Multi-fidelity Bayesian Optimisation with Continuous Approximations

Kirthevasan Kandasamy

Gautam Dasarathy

Jeff Schneider

Barnabás Póczos

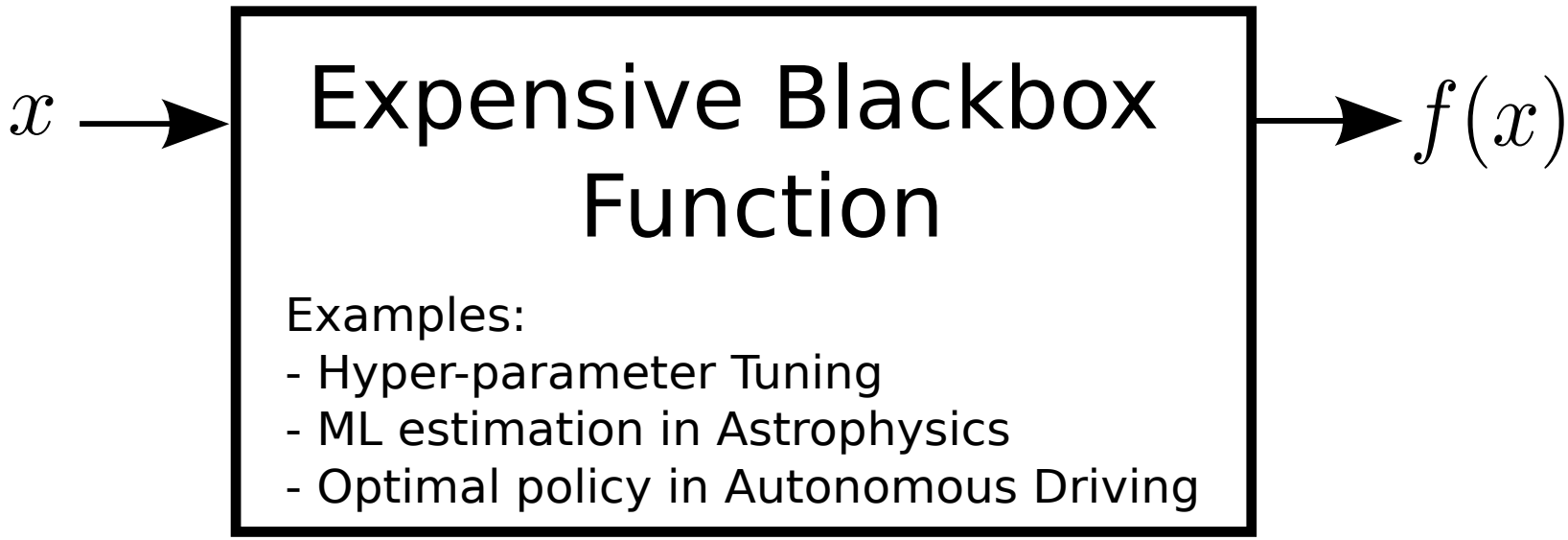
ICML '17

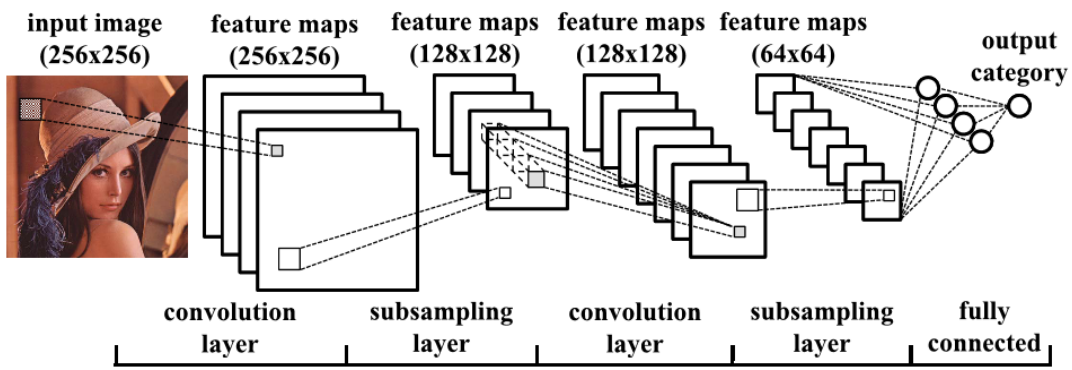
Carnegie Mellon University

RICE

Auton Lab

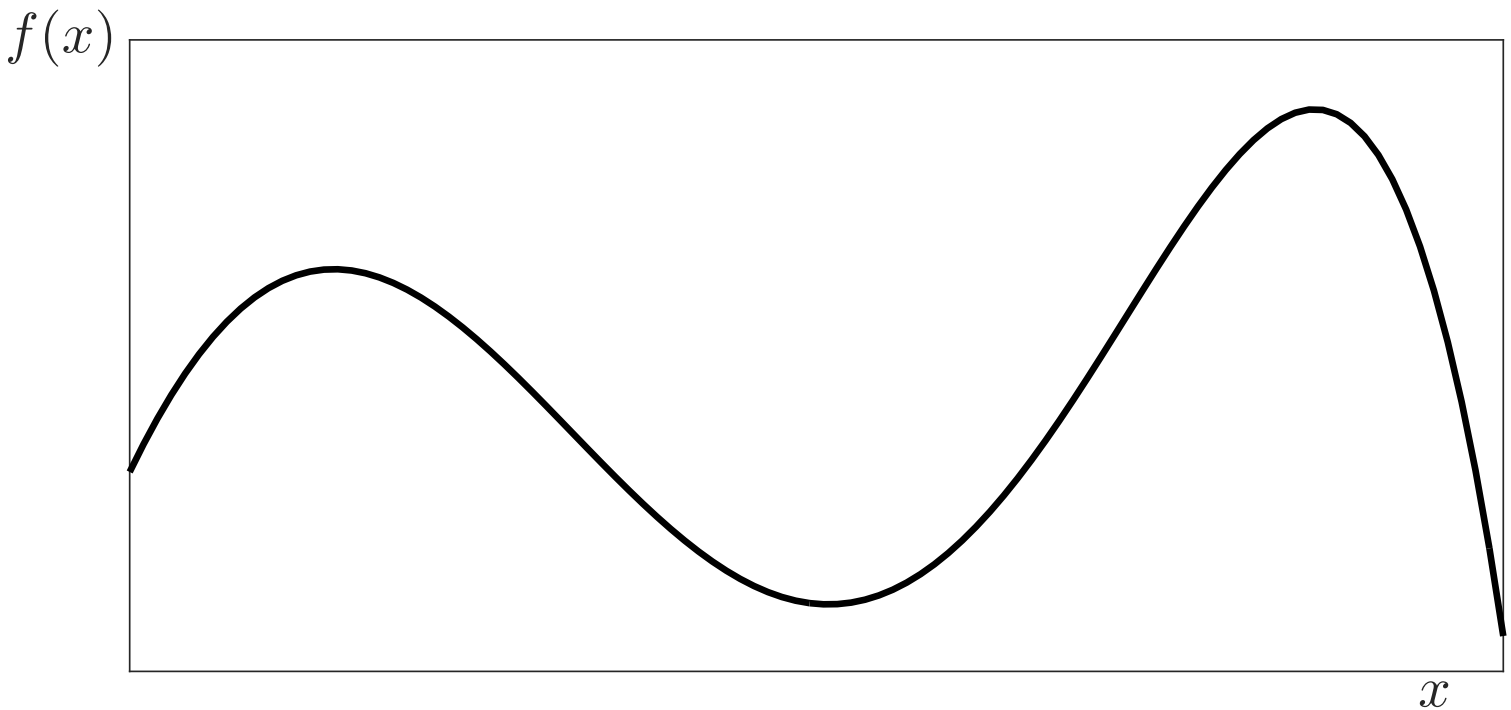
Black-box Optimisation





Black-box Optimisation

$f : \mathcal{X} \to \mathbb{R}$ is an expensive, black-box, noisy function.



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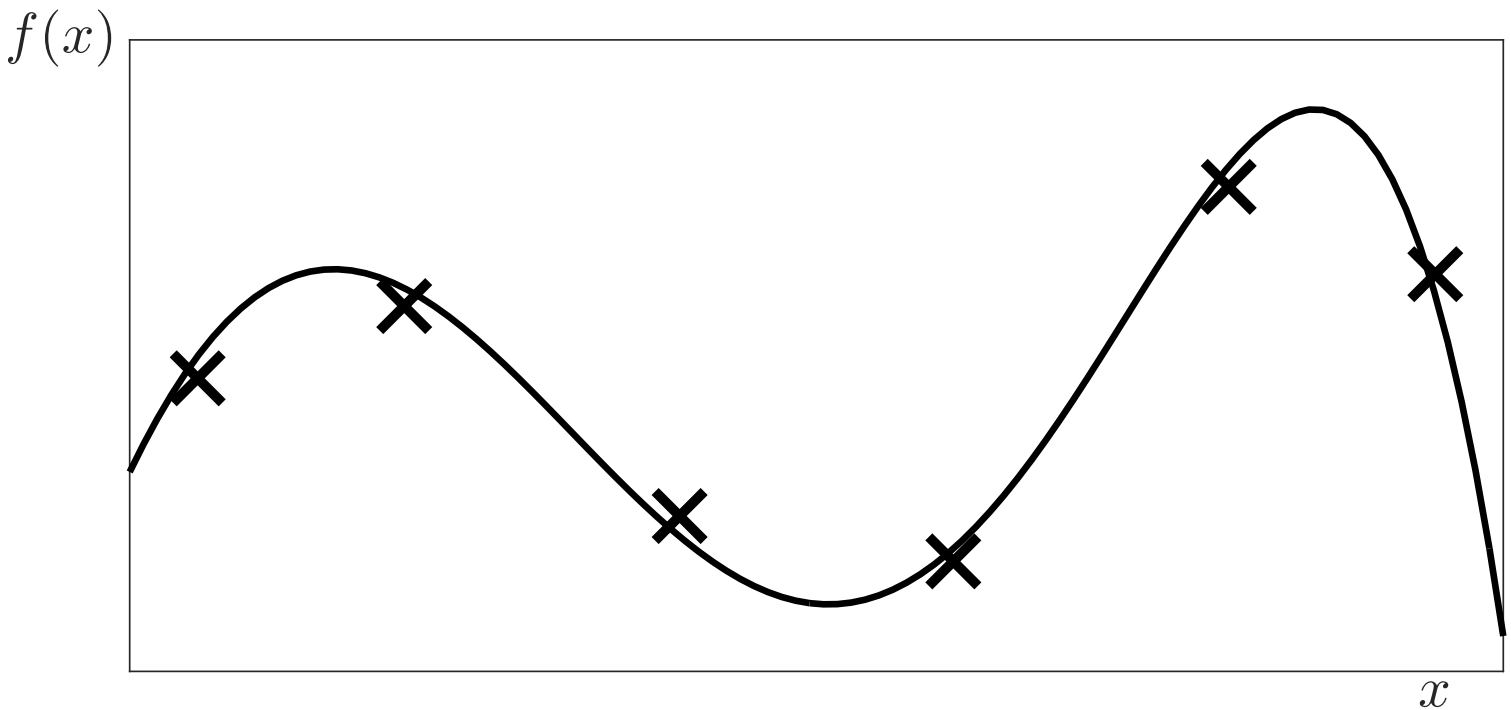

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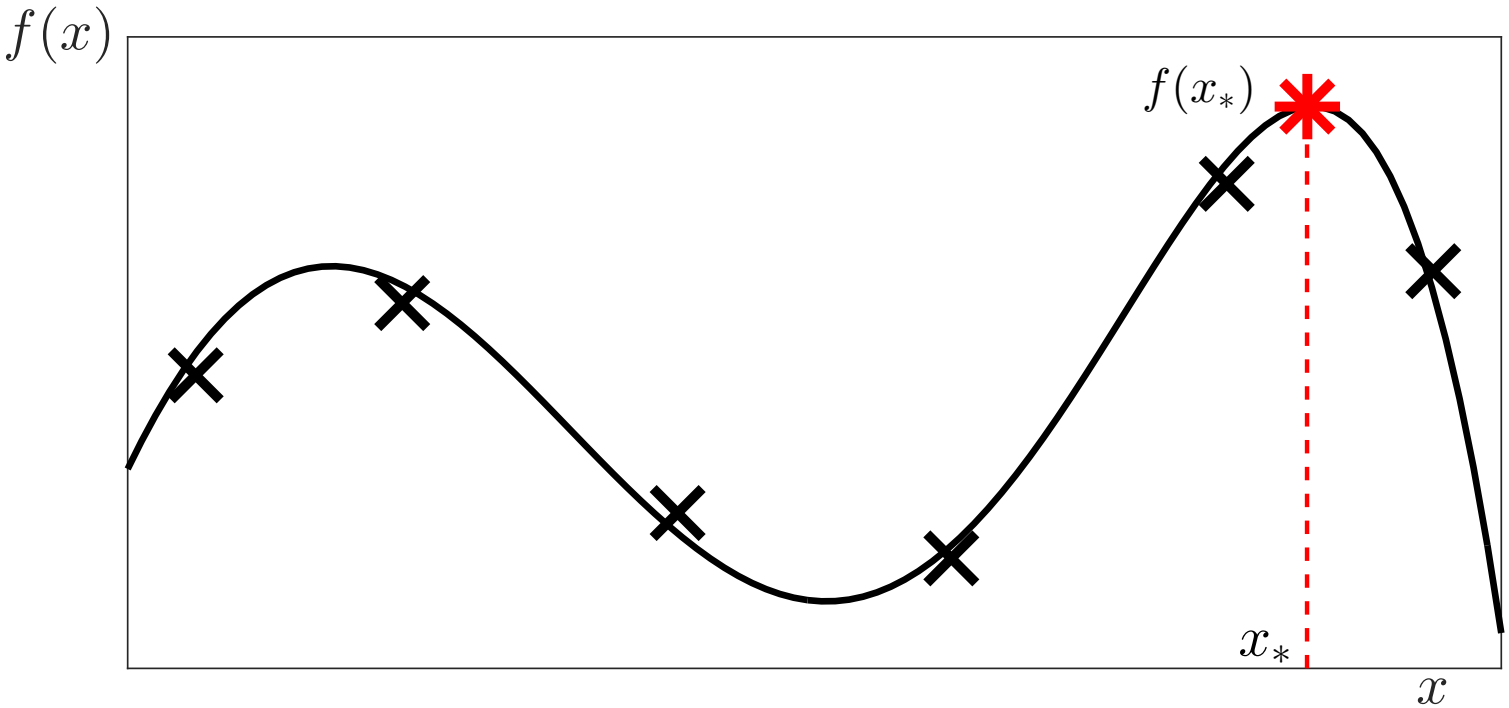

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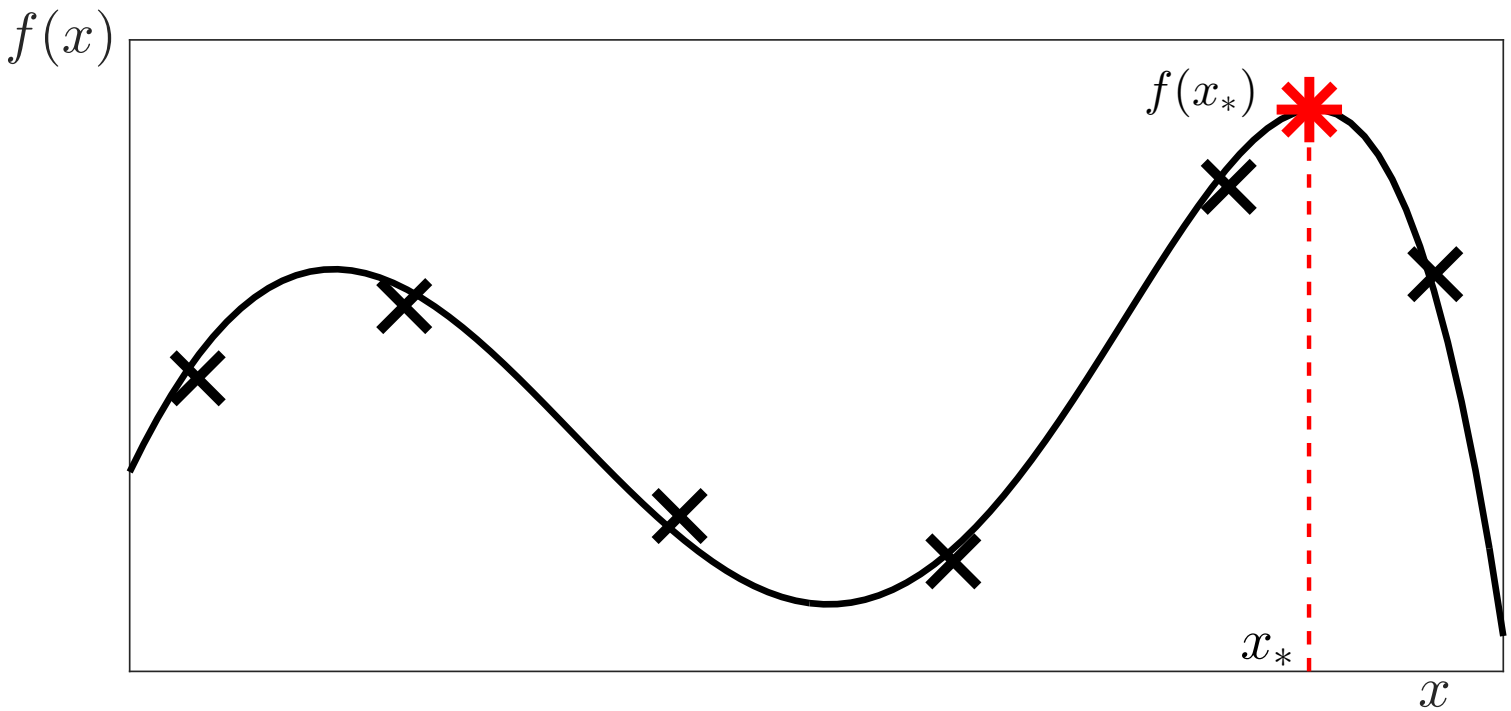


Simple Regret after n evaluations

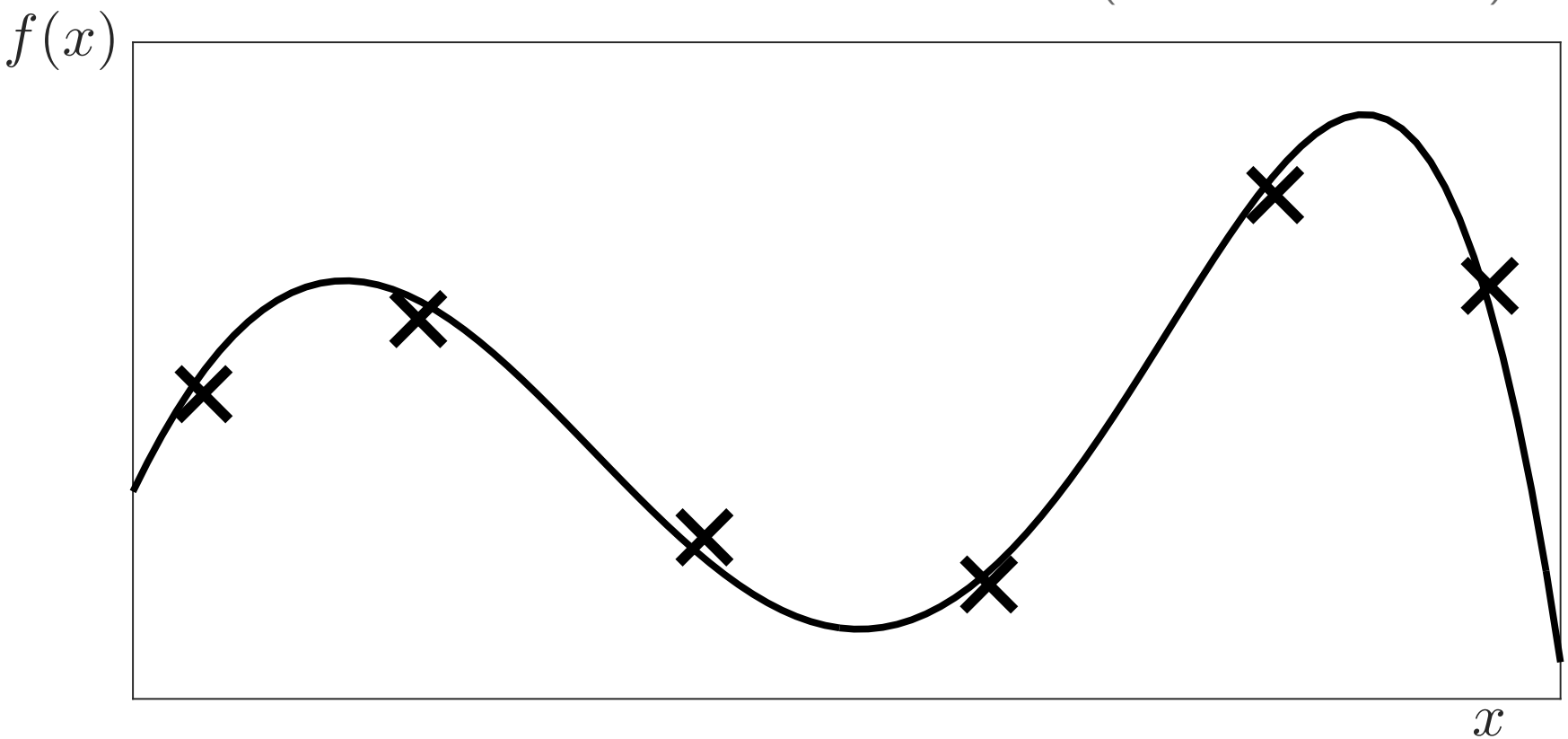
$$S_n = f(x_\star) - \max_{t=1,\ldots,n} f(x_t).$$

Gaussian Process (Bayesian) Optimisation

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

Gaussian Process Upper Confidence Bound (GP-UCB)

(Srinivas et al. 2010).



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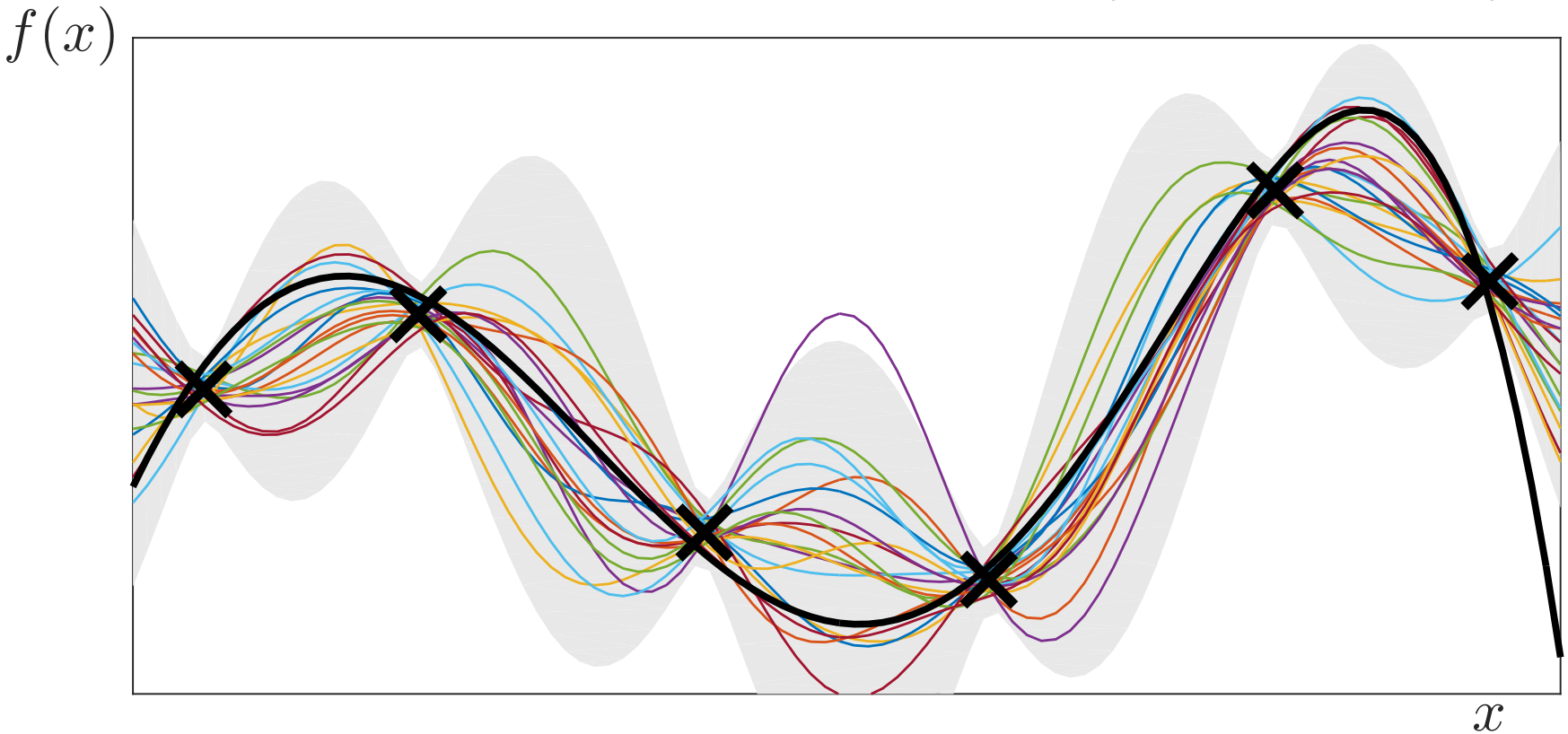

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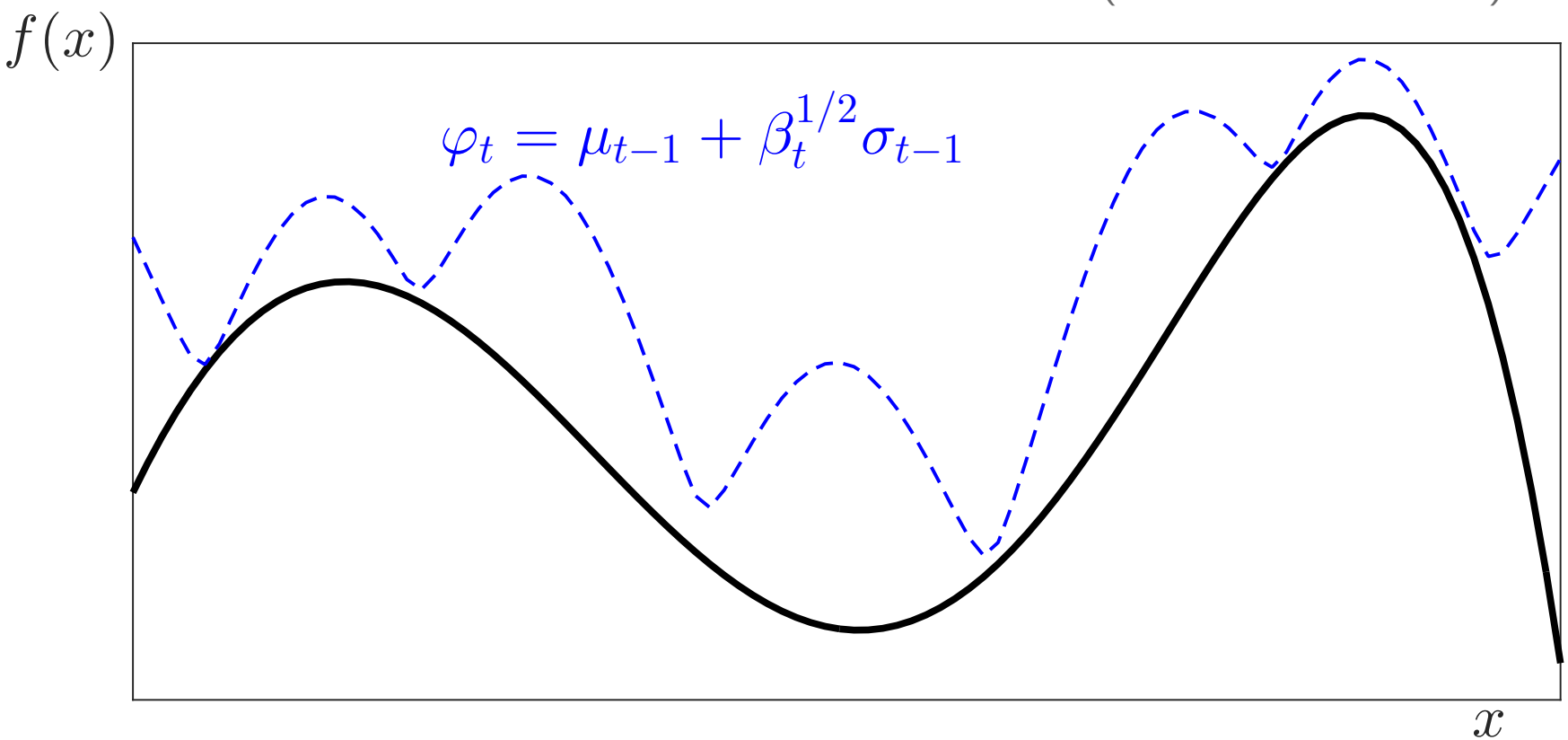

Construct upper conf. bound: $\varphi_t(x) = \mu_{t-1}(x) + \beta_t^{1/2}\sigma_{t-1}(x)$.

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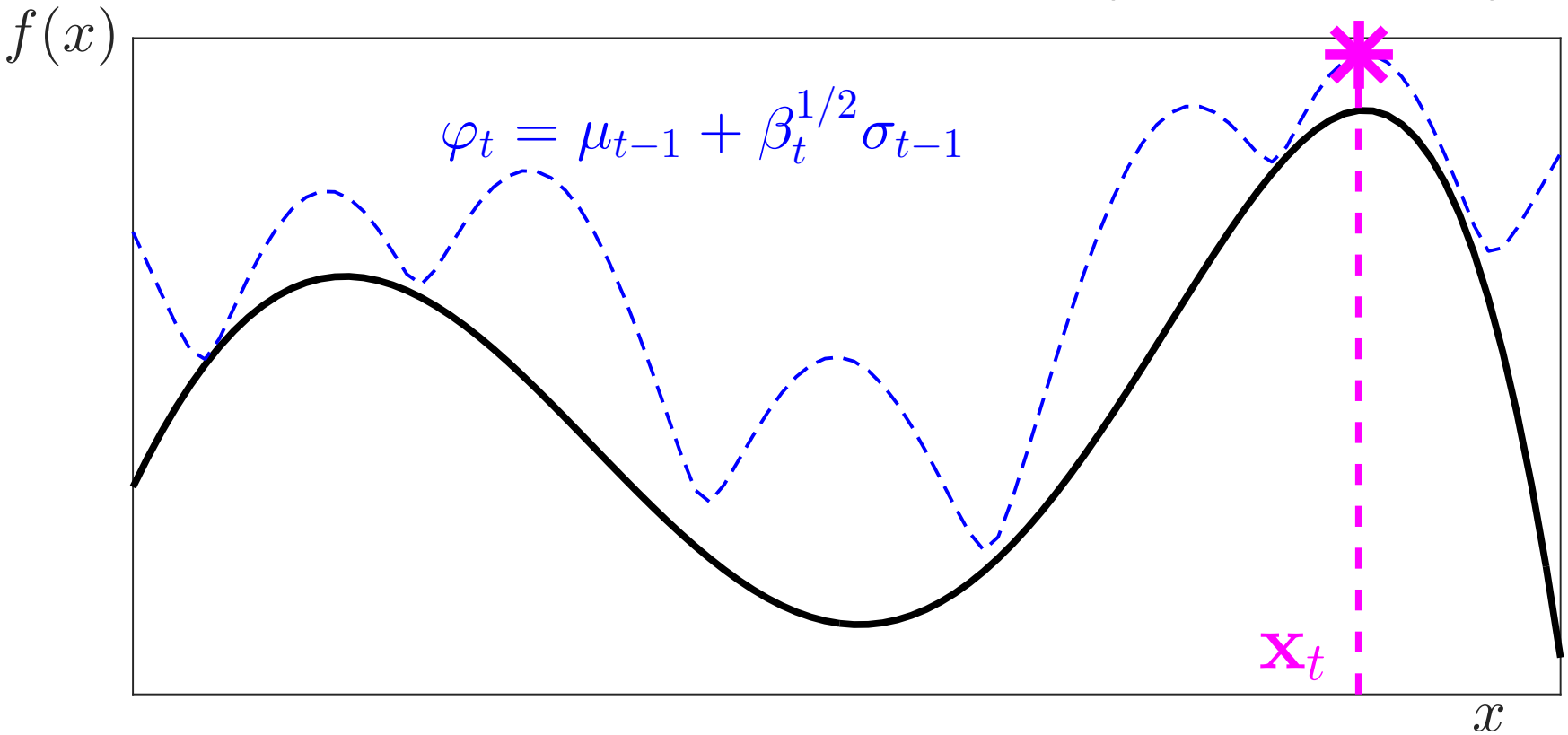

Maximise upper confidence bound.

This work: What if we have cheap approximations to f ?

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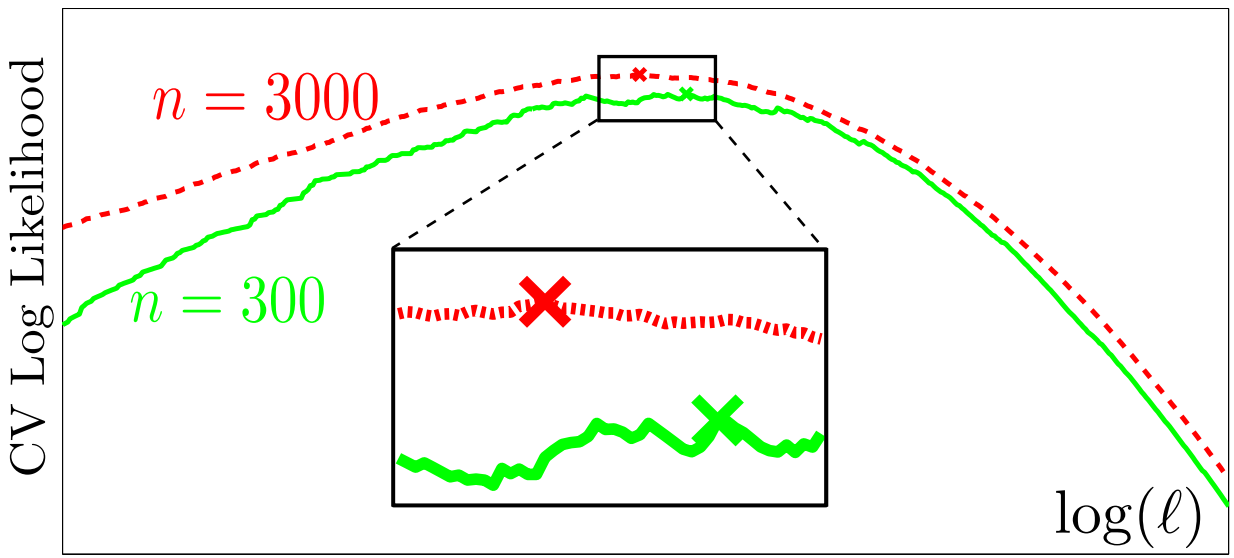
E.g. Hyper-parameter tuning: Train & validate with a subset of the data.

Bandwidth (ℓ) selection in kernel density estimation.



Prior work in **Multi-fidelity** Methods

For specific applications, such as hyper-parameter tuning, active learning, robotics etc. (Agarwal et al. 2011, Cutler et al. 2014, Zhang & Chaudhuri 2015, Klein et al. 2015, Li et al. 2016)

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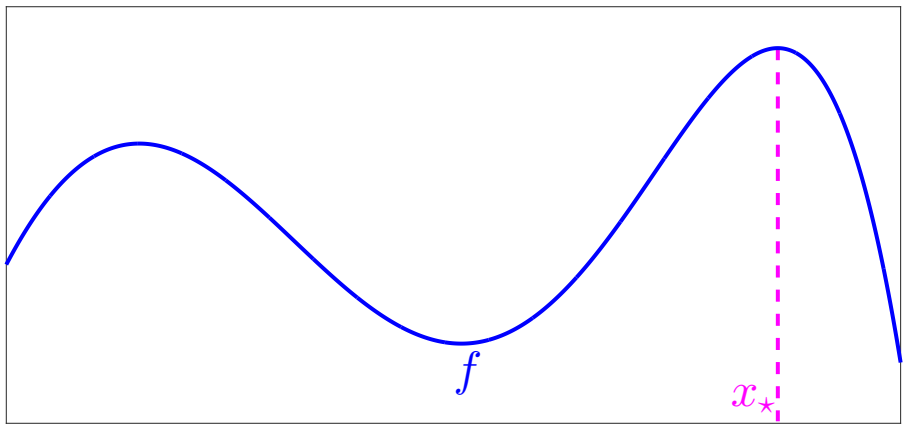

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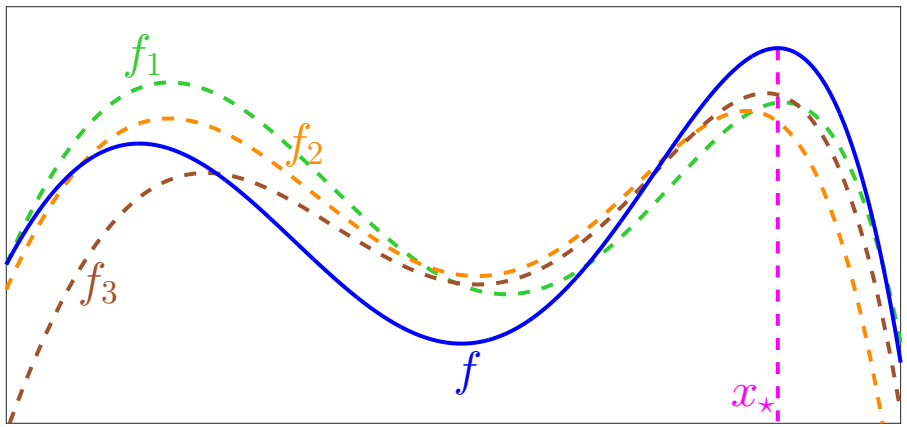
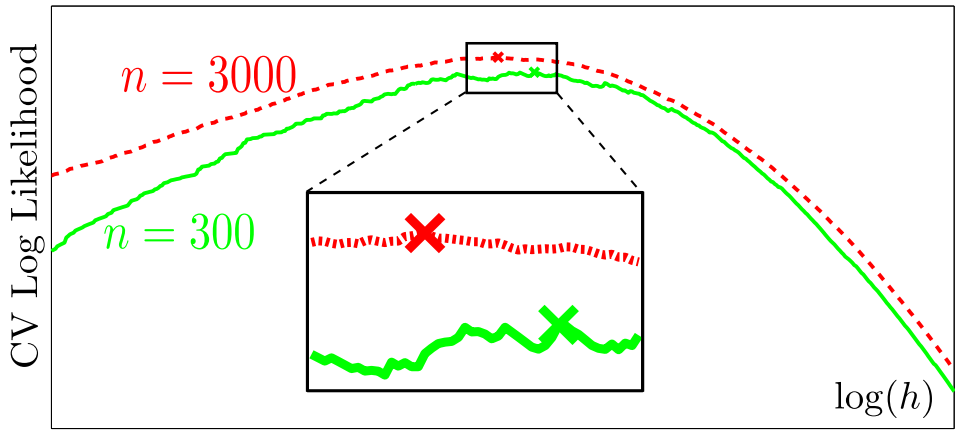


$f_1, f_2, f_3 \approx f$ which are cheaper to evaluate.

Why continuous approximations?



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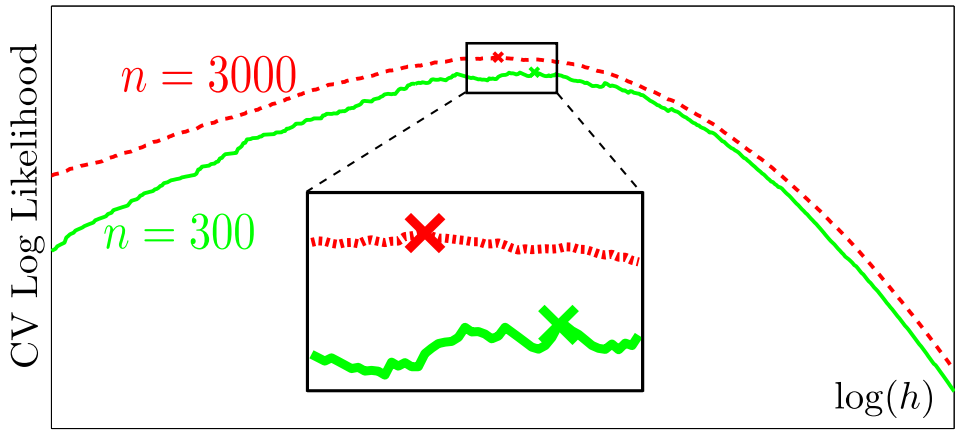

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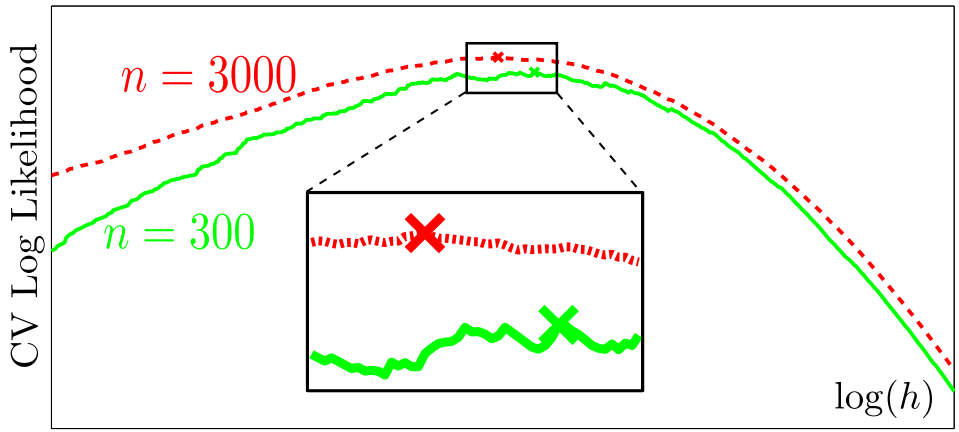

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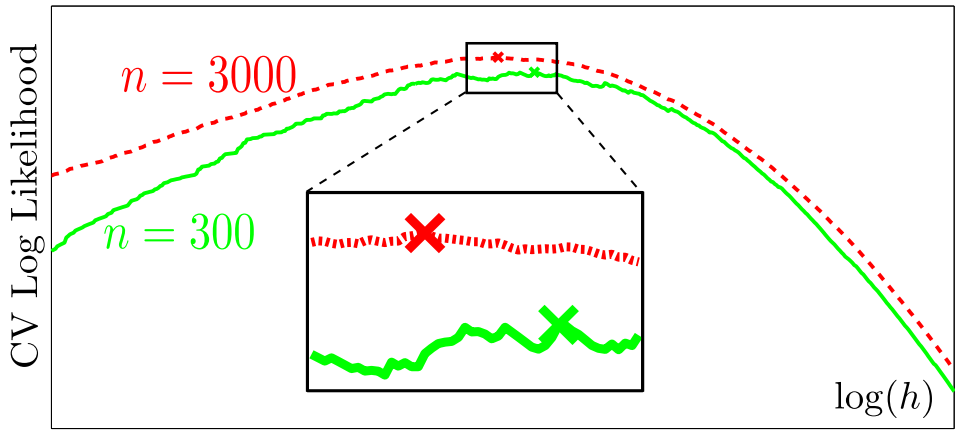

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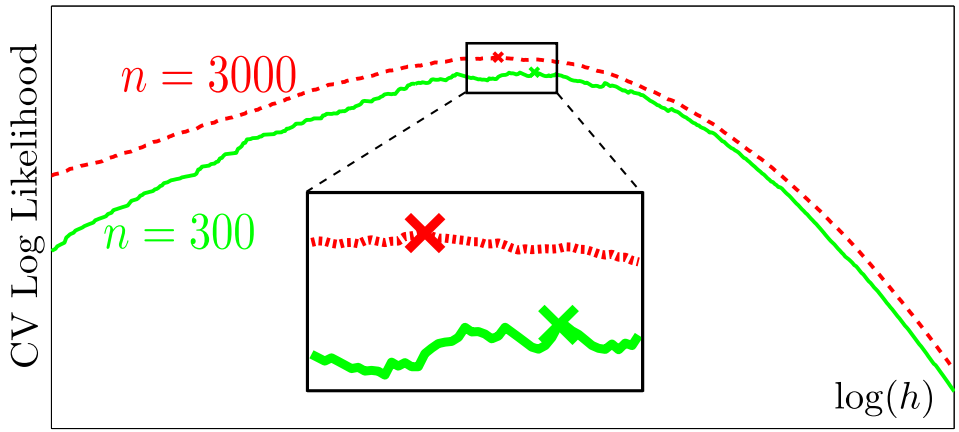

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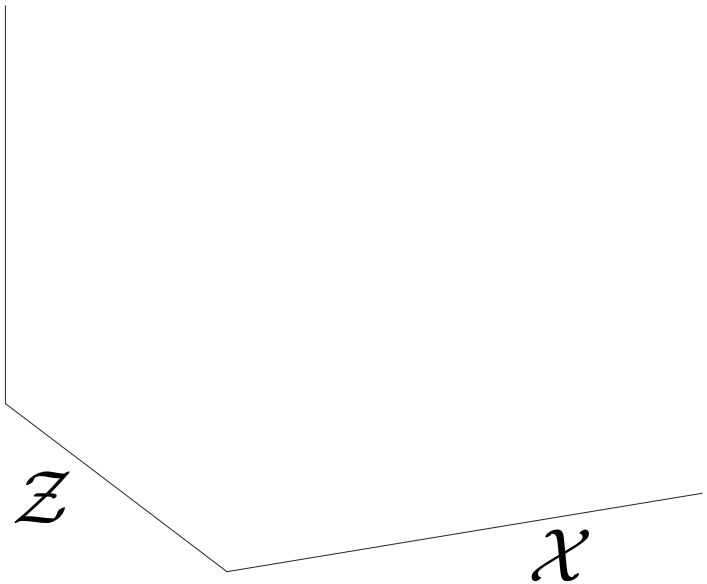
Approximations from a *continuous* 2D "fidelity space" (N, T).

Multi-fidelity Optimisation with Continuous Approximations

(Kandasamy et al. ICML 2017)



A fidelity space $\mathcal{Z}$ and domain $\mathcal{X}$

$\mathcal{Z} \leftarrow$ all (N, T) values.

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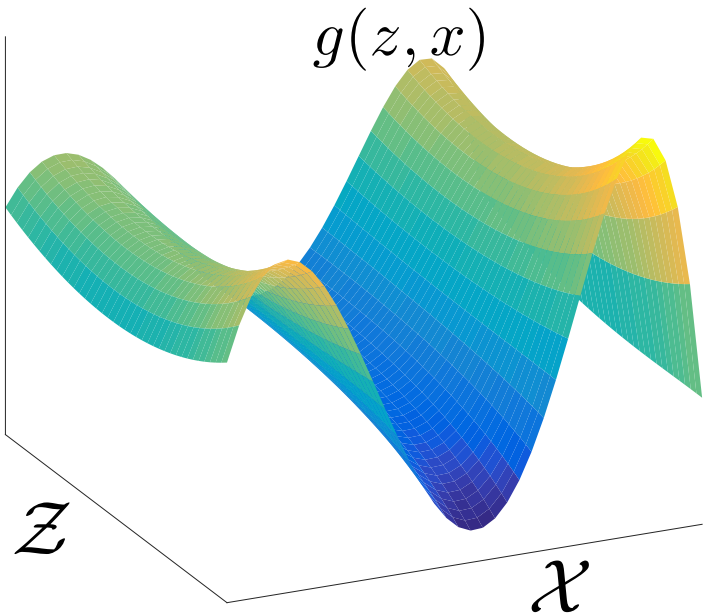

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$g([N, T], x) \leftarrow$ cv accuracy when training with N data for T iterations at hyper-parameter x.

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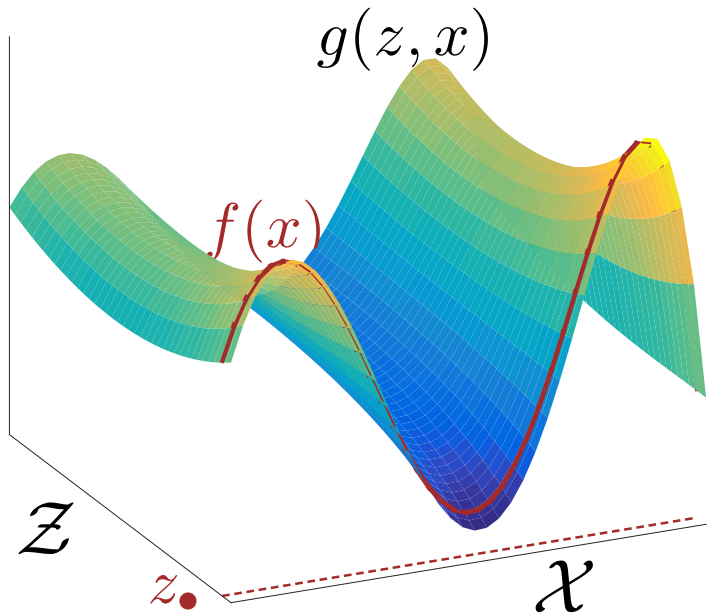

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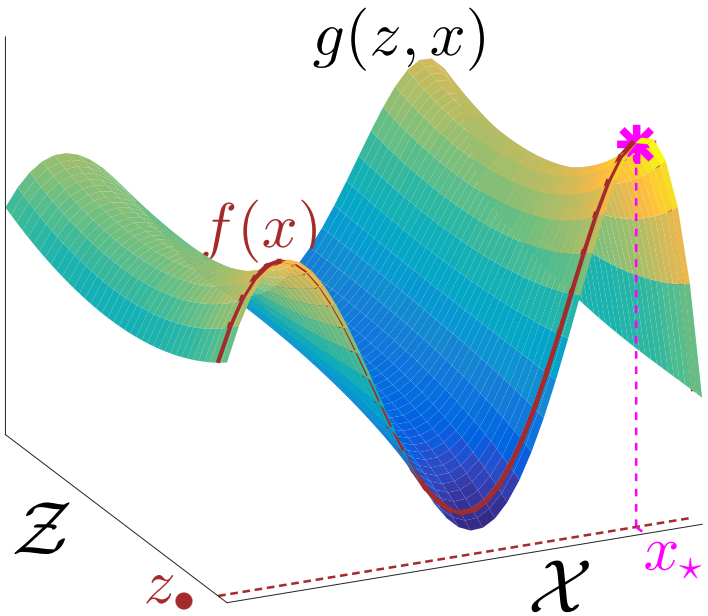

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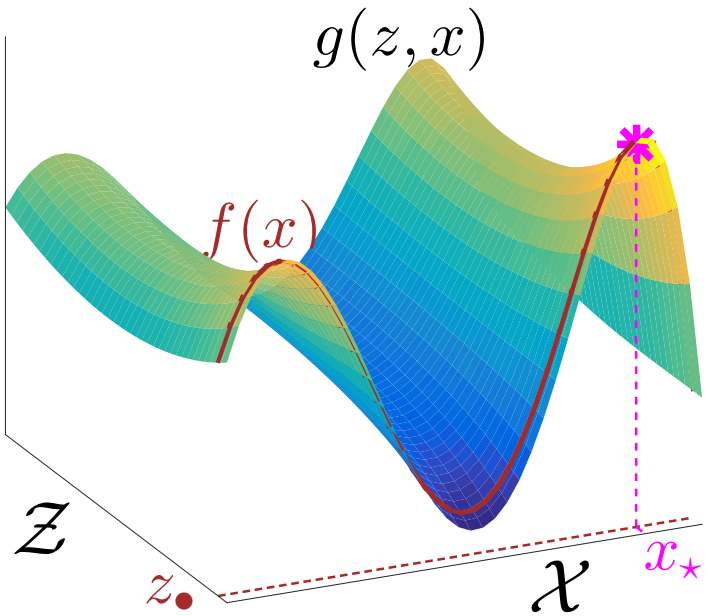

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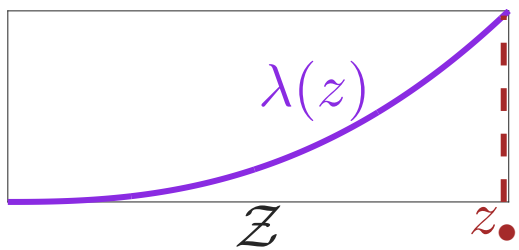
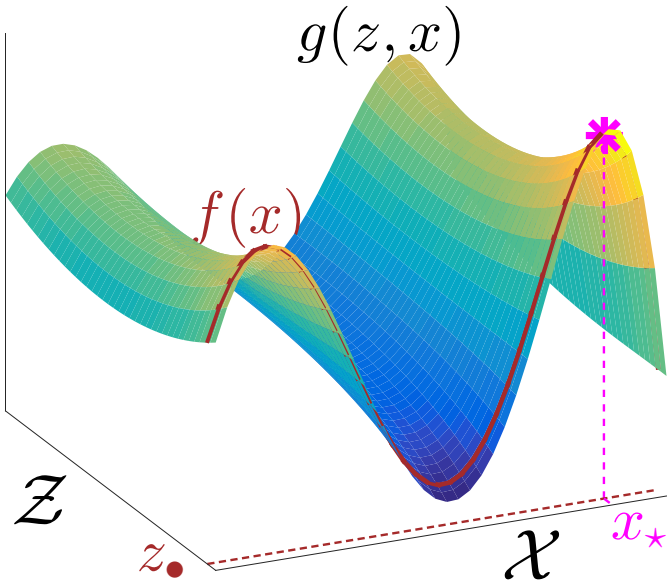
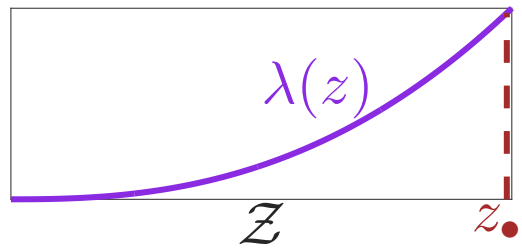
A cost function, $\lambda : \mathcal{Z} \rightarrow \mathbb{R}_+$.

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



Multi-fidelity Simple Regret (Kandasamy et al. ICML 2017)





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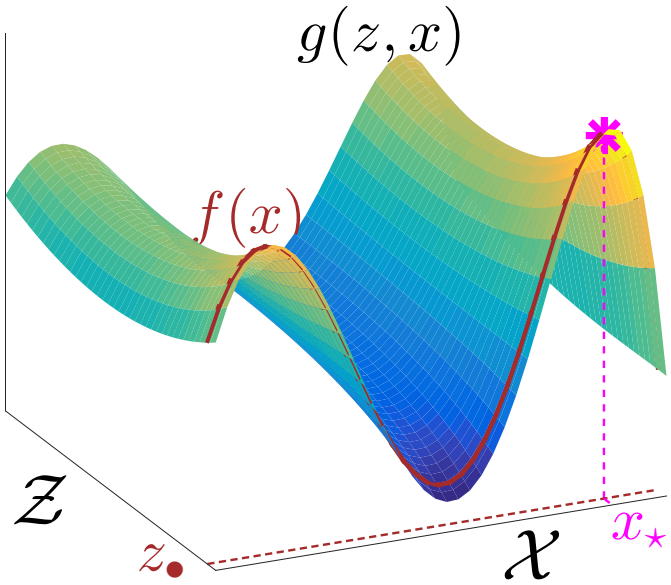

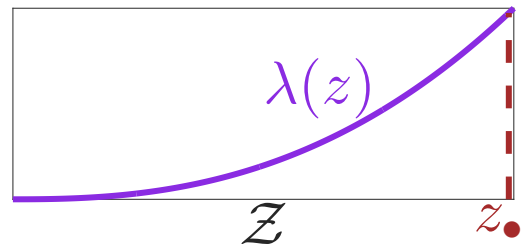

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Simple Regret after *capital* Λ: $S(\Lambda) = f(x_\star) - \max_{t:\, z_t = z_\bullet} f(x_t)$.

$\Lambda \leftarrow$ amount of a resource spent, e.g. computation time or money.

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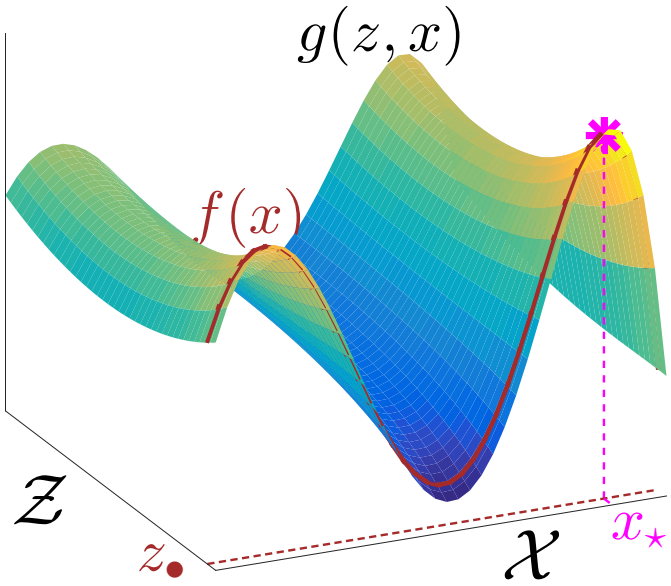

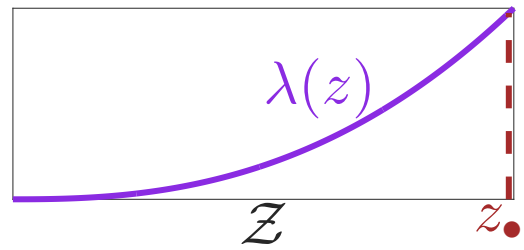

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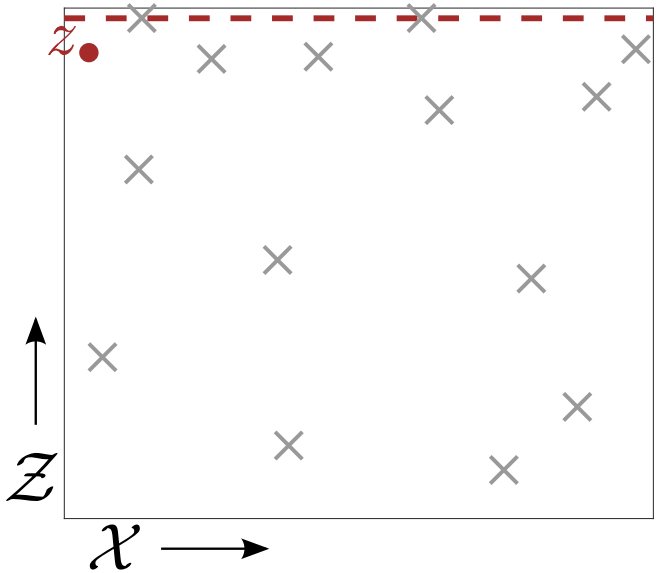
No reward for maximising low fidelities, but use cheap evaluations at $z \neq z_\bullet$ to speed up search for $x_\star$.

BOCA: Bayesian Optimisation with Continuous Approximations

(Kandasamy et al. ICML 2017)



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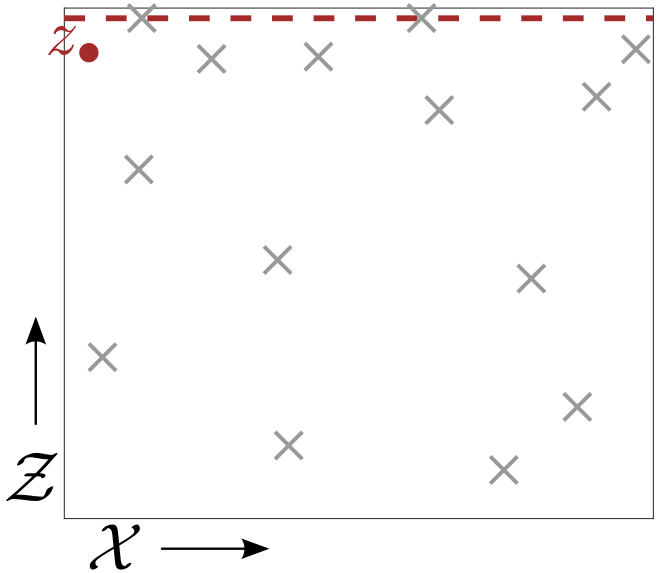

Model $g \sim \mathcal{GP}(0, \kappa)$ and compute posterior $\mathcal{GP}$:

mean $\quad \mu_{t-1} : \mathcal{Z} \times \mathcal{X} \to \mathbb{R}$

std-dev $\quad \sigma_{t-1} : \mathcal{Z} \times \mathcal{X} \to \mathbb{R}_+$

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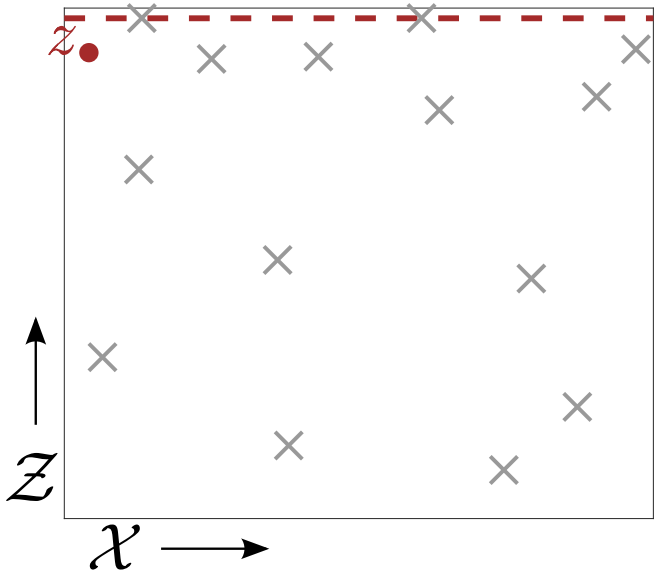

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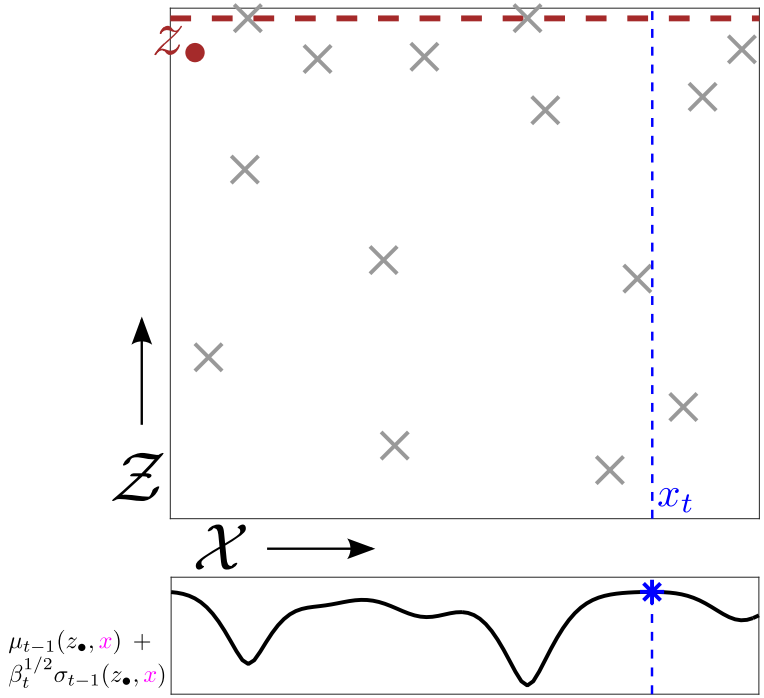

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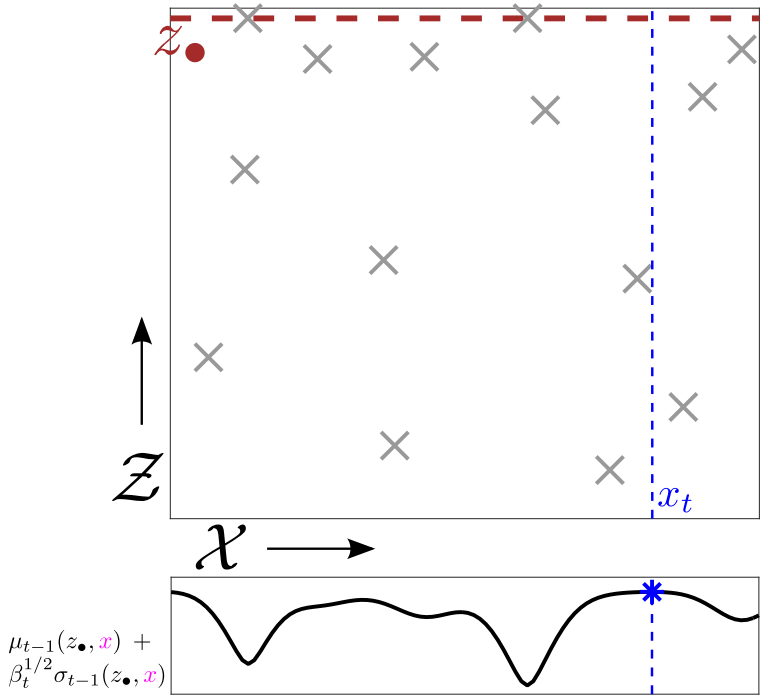

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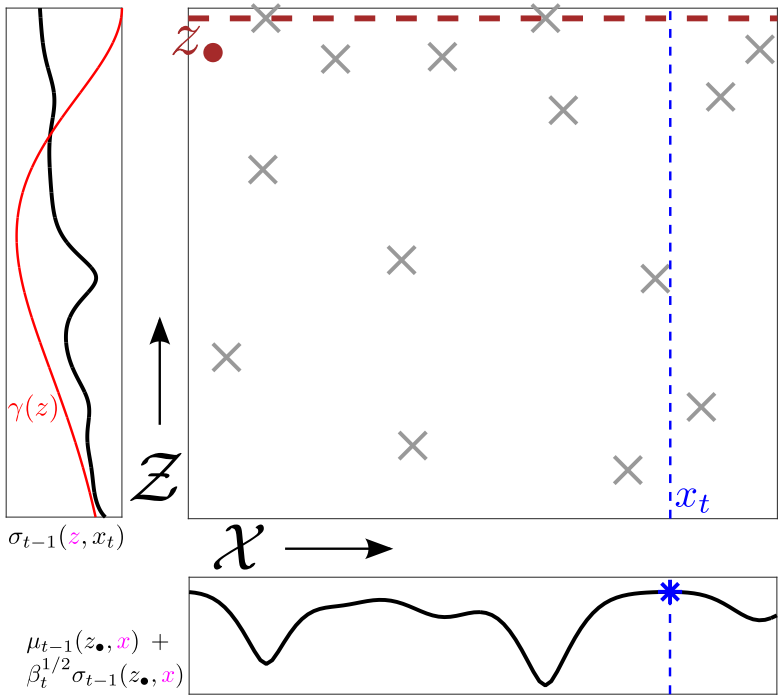
(2) $$\mathcal{Z}_t \approx \{z_\bullet\} \cup \left\{ z \ : \ \sigma_{t-1}(z, x_t) \geq \gamma(z) \right\}$$

(3) $$z_t = \underset{z \in \mathcal{Z}_t}{\operatorname{argmin}} \ \lambda(z) \qquad \text{(cheapest } z \text{ in } \mathcal{Z}_t\text{)}$$

BOCA: Bayesian Optimisation with Continuous Approximations

(Kandasamy et al. ICML 2017)



Model $g \sim \mathcal{GP}(0, \kappa)$ and compute posterior $\mathcal{GP}$:

mean $\quad \mu_{t-1} : \mathcal{Z} \times \mathcal{X} \to \mathbb{R}$

std-dev $\quad \sigma_{t-1} : \mathcal{Z} \times \mathcal{X} \to \mathbb{R}_+$

(1) $x_t \leftarrow$ maximise upper confidence bound for $f(x) = g(z_\bullet, x)$.

$$x_t = \underset{x \in \mathcal{X}}{\operatorname{argmax}} \ \mu_{t-1}(z_\bullet, x) + \beta_t^{1/2}\sigma_{t-1}(z_\bullet, x)$$

(2) $$\mathcal{Z}_t \approx \{z_\bullet\} \cup \left\{ z \ : \ \sigma_{t-1}(z, x_t) \geq \gamma(z) \right\}$$

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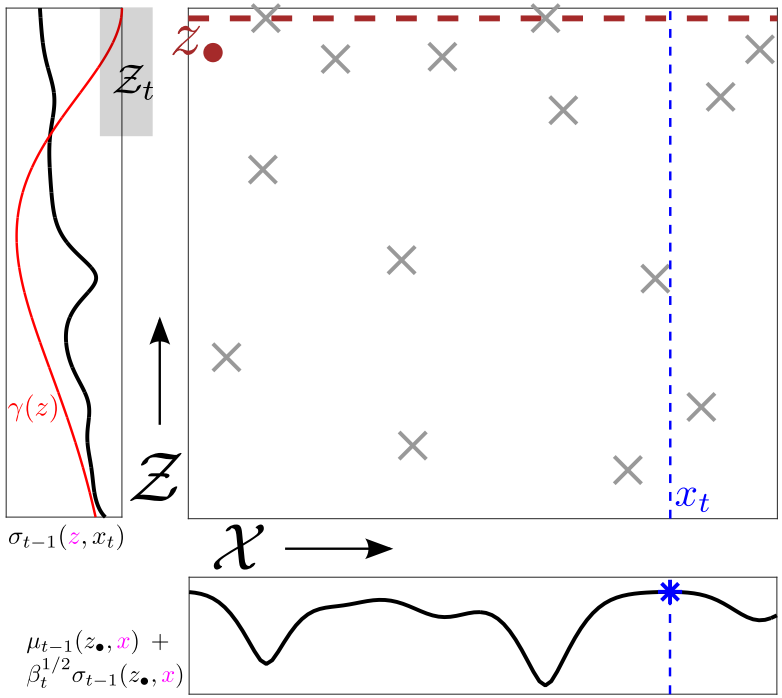

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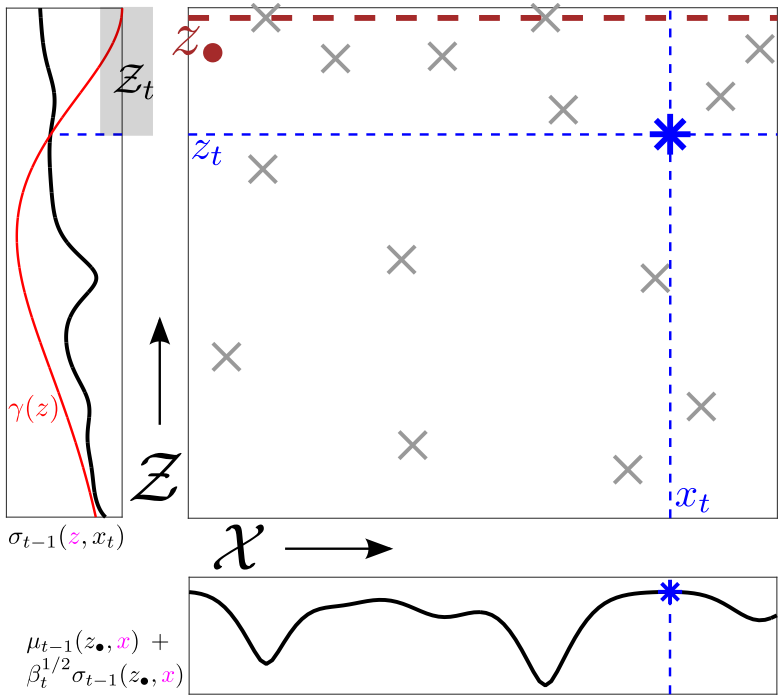

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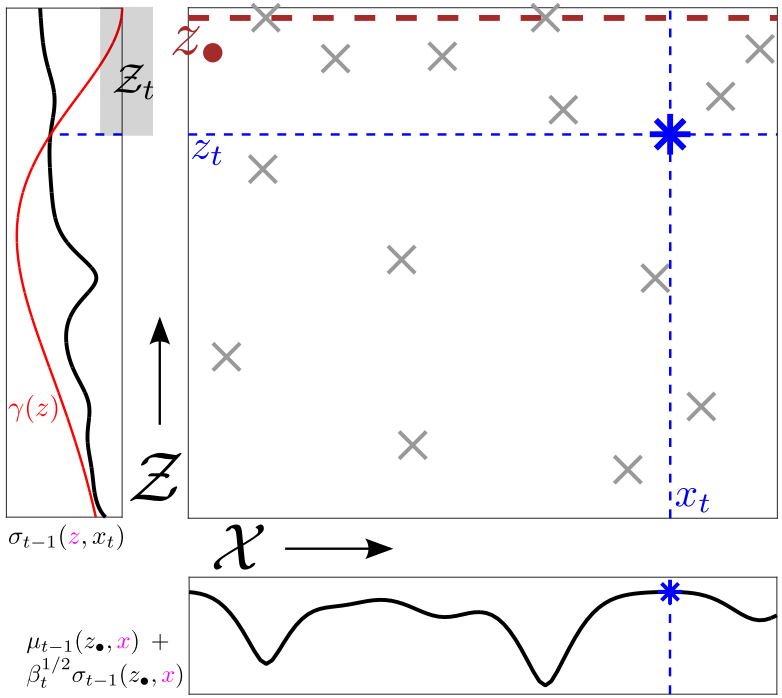

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Theoretical Results for BOCA

$$g \sim \mathcal{GP}(\mathbf{0}, \kappa), \quad \kappa : (\mathcal{Z} \times \mathcal{X})^2 \to \mathbb{R}.$$

$$\kappa([z, x], [z', x']) = \kappa_{\mathcal{X}}(x, x') \cdot \kappa_{\mathcal{Z}}(z, z')$$

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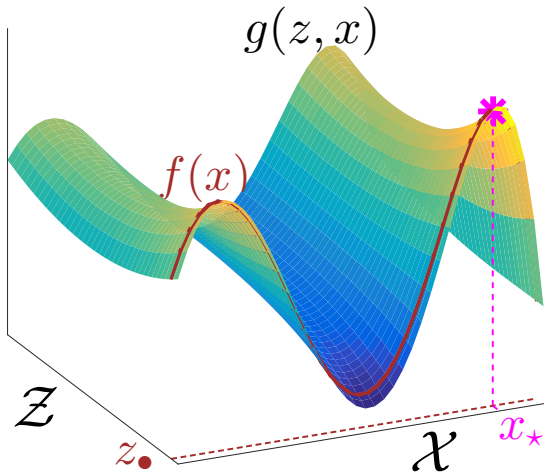

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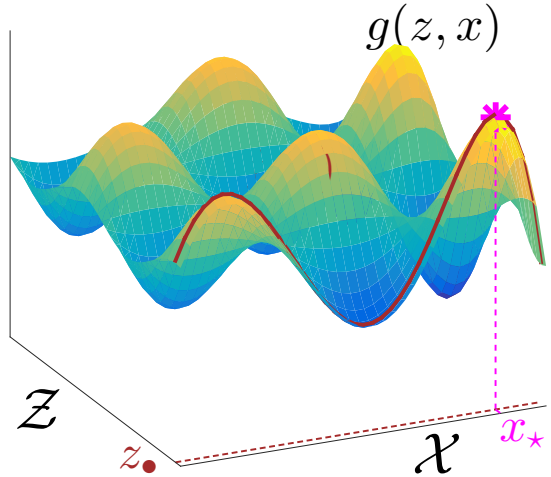

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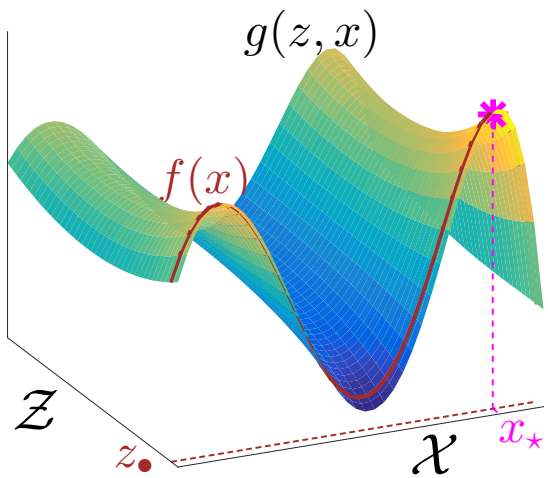

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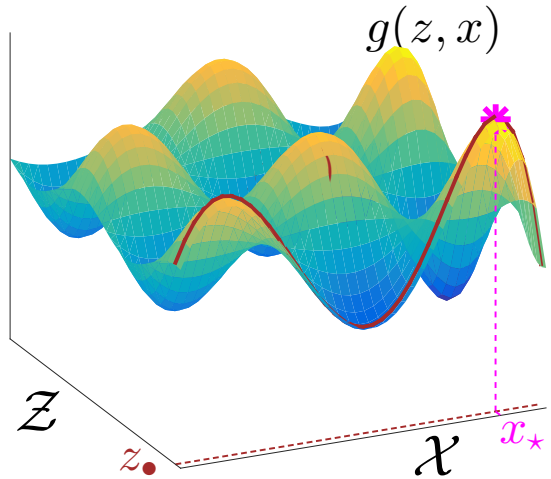

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E.g.: If $\kappa_{\mathcal{Z}}$ is an SE kernel, bandwidth $h_{\mathcal{Z}}$ controls smoothness.

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GP-UCB $\kappa_{\mathcal{X}}$ is an SE kernel, (Srinivas et al. 2010)

$$\text{w.h.p} \qquad S(\Lambda) \lesssim \sqrt{\frac{\mathrm{vol}(\mathcal{X})}{\Lambda}}$$

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$$\text{w.h.p} \quad \forall \alpha > 0, \quad S(\Lambda) \lesssim \sqrt{\frac{\mathrm{vol}(\mathcal{X}_\alpha)}{\Lambda}} + \sqrt{\frac{\mathrm{vol}(\mathcal{X})}{\Lambda^{2-\alpha}}}$$

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If $h_{\mathcal{Z}}$ is large (good approximations), $\text{vol}(\mathcal{X}_\alpha) \ll \text{vol}(\mathcal{X})$, and BOCA is much better than GP-UCB.

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).

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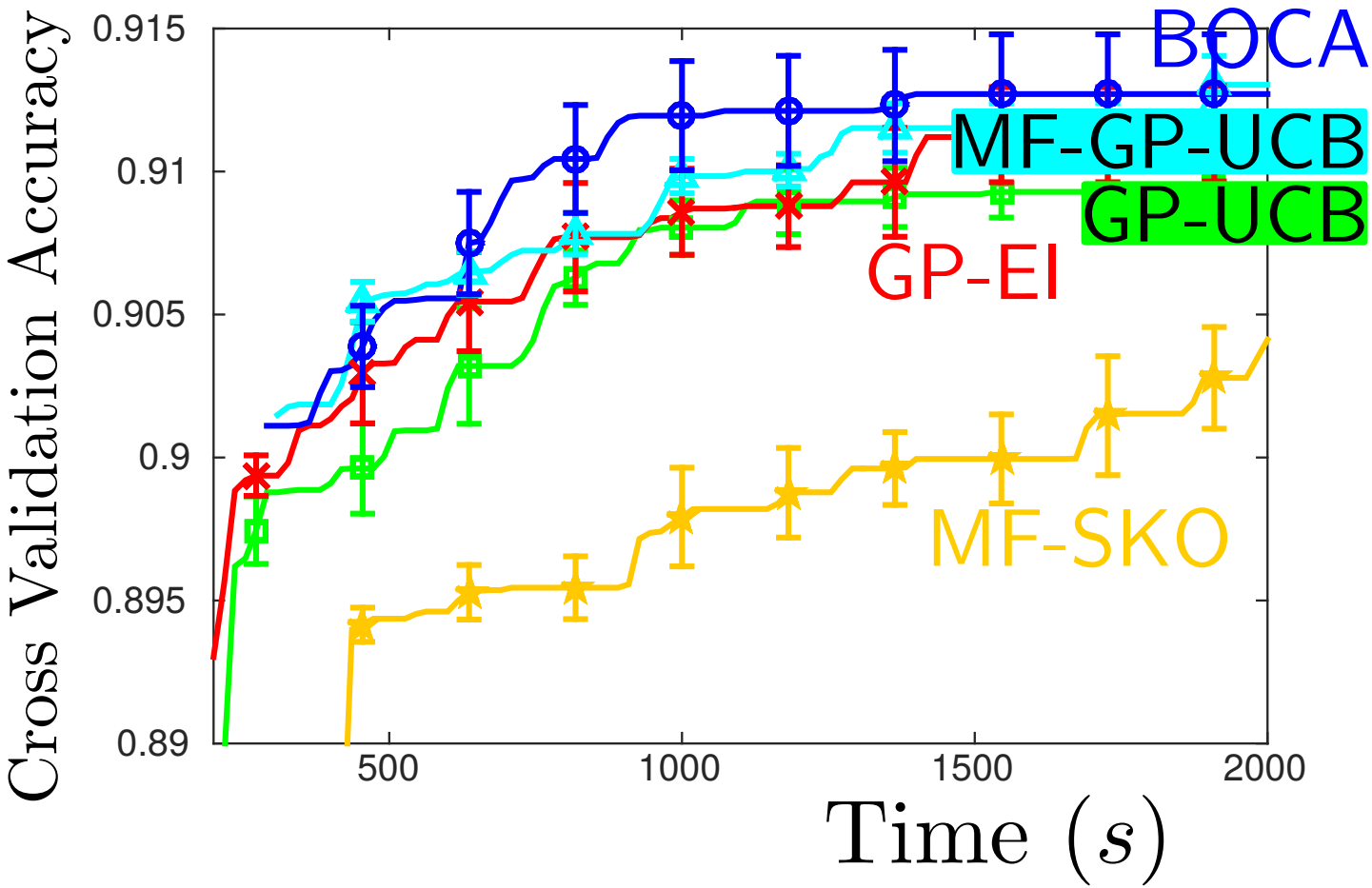

Take-aways

- BOCA: a multi-fidelity optimisation algorithm when you have access to continuous approximations.
- Choose higher fidelity only after controlling uncertainty/variance at lower fidelities.
- Theoretically/empirically outperforms strategies that ignore the approximations or use only a finite number of fidelities.

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Thank you.

Poster tonight @ Gallery #49.