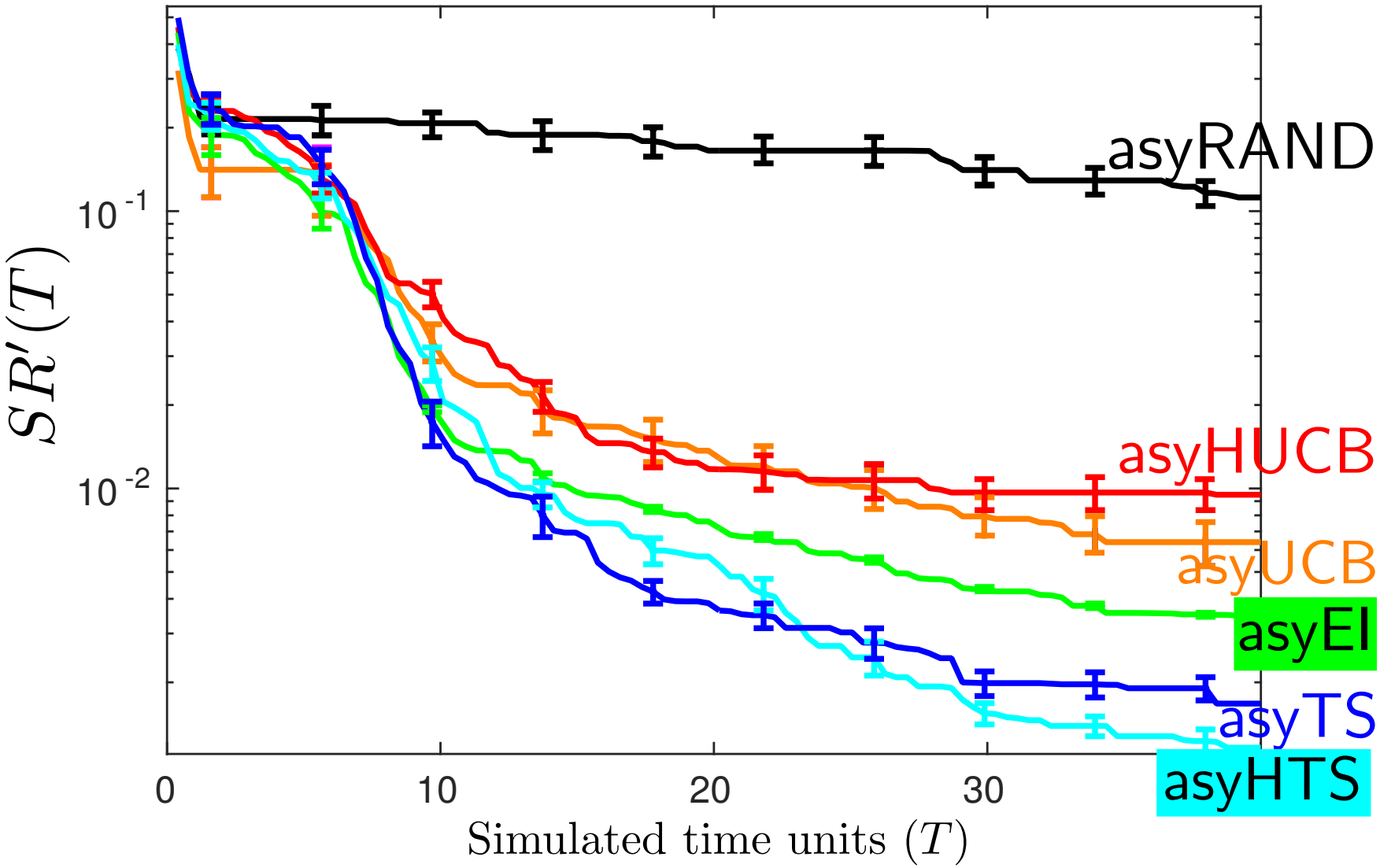

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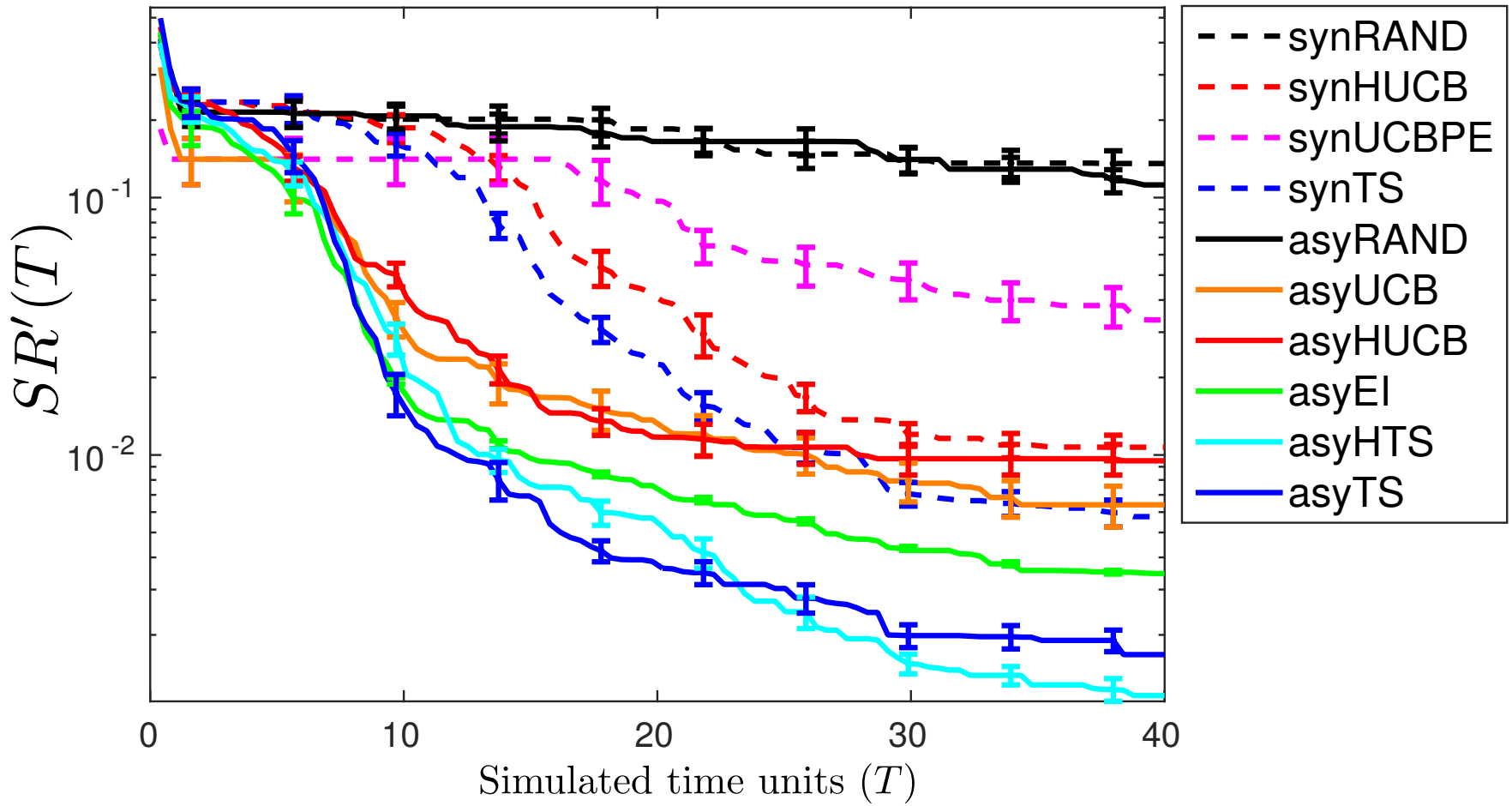
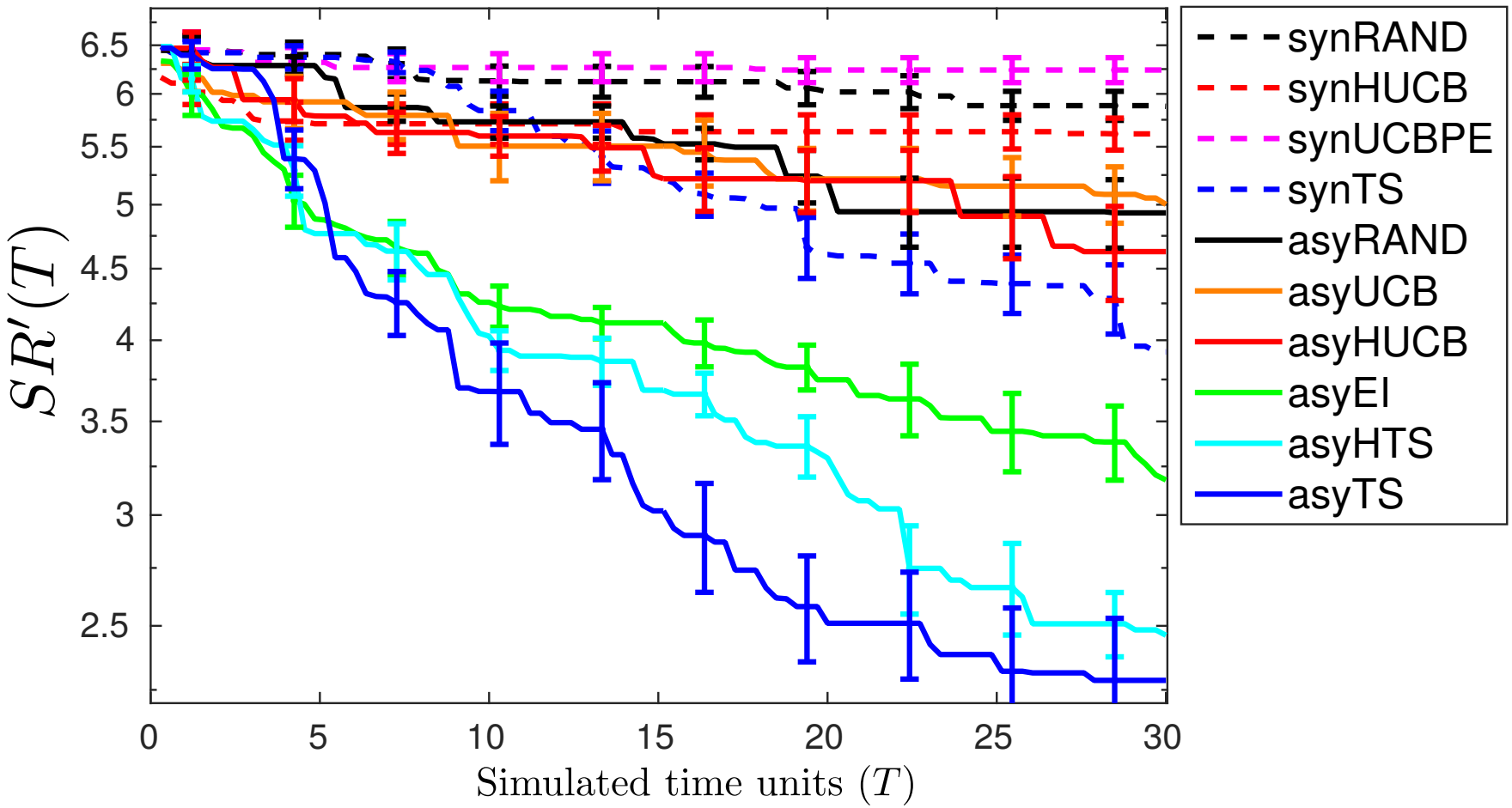


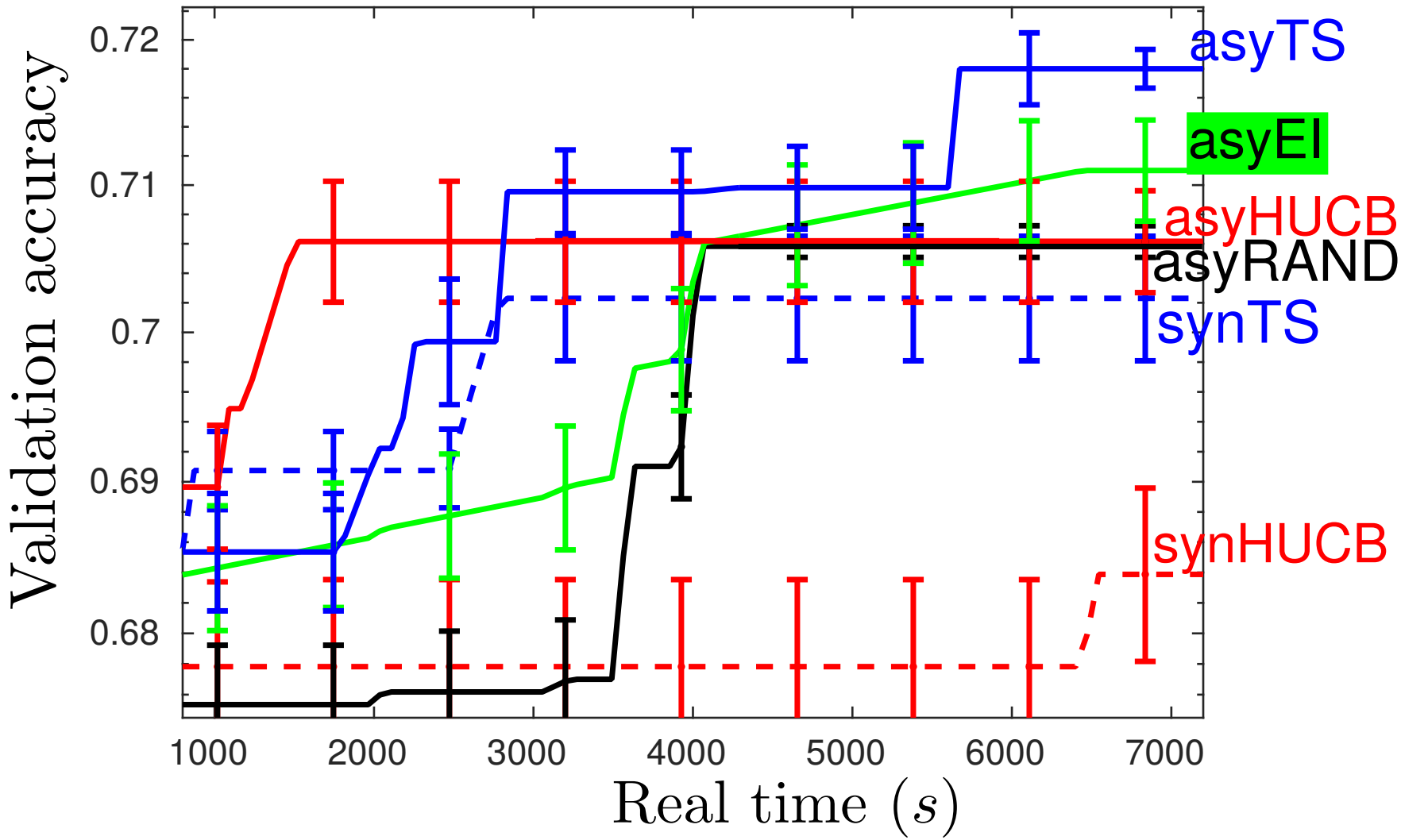
Experiment: Hartmann-18D $M = 25$

Evaluation time sampled from an exponential distribution



Experiment: Model Selection in Cifar10 $M = 4$

Tune # filters in in range $(32, 256)$ for each layer in a 6 layer CNN.
Time taken for an evaluation: 4 - 16 minutes.



Parallelised Thompson Sampling in Neural Networks

(Hernandez-Lobato et al. 2017)

Algorithm 2 Parallel and distributed Thompson sampling

Input: initial data $\mathcal{D}_{\mathcal{I}(1)} = \{\mathbf{x}_i, y_i\}_{i \in \mathcal{I}(1)}$, batch size S

for $t = 1$ **to** T **do**

  Compute current posterior $p(\boldsymbol{\theta}|\mathcal{D}_{\mathcal{I}(t)})$

  for $s = 1$ **to** S **do**

    Sample $\boldsymbol{\theta}$ from $p(\boldsymbol{\theta}|\mathcal{D}_{\mathcal{I}(t)})$

    Select $k(s) \leftarrow \text{argmax}_{j \notin \mathcal{I}(t)} \mathbf{E}[y_j|\mathbf{x}_j, \boldsymbol{\theta}]$

    Collect $y_{k(s)}$ by evaluating f at $\mathbf{x}_{k(s)}$

  Executed in parallel in node s

  end for

  $\mathcal{D}_{\mathcal{I}(t+1)} = \mathcal{D}_{\mathcal{I}(t)} \cup \{\mathbf{x}_{k(s)}, y_{k(s)}\}_{s=1}^{S}$

end for

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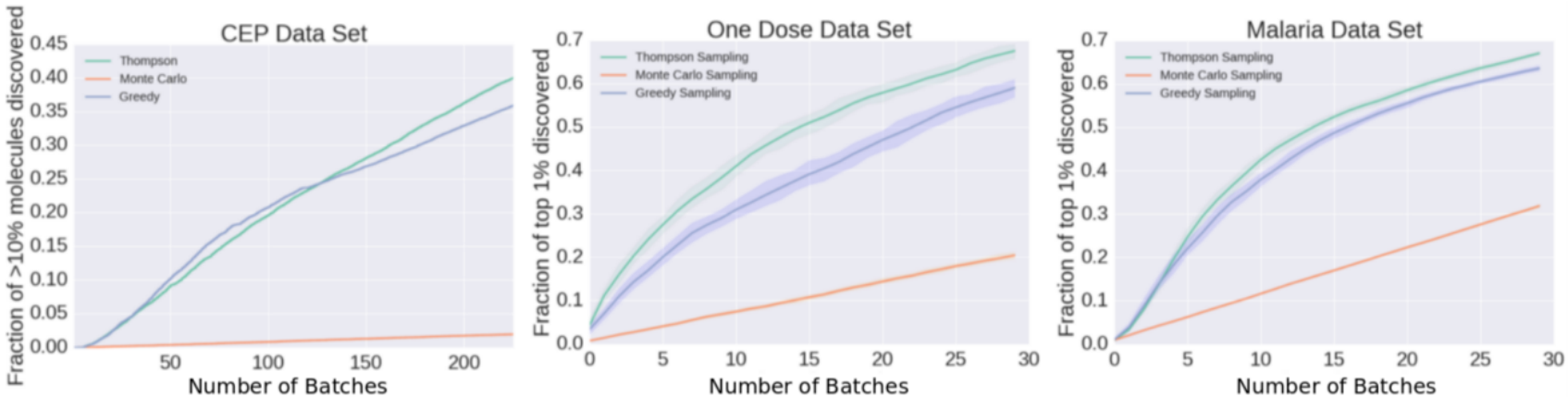

Outline

- Part I: Bandits in the Bayesian Paradigm
  1. Gaussian processes
  2. Algorithms: Upper Confidence Bound (UCB) & Thompson Sampling (TS)
- Part II: Scaling up Bandits
  1. Multi-fidelity bandit: cheap approximations to an expensive experiment
  2. Parallelising function evaluations
  3. High dimensional input spaces

Part 2.3: Optimisation in High Dimensional Input Spaces

E.g. Tuning a machine learning model with several hyper-parameters

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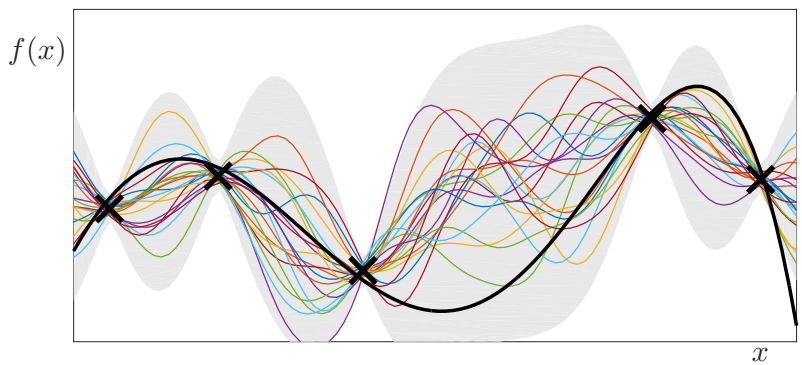
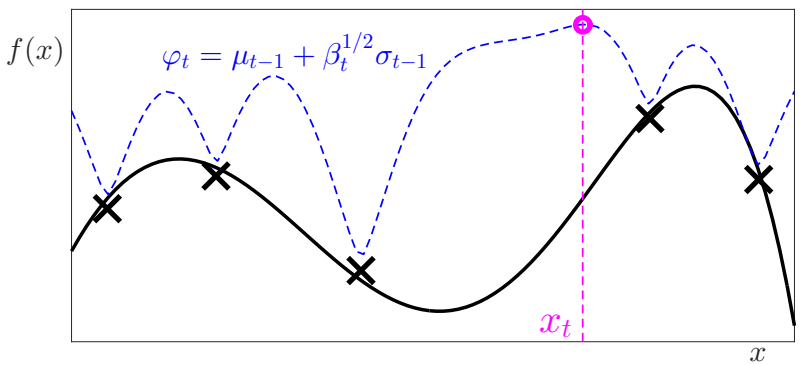
At each time step





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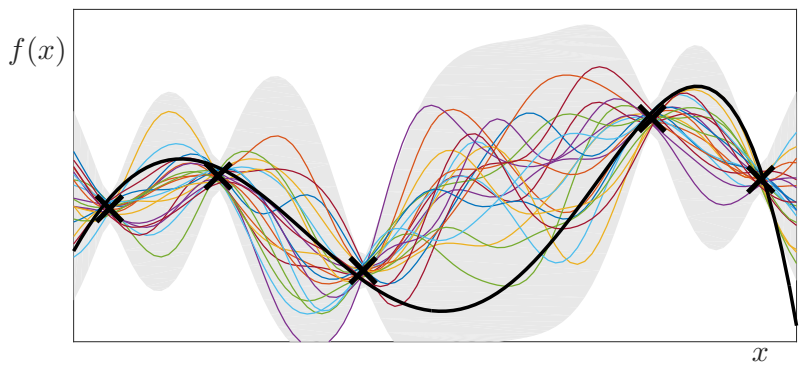

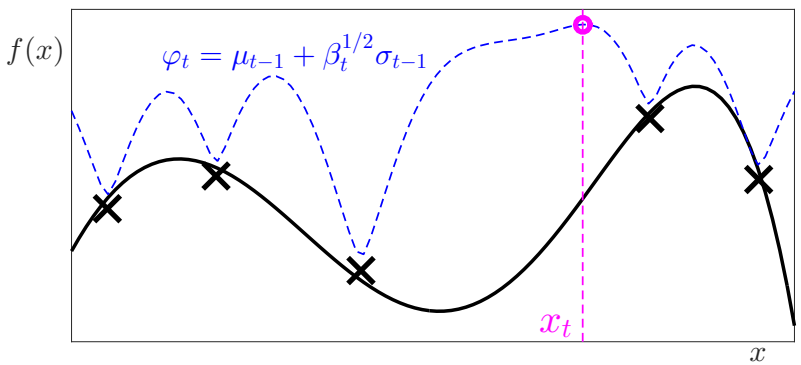

1. **Statistical Difficulty:** estimating a high dimensional GP.
2. **Computational Difficulty:** maximising a high dimensional acquisition (e.g. upper confidence bound) φ_t.

Additive Models for High Dimensional BO

(Kandasamy et al. ICML 2015)

E.g. $f(x_{\{1,\ldots,10\}}) = f^{(1)}(x_{\{1,3,9\}}) + f^{(2)}(x_{\{2,4,8\}}) + f^{(3)}(x_{\{5,6,10\}})$.

Additive Models for High Dimensional BO

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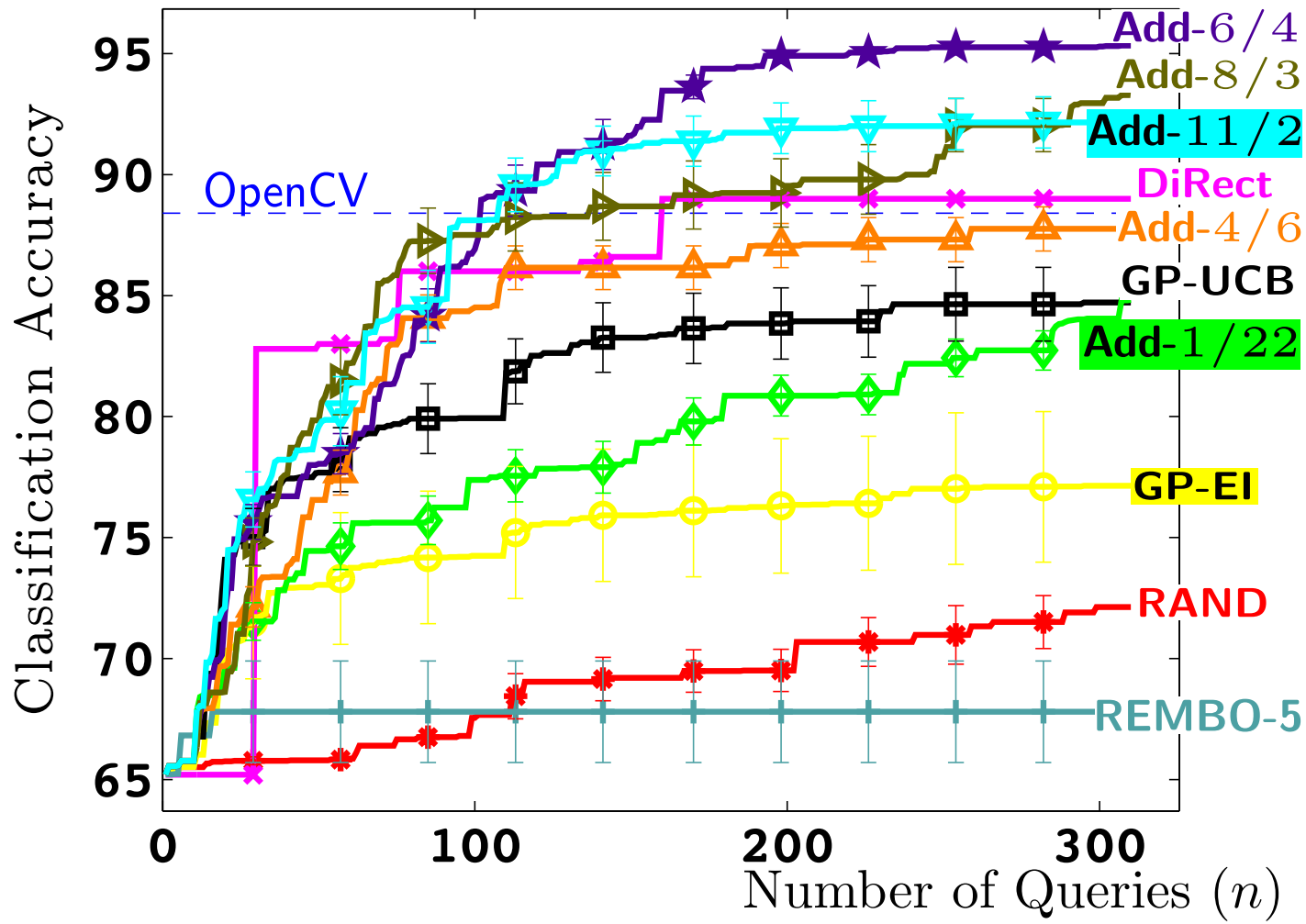
E.g. $f(x_{\{1,\ldots,10\}}) = f^{(1)}(x_{\{1,3,9\}}) + f^{(2)}(x_{\{2,4,8\}}) + f^{(3)}(x_{\{5,6,10\}})$.

- Better statistical properties: sample complexity improves from exponential in d to linear in d.
- **Add-GP-UCB** algorithm: computationally tractable even for large d.
- Better bias variance trade-off in practice: algorithm does well even if f is not additive.

Experiment: Viola & Jones Cascade classifier

Tune 22 hyper-parameters in the V&J classifier.



Summary

- Bandits are a framework for studying exploration vs exploitation trade-offs when optimising black-box functions.
- Several applications: Hyper-parameter Tuning, materials synthesis, scientific experiments etc.
- Several algorithms: UCB, TS, EI etc.

Summary

- Bandits are a framework for studying exploration vs exploitation trade-offs when optimising black-box functions.
- Several applications: Hyper-parameter Tuning, materials synthesis, scientific experiments etc.
- Several algorithms: UCB, TS, EI etc.

- **Multi-fidelity Bandits:** Use cheap approximations to a an expensive experiment to speed up optimisation.
- **Parallelised TS:** Simple and intuitive way to deal with multiple workers.
- **High dimensional optimisation:** Additive models have favourable statistical and computational properties.

Akshay

Barnabás

Gautam

Jeff

Junier

Thank You

Slides: `www.cs.cmu.edu/~kkandasa/talks/pitt-hptune-slides.pdf`