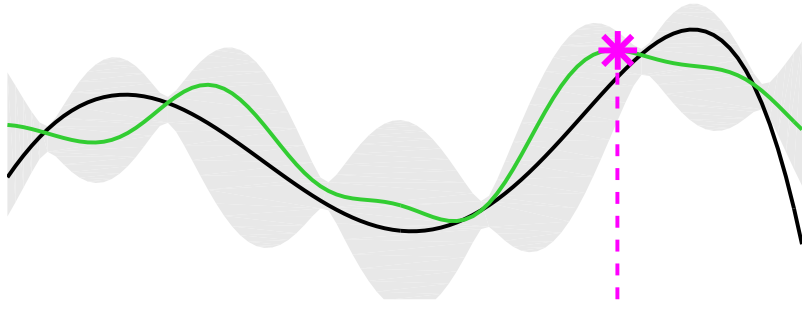
Bayesian Design of Experiments via Posterior Sampling

Applications in Hyper-parameter tuning, Astrophysics, and Materials Science



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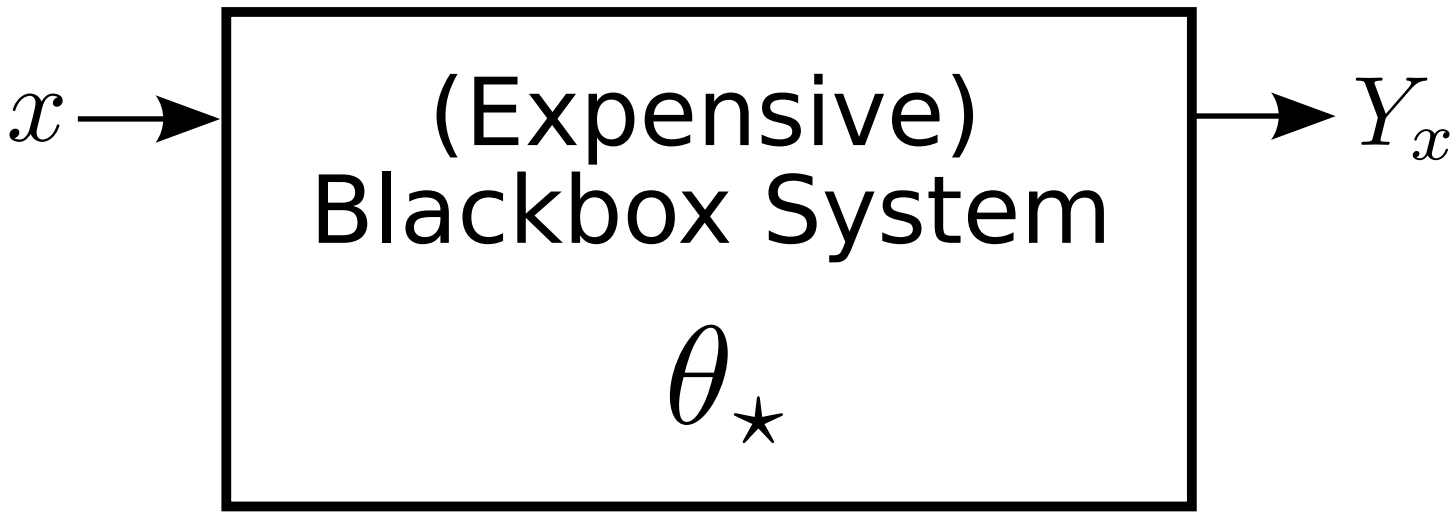
June 1, 2018

Lawrence Berkeley National Lab, CA

slides: `www.cs.cmu.edu/~kkandasa`

Design of Experiments



- Choose an experiment $x \in \mathcal{X}$.
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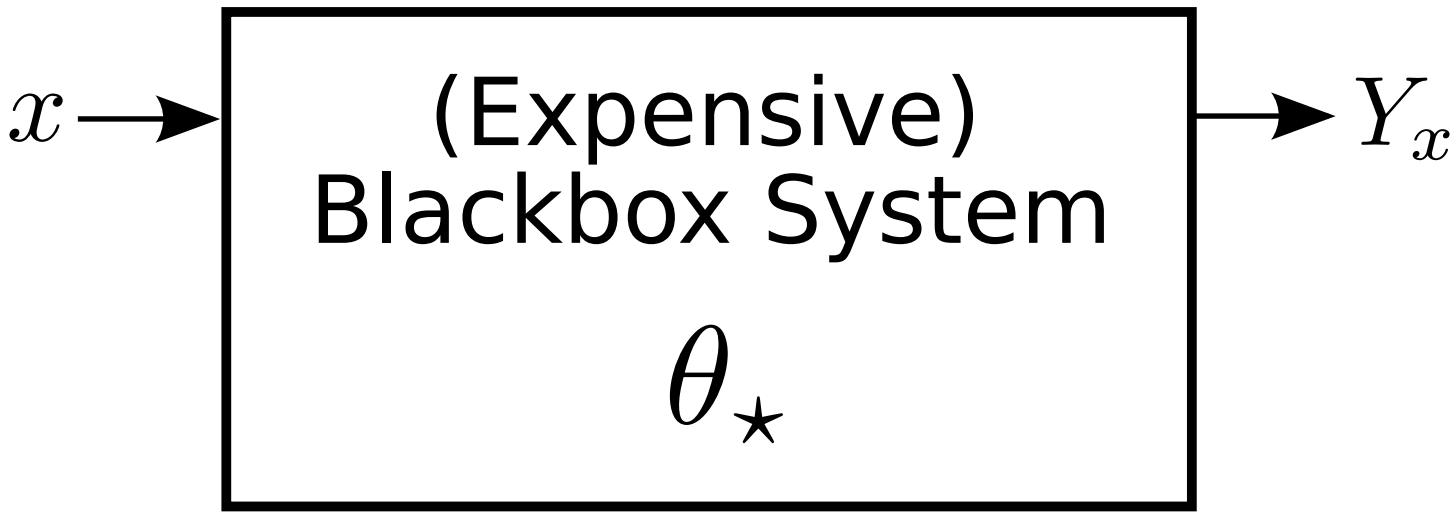

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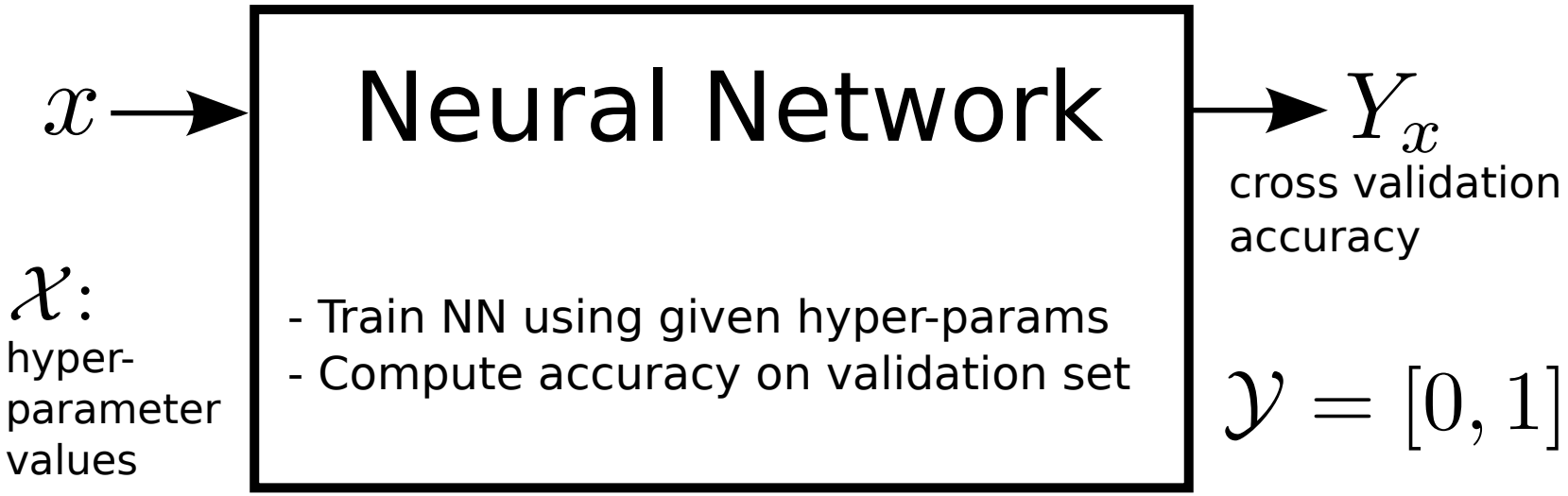
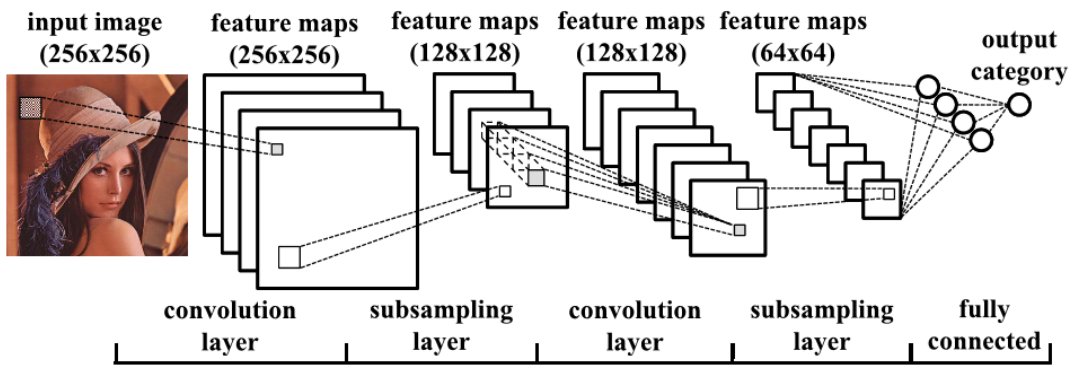
- Repeat in an adaptive sequence to collect data
  $D_t = \{(x_t, Y_{x_t})\}_{t=1}^n$.
- Typically some "goal/objective" in mind.

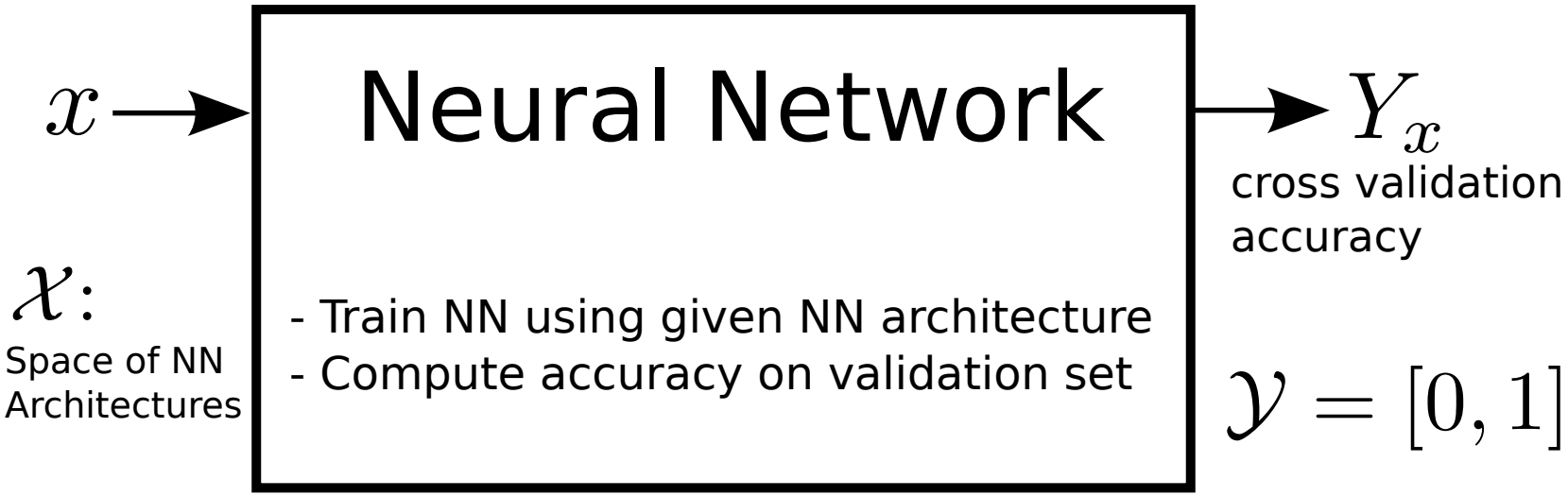
Black-box Optimisation: Model Selection

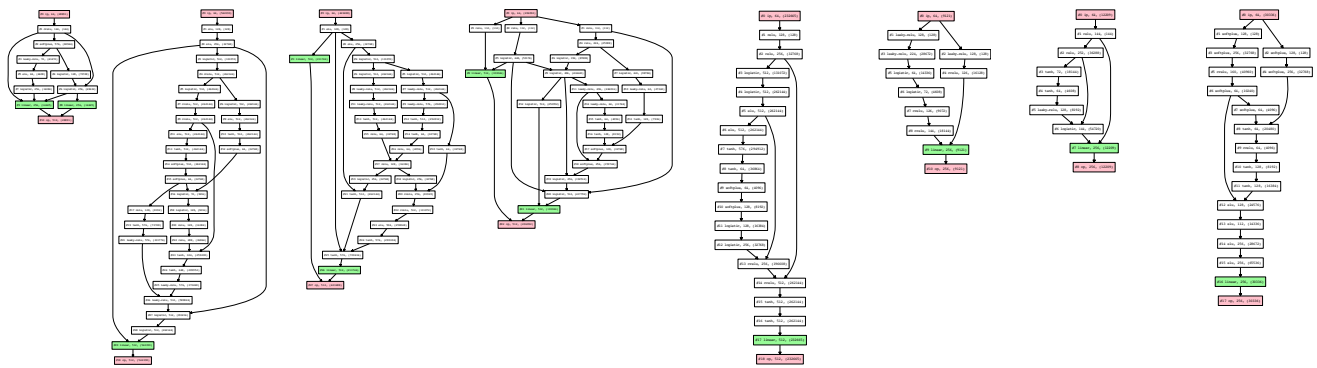




Goal: Find hyper-parameters with highest CV accuracy.

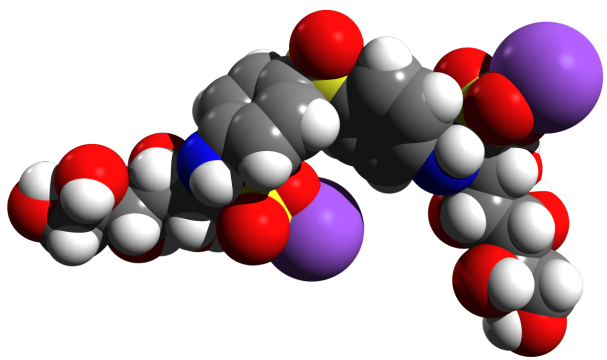
Black-box Optimisation: Architecture Search





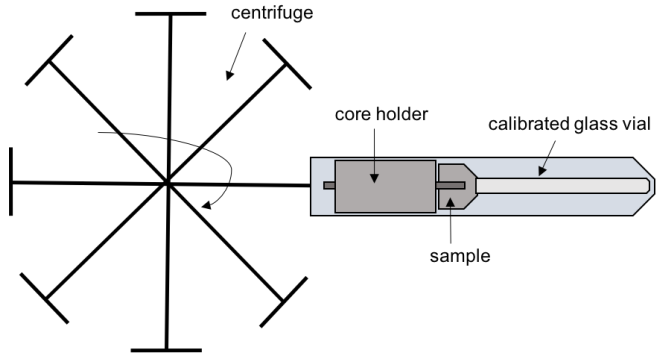
Goal: Find NN architecture with highest CV accuracy.

Multi-objective Optimisation: Drug Discovery



Goal: Find drug with "good value" on all objectives.

Active Learning: Materials Science



Goal: Estimate relation between solution and interfacial tension.

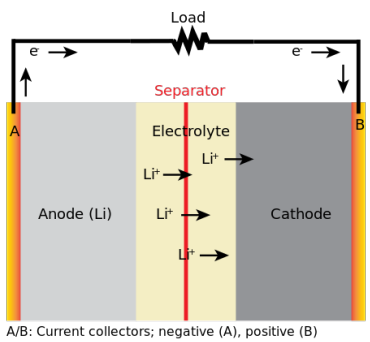
Multiple Goals: Materials Science

x → MD/DFT Simulations, Viscometer tests, Impedance spectroscopy, UV-vis spectroscopy → Y_x

$\mathcal{X}$: solvents/salt concentrations, physical/process conditions

solvation energy, viscosity, conductivity

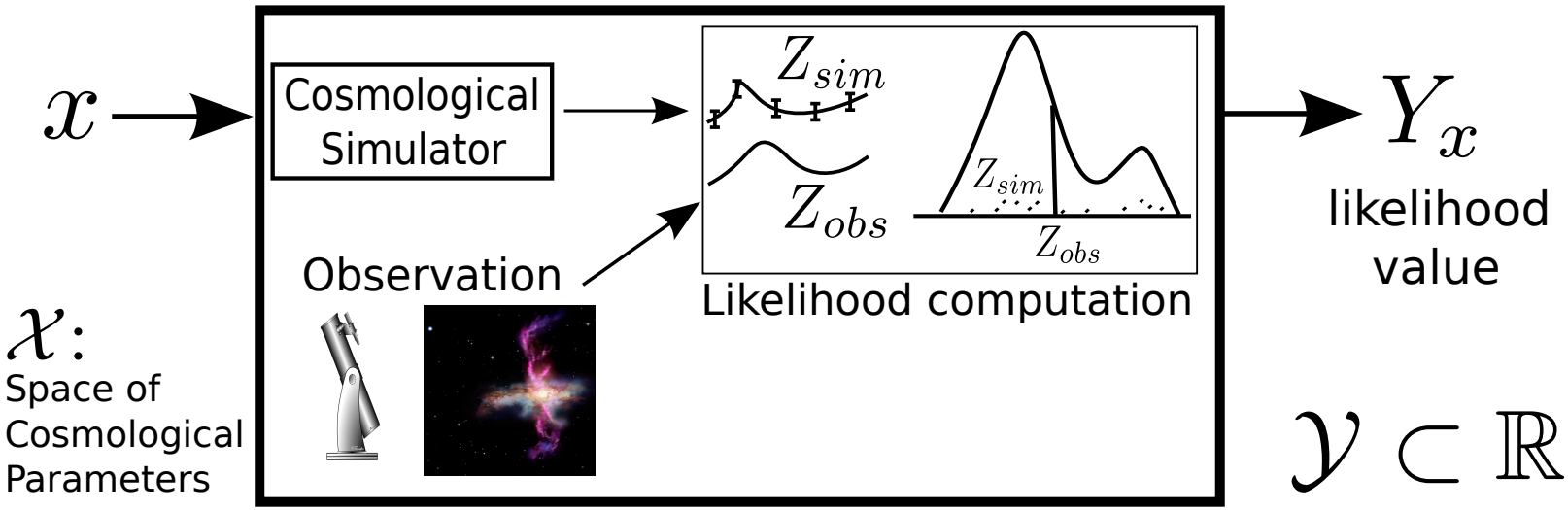
$\mathcal{Y} \subset \mathbb{R}^K$

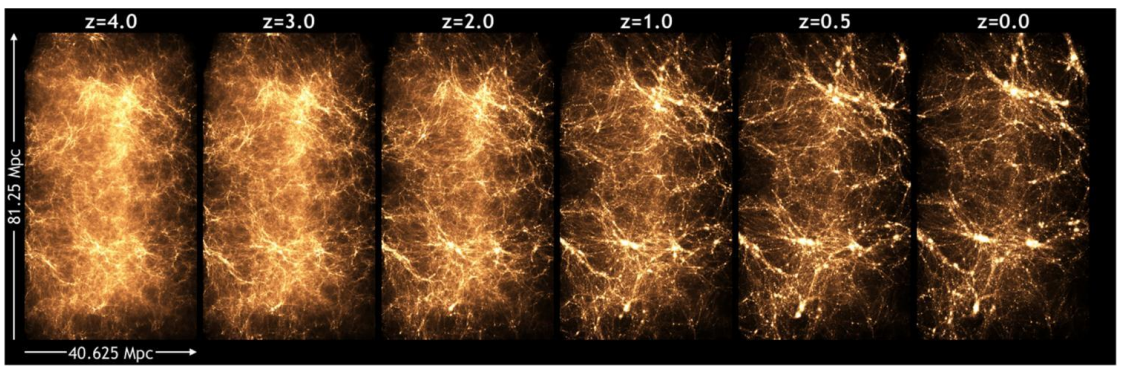


A/B: Current collectors; negative (A), positive (B)

Goal: Estimate relation between electrolyte solution and viscosity, while simultaneously optimising conductivity.

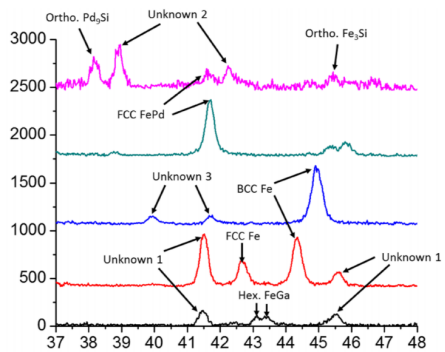
Posterior Estimation: Astrophysics

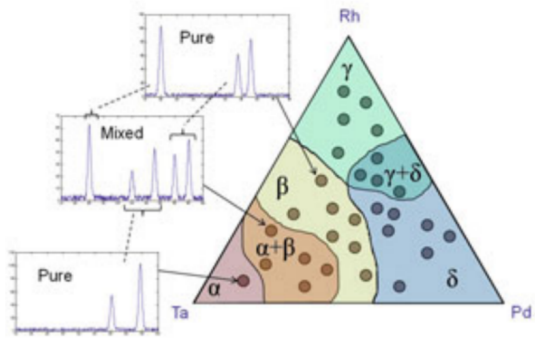




Goal: Estimate posterior for cosmological parameters given data.

Phase Identification: Materials Science





Goal: Identify changes in crystal structure in an alloy.

Outline

- Part I: Preliminaries (Black-box Optimisation)
  1. Bayesian Models
  2. Black-box Optimisation via Thompson Sampling
- Part II: DOE via posterior sampling
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  1. Parallelising experiments
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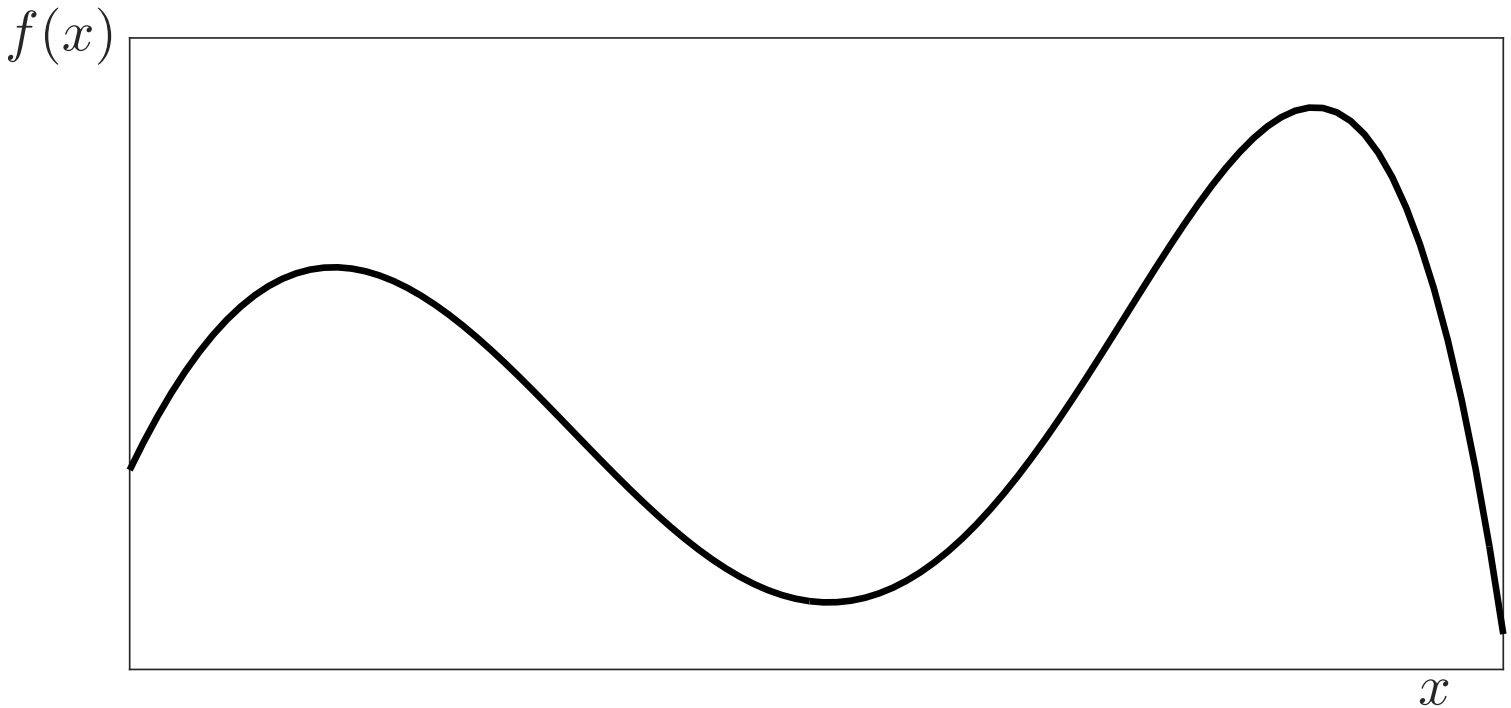
Black-box Optimisation

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



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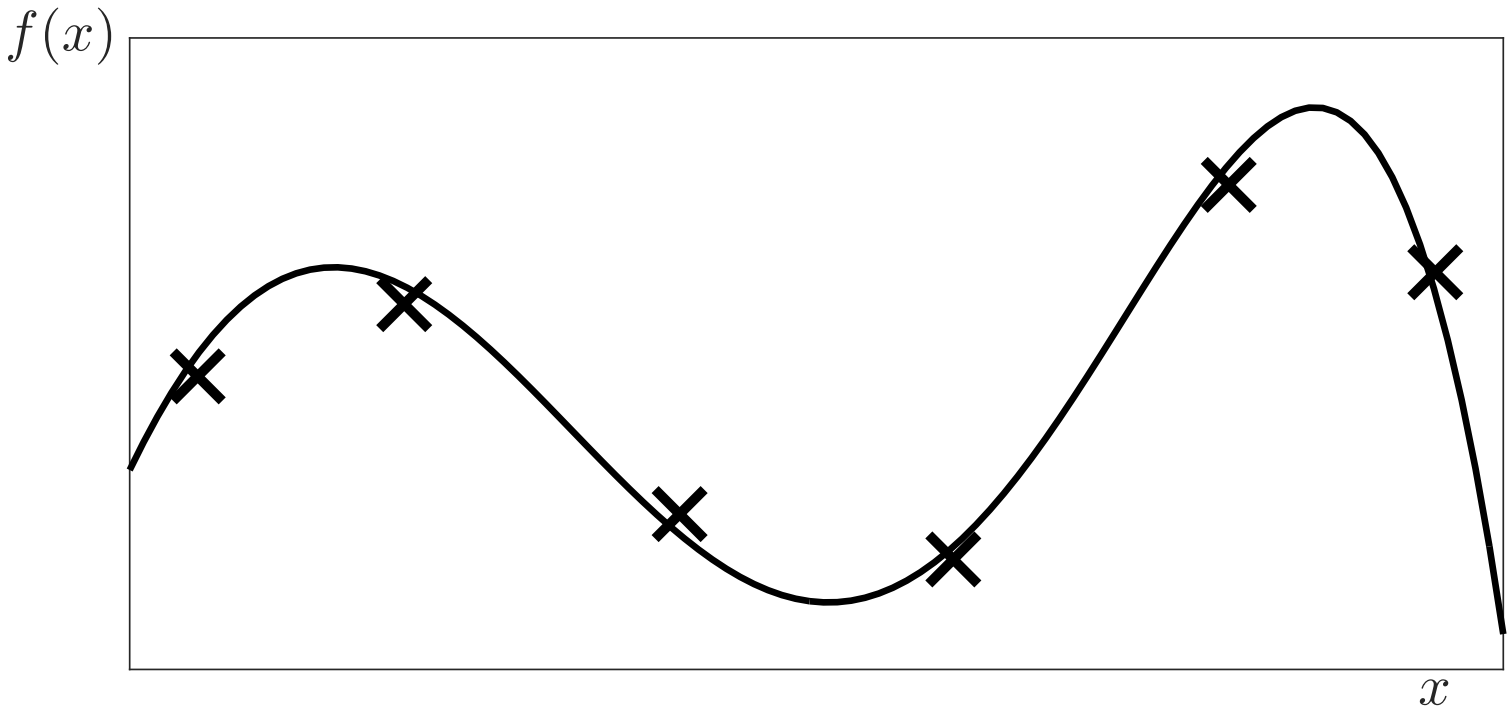

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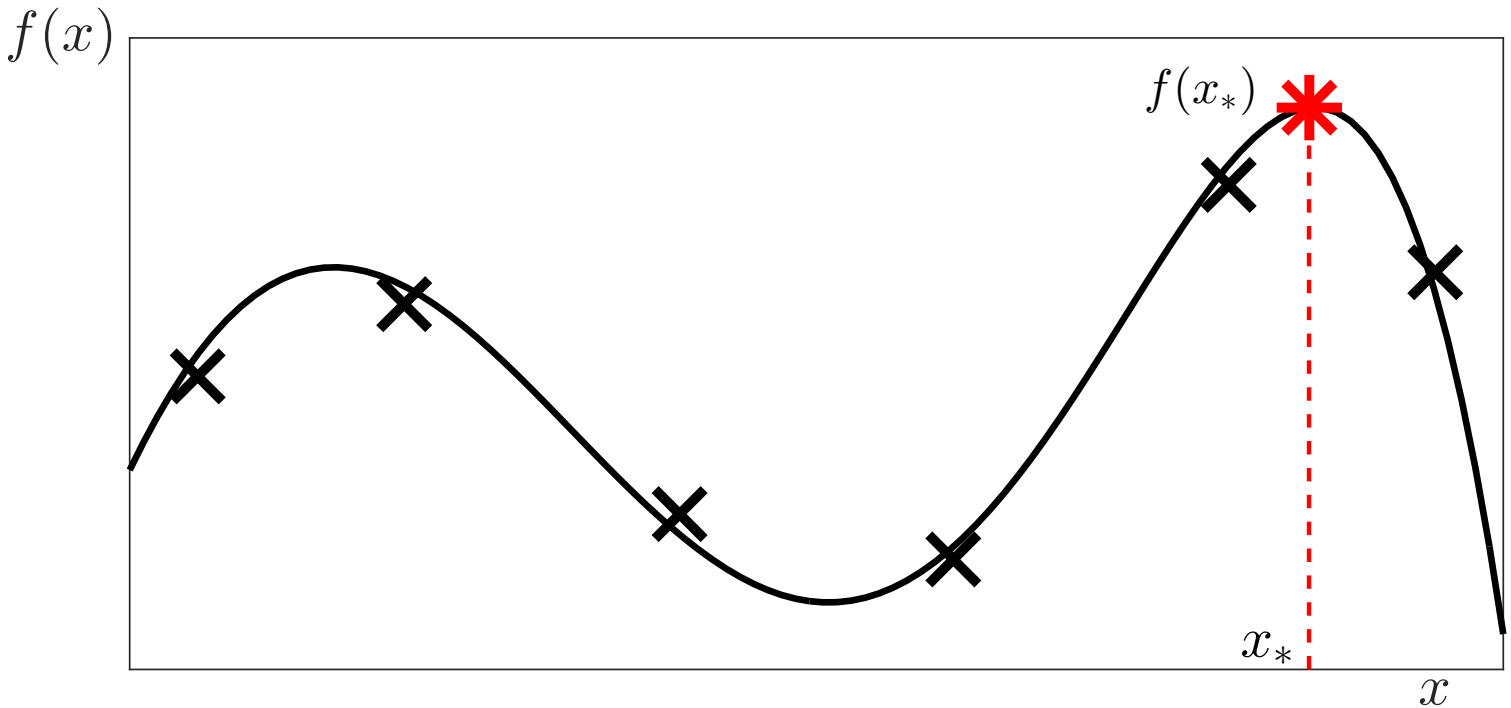
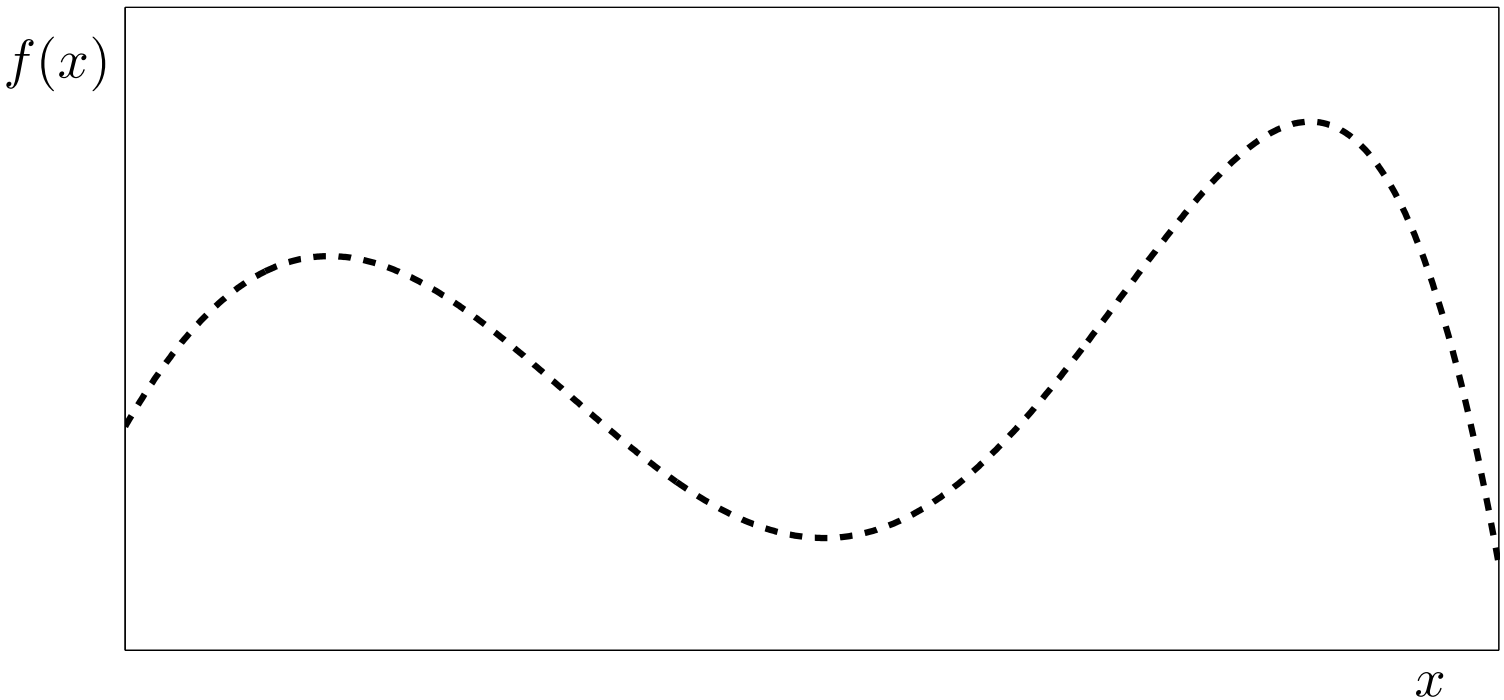


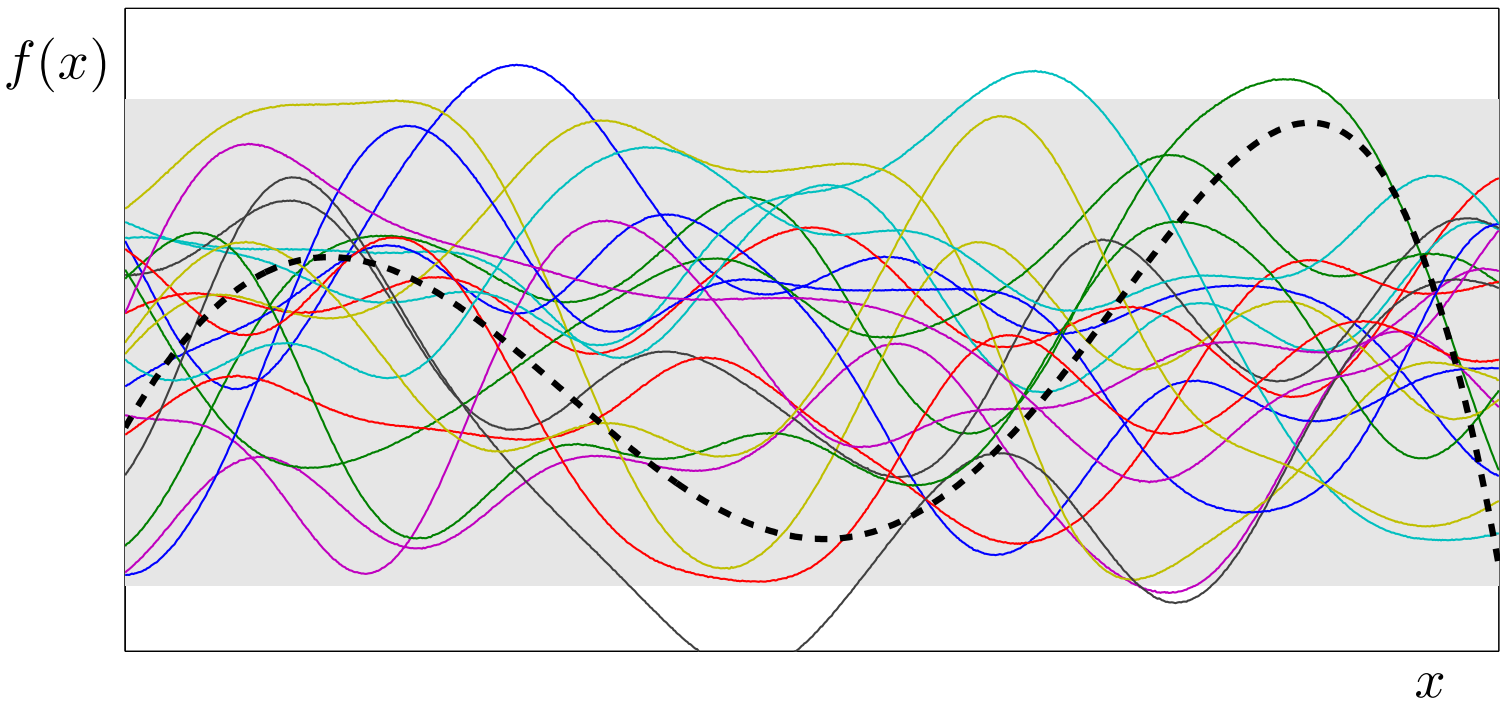
Bayesian Models for f

Functions with no observations



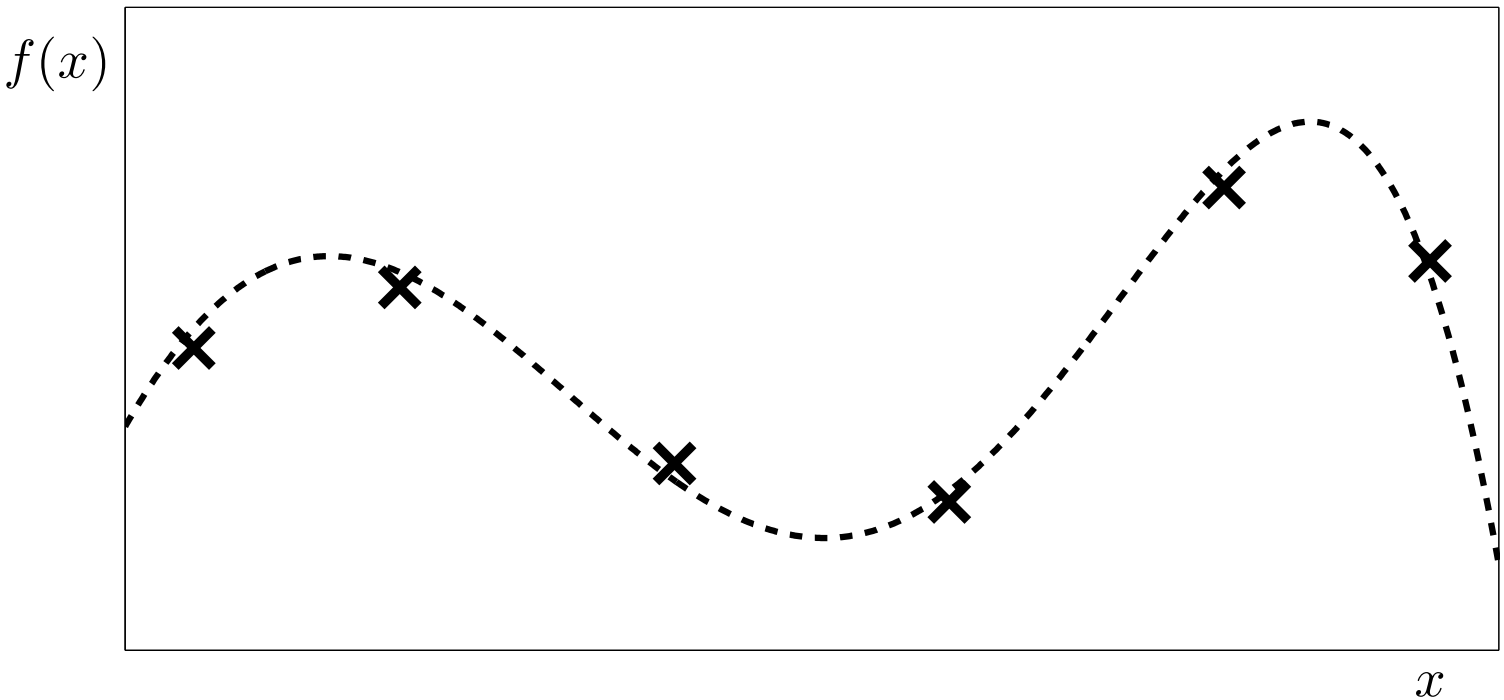
Bayesian Models for f

Prior $\mathbb{P}(\theta_\star)$



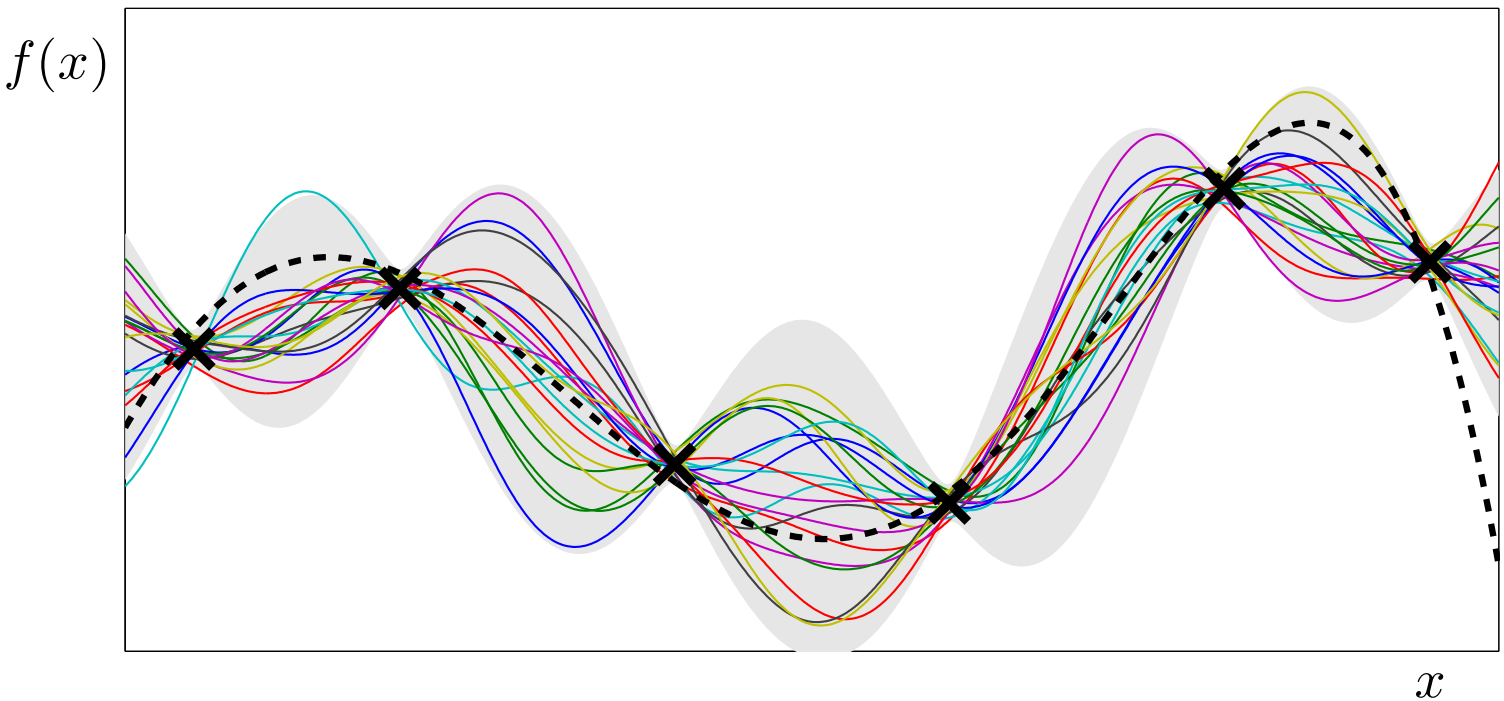
Bayesian Models for f

Observations



Bayesian Models for f

Posterior given observations $\mathbb{P}(\theta_\star | D_t)$



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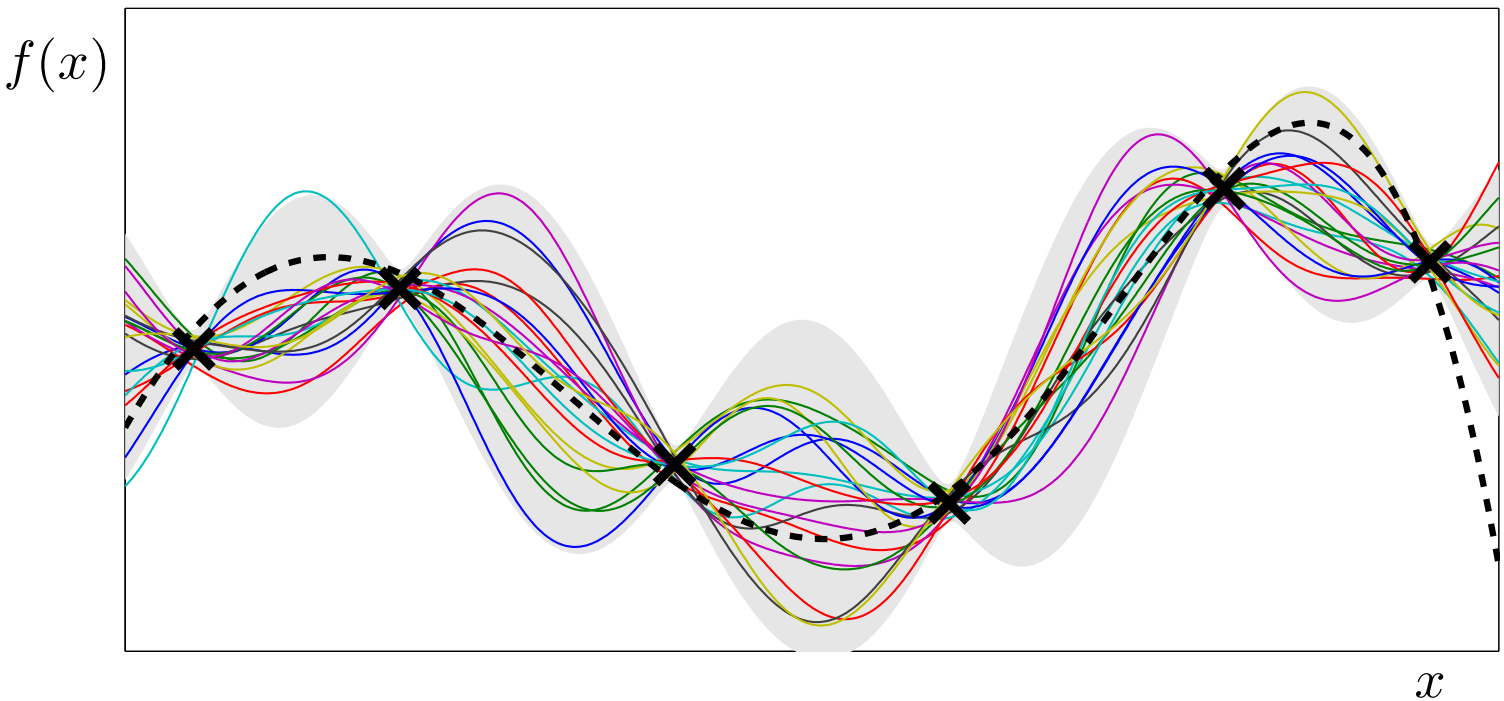
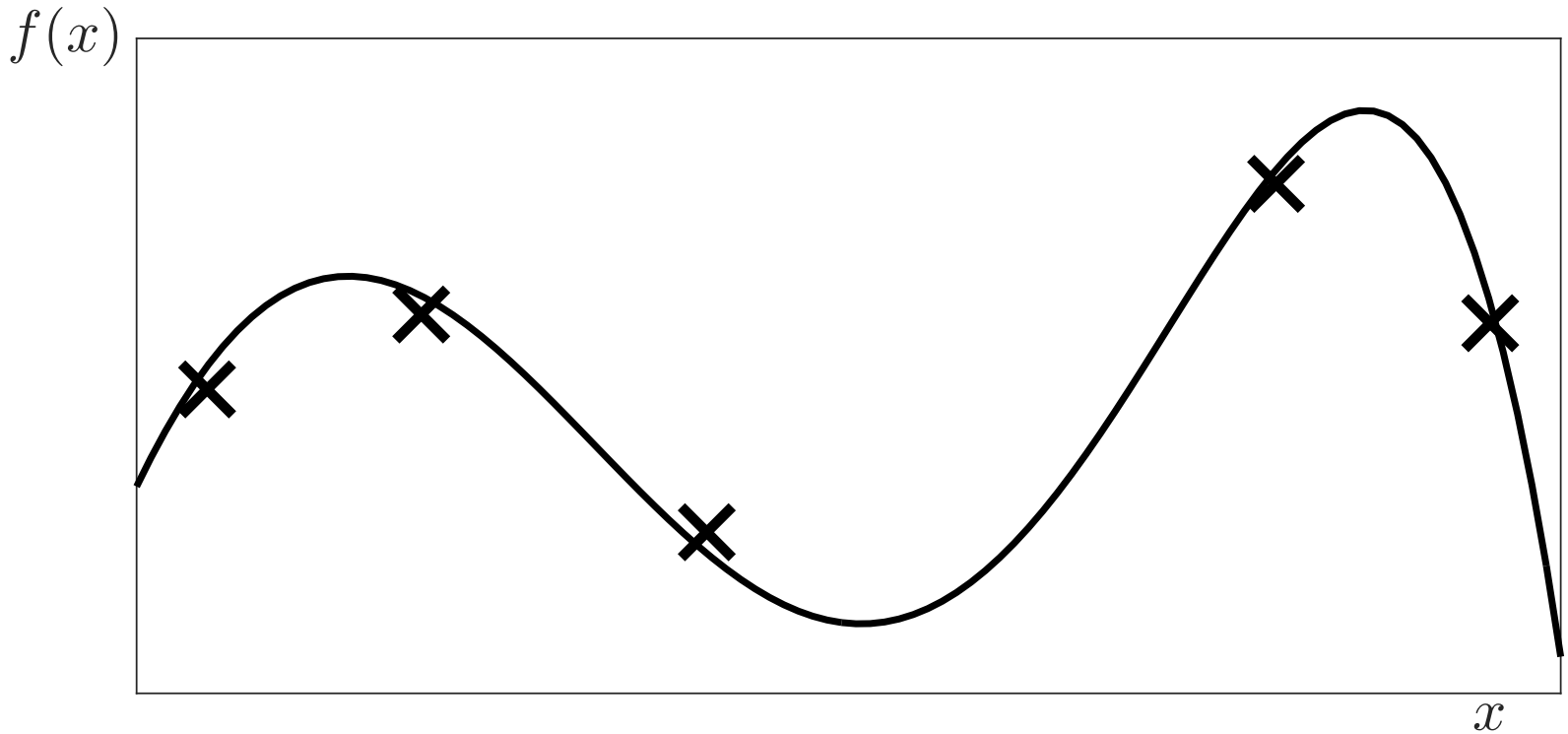


Thompson Sampling for Black-box Optimisation

(Thompson, 1933)



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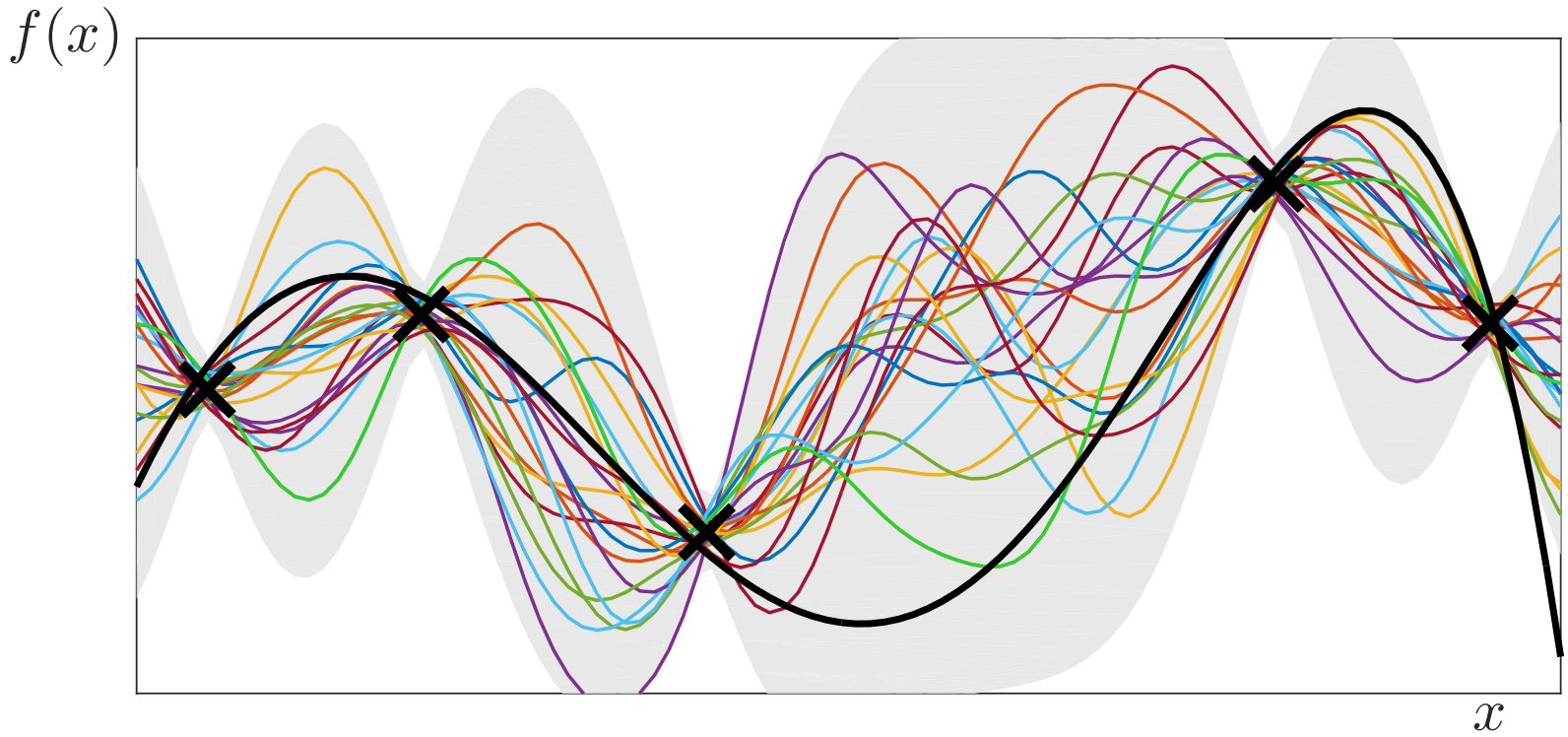

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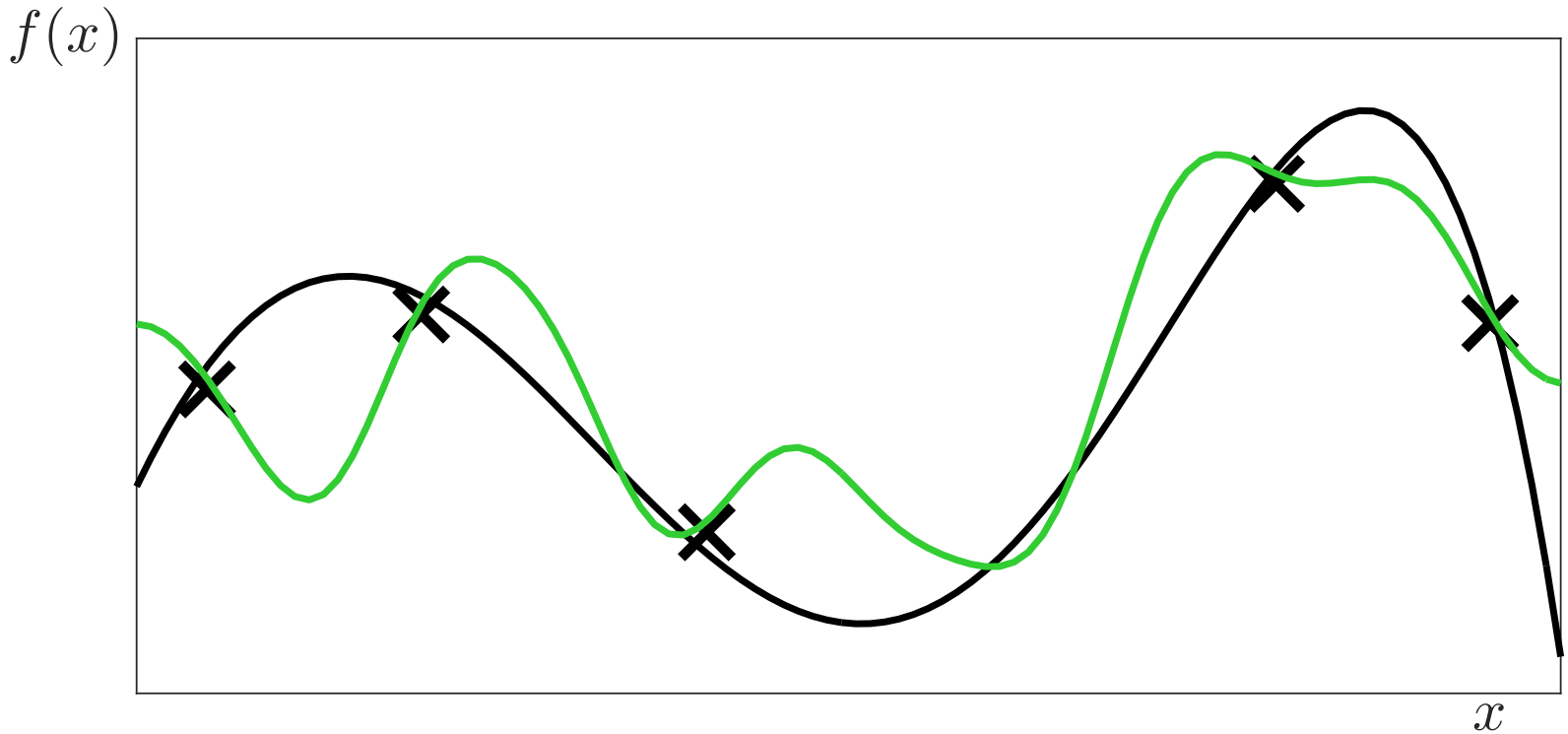

1) Construct posterior $\mathbb{P}(\theta_\star|D_t)$. 2) Draw sample g from posterior.

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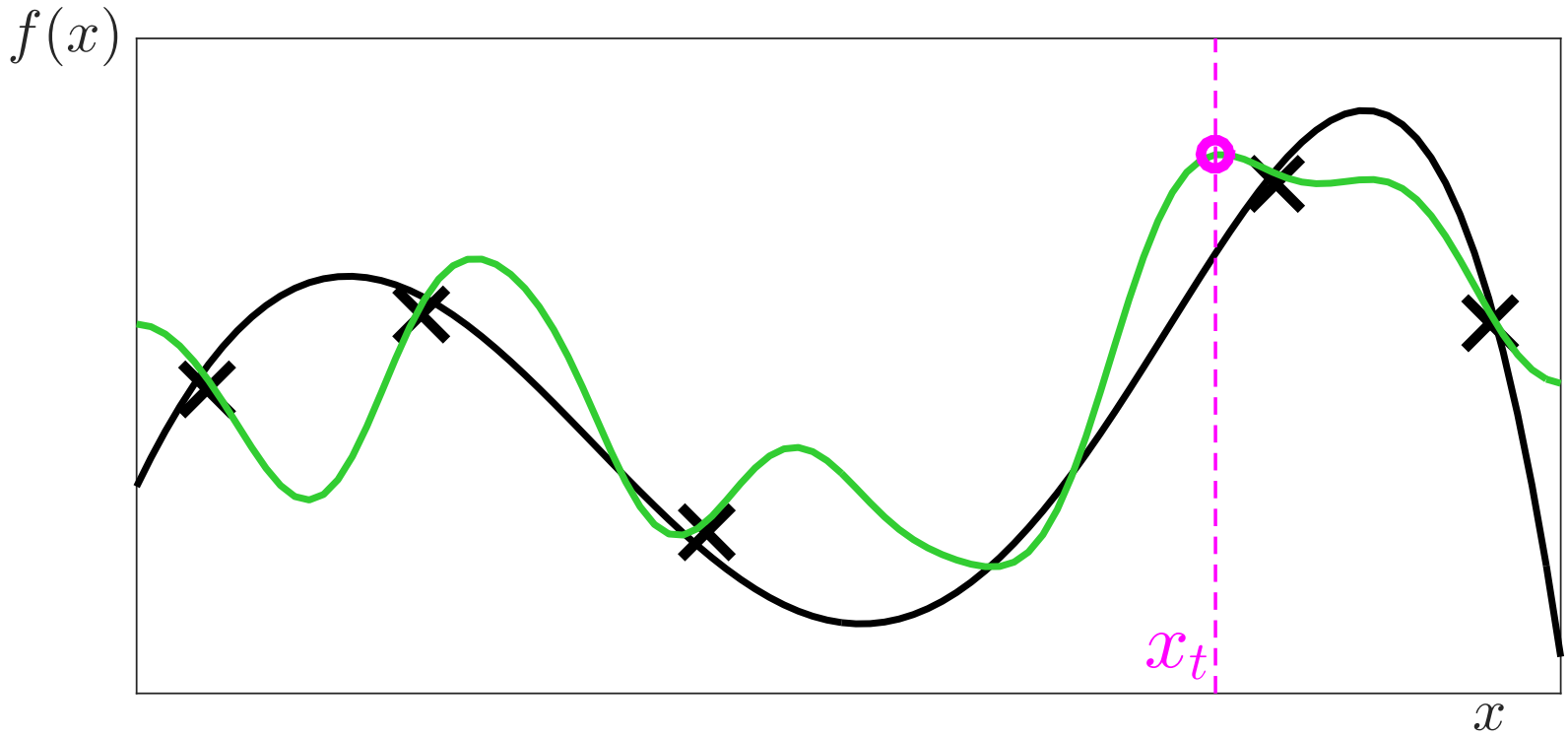

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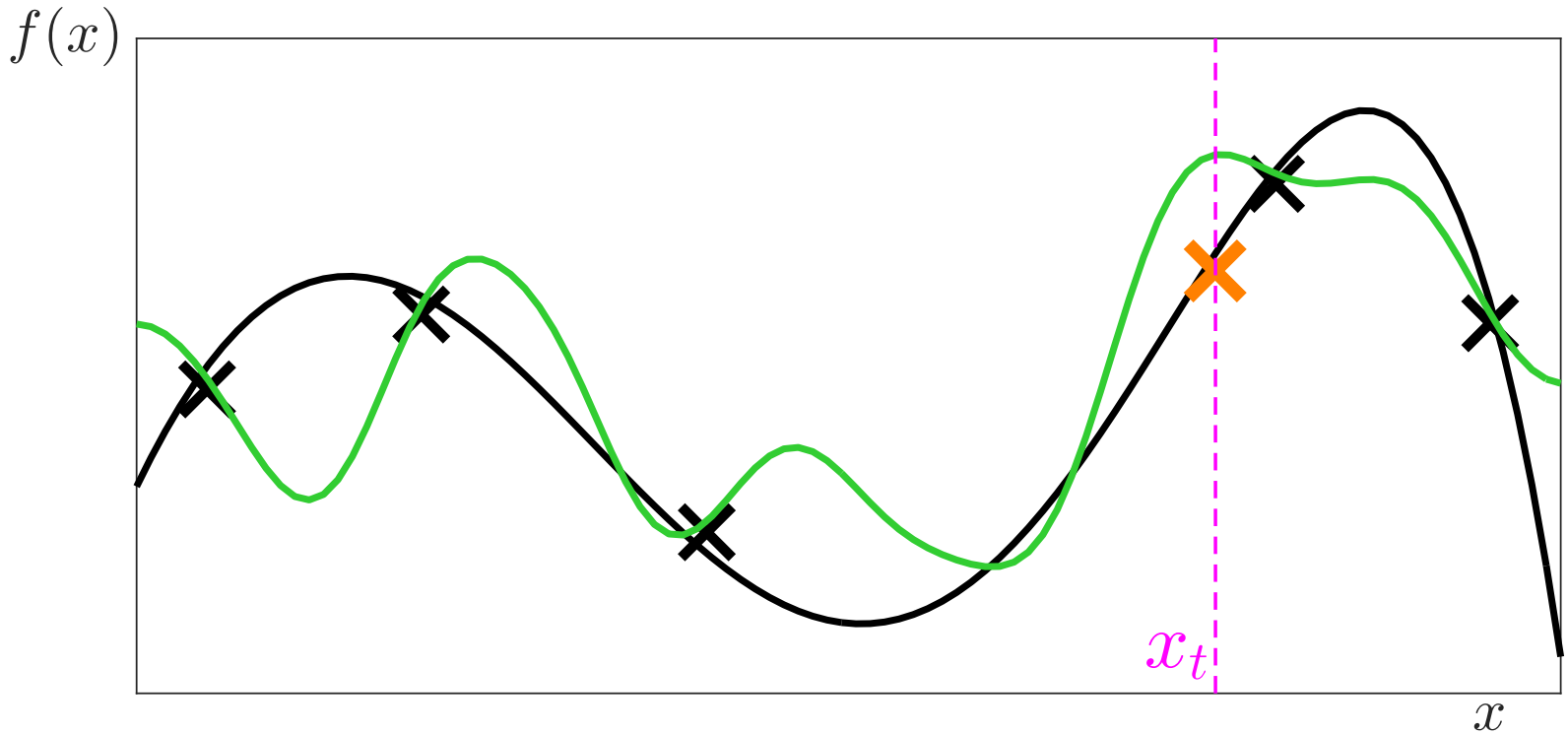

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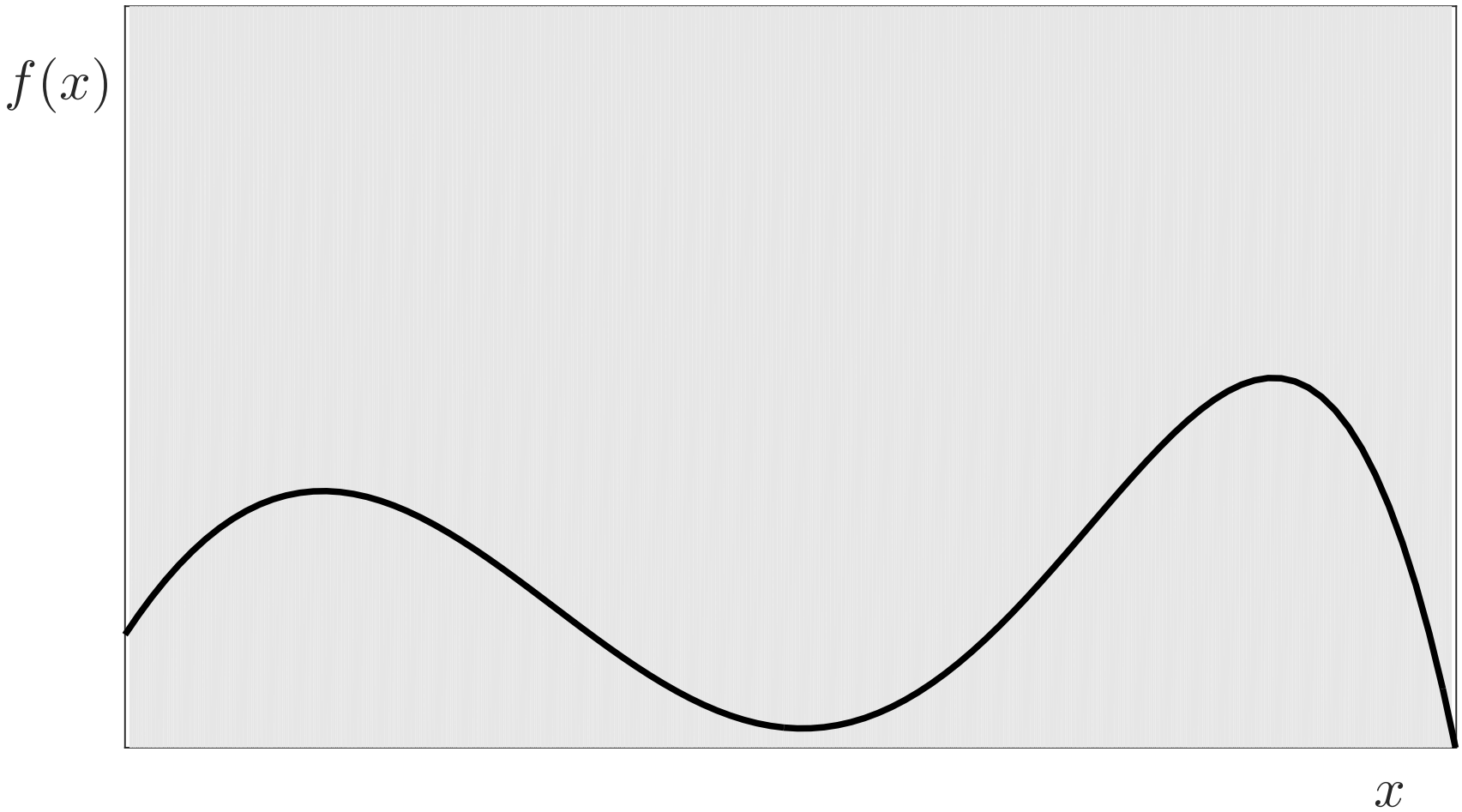

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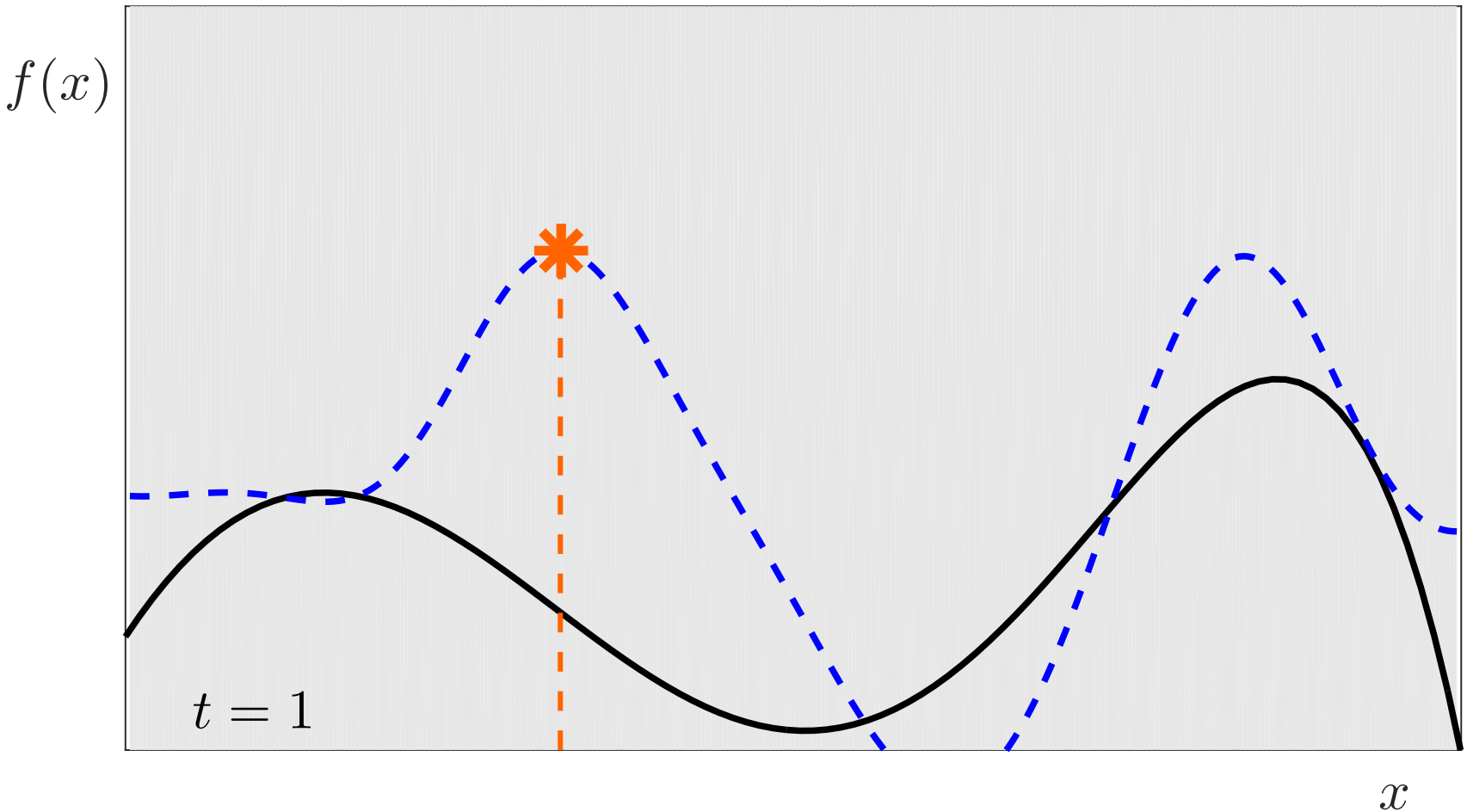

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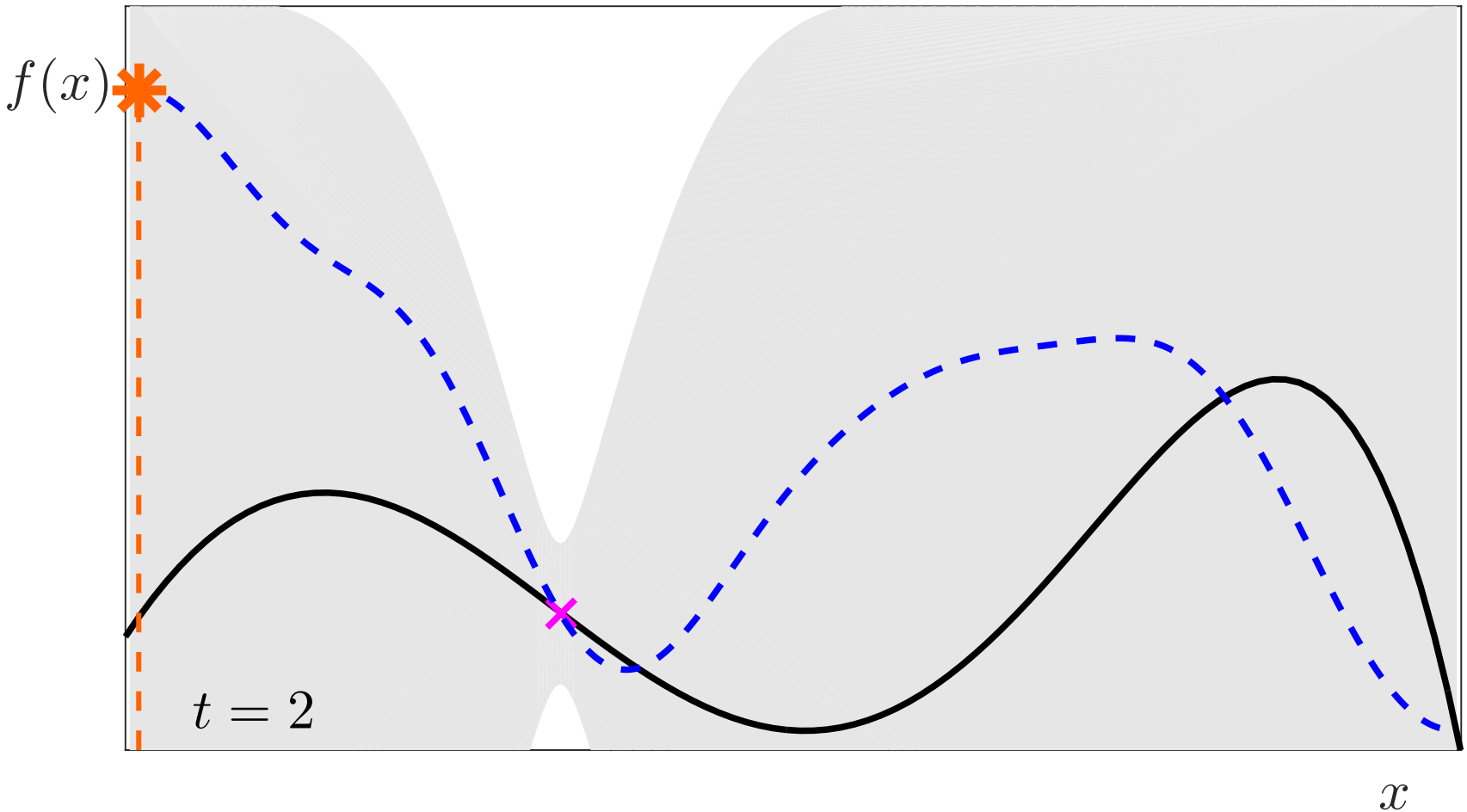

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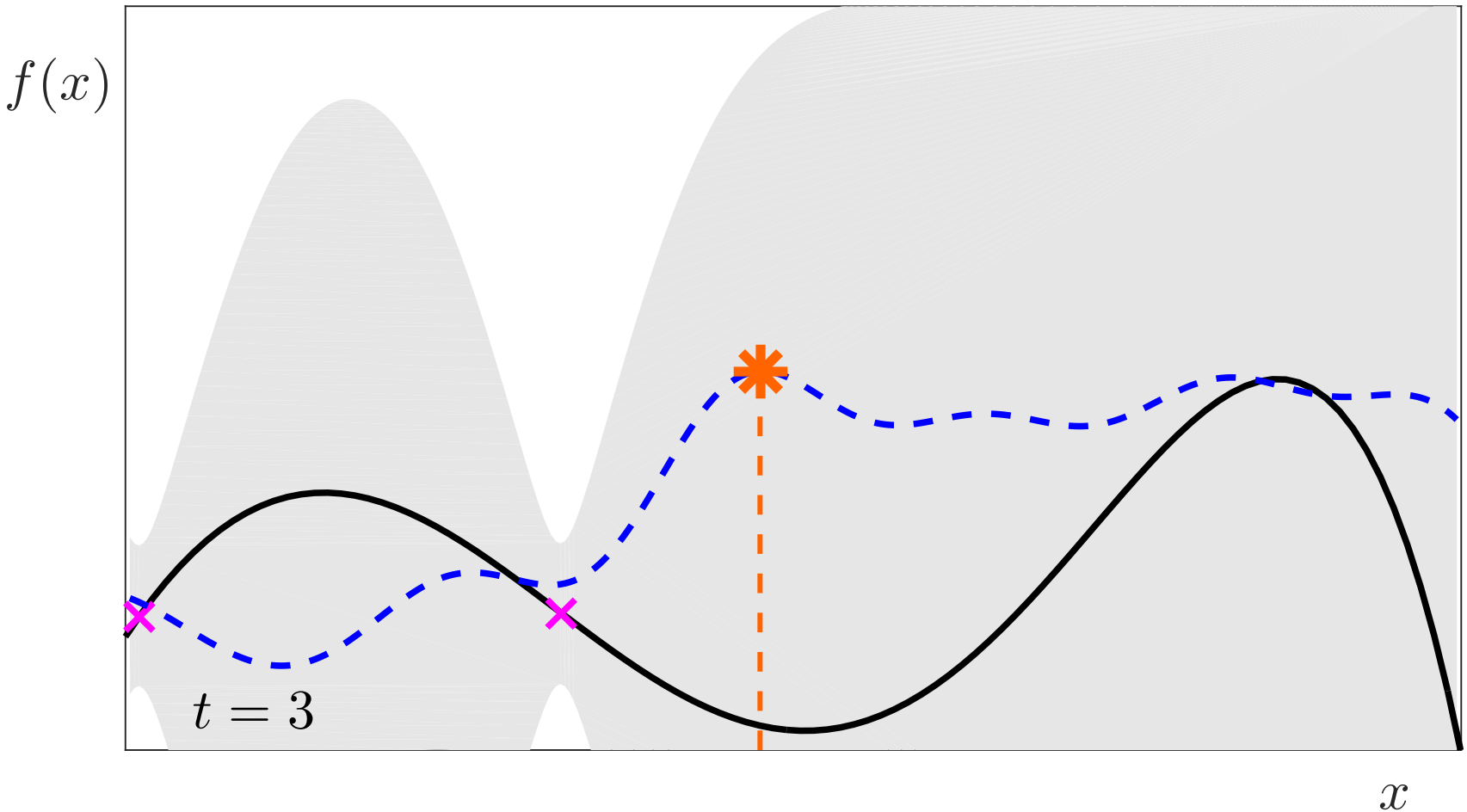

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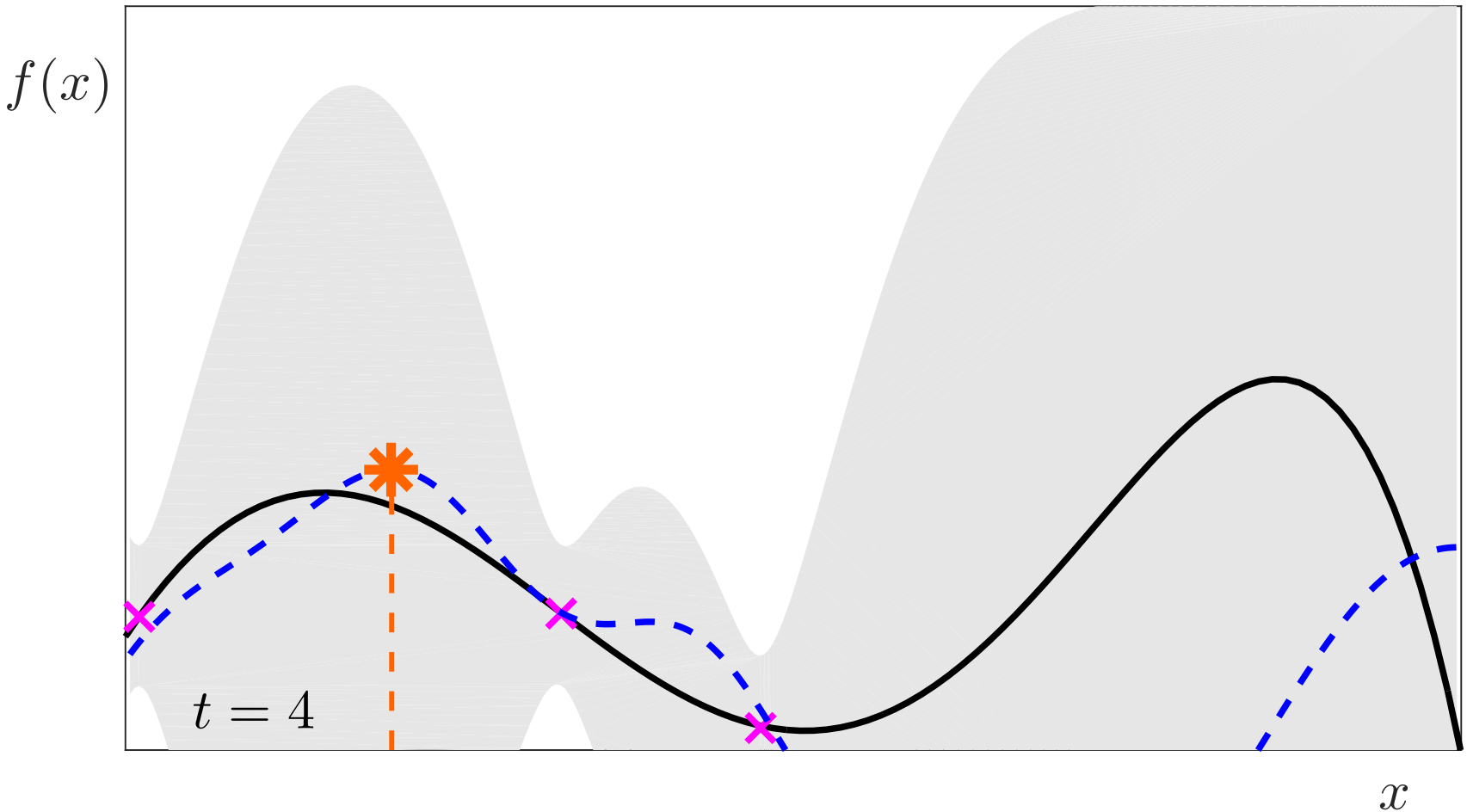

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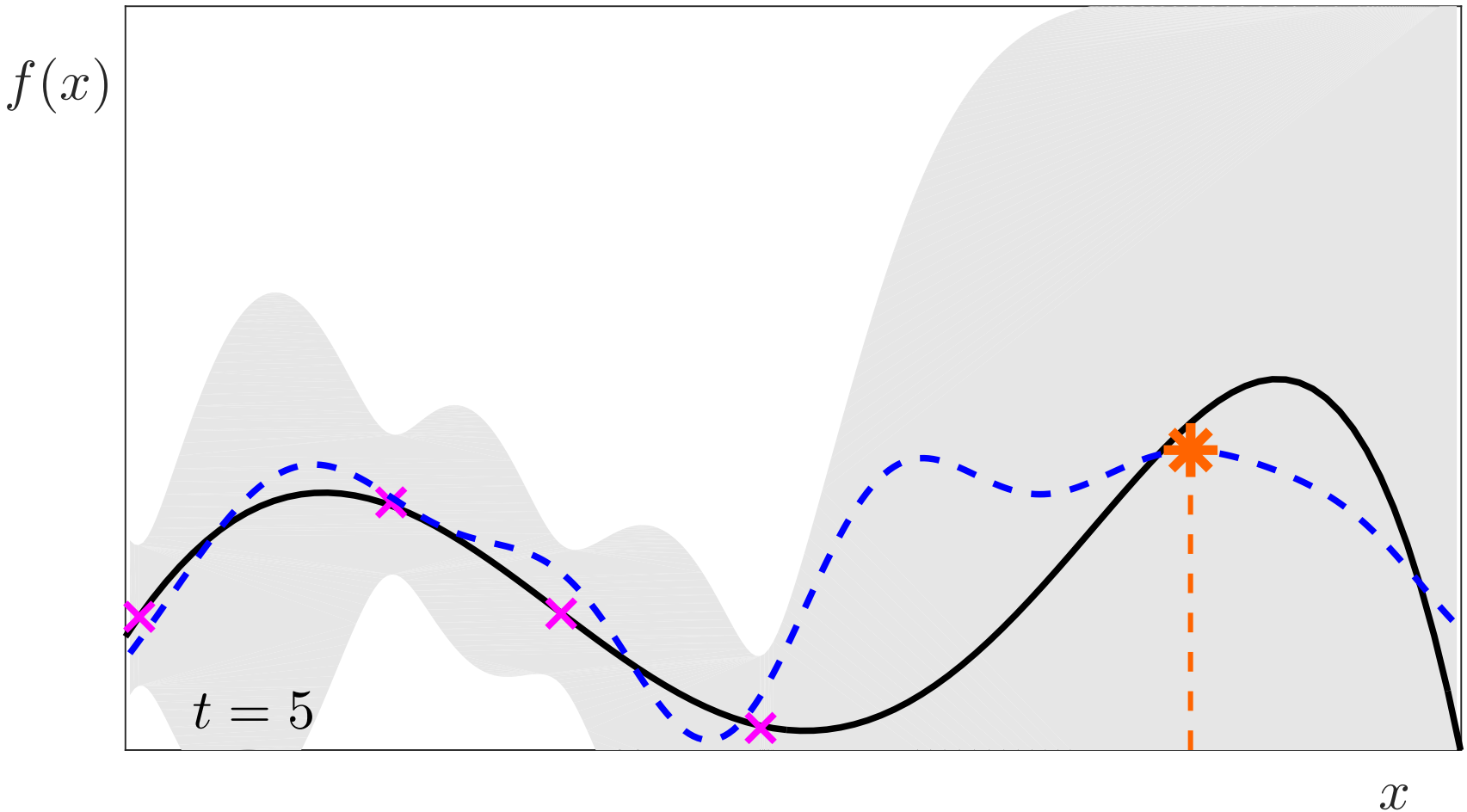

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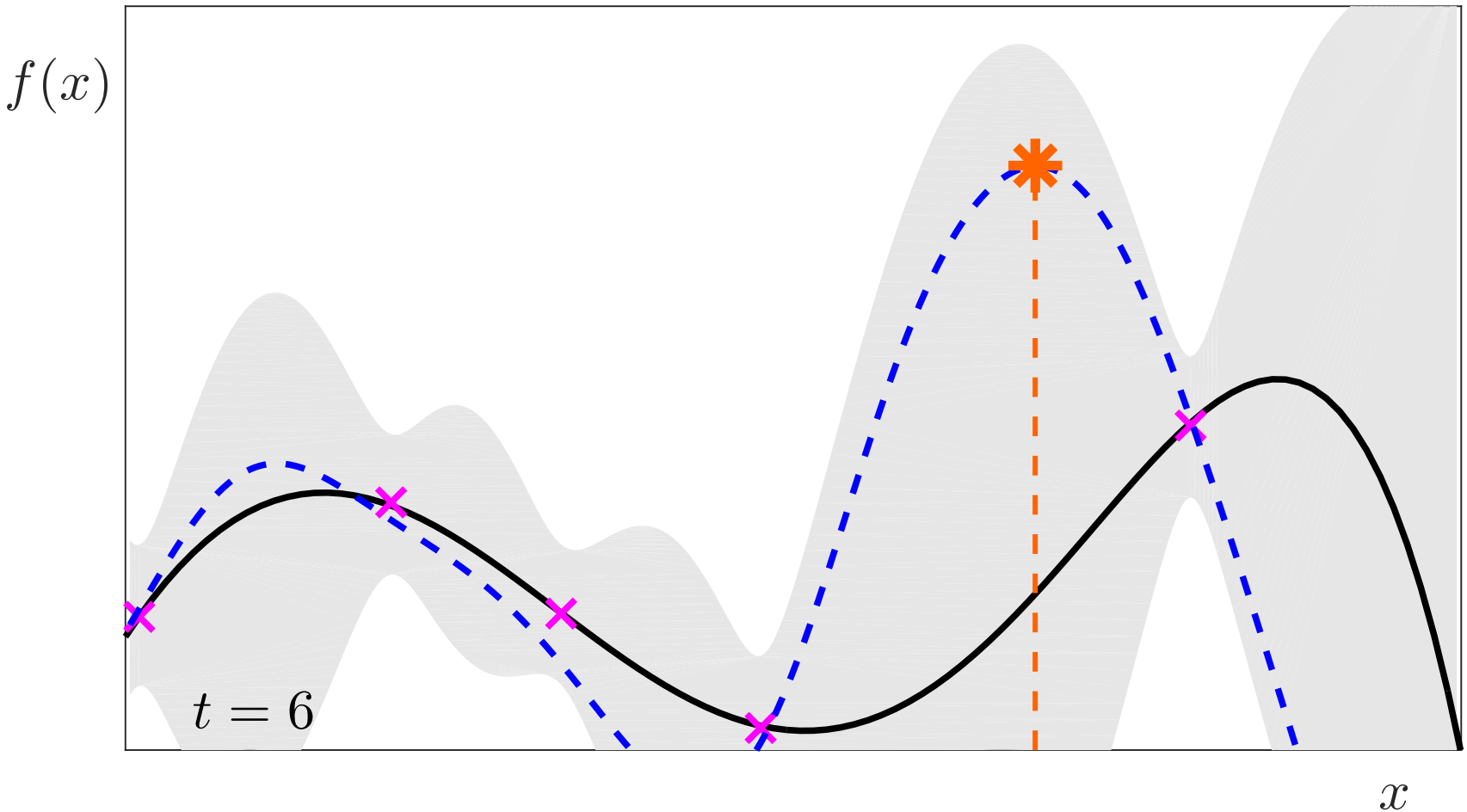

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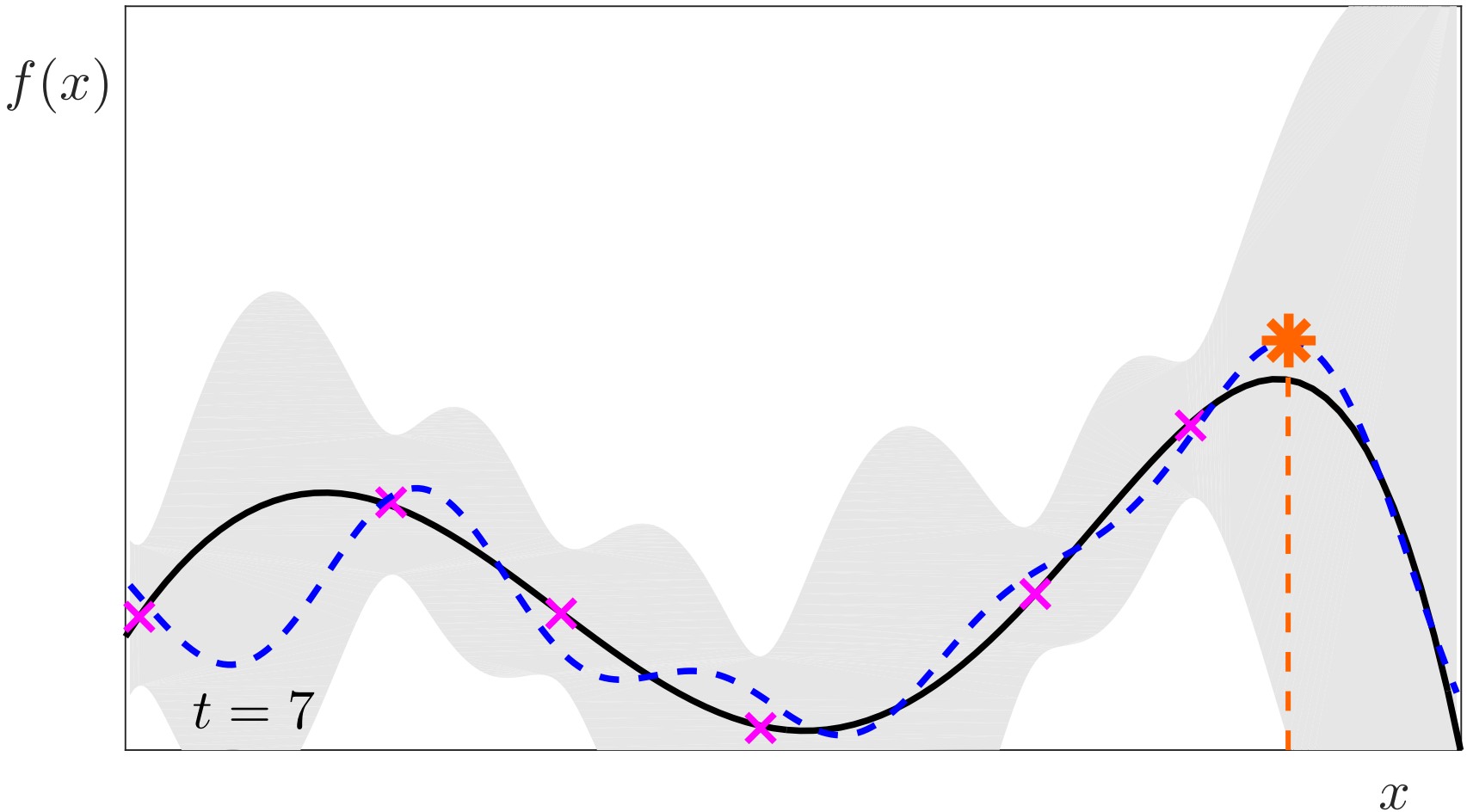

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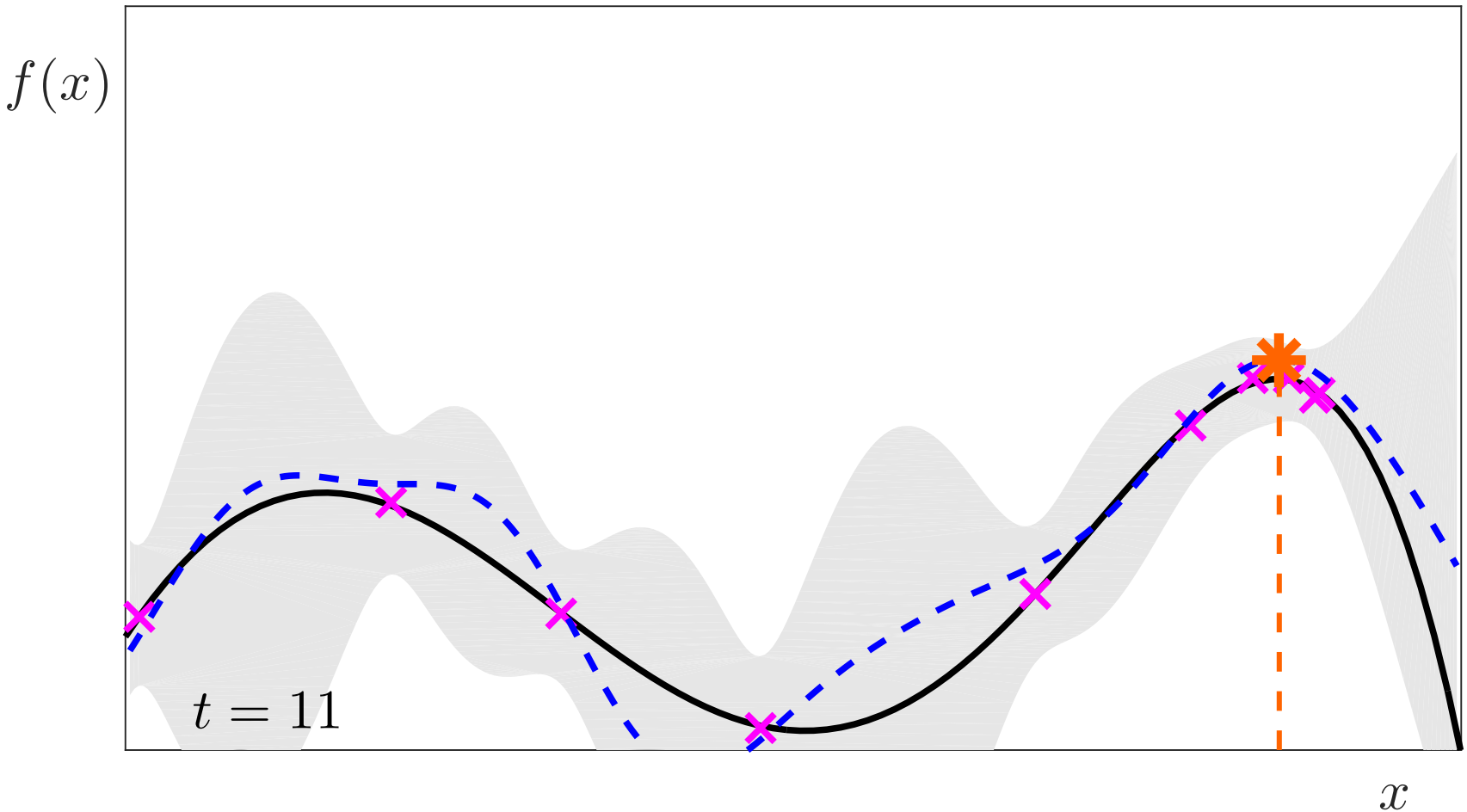

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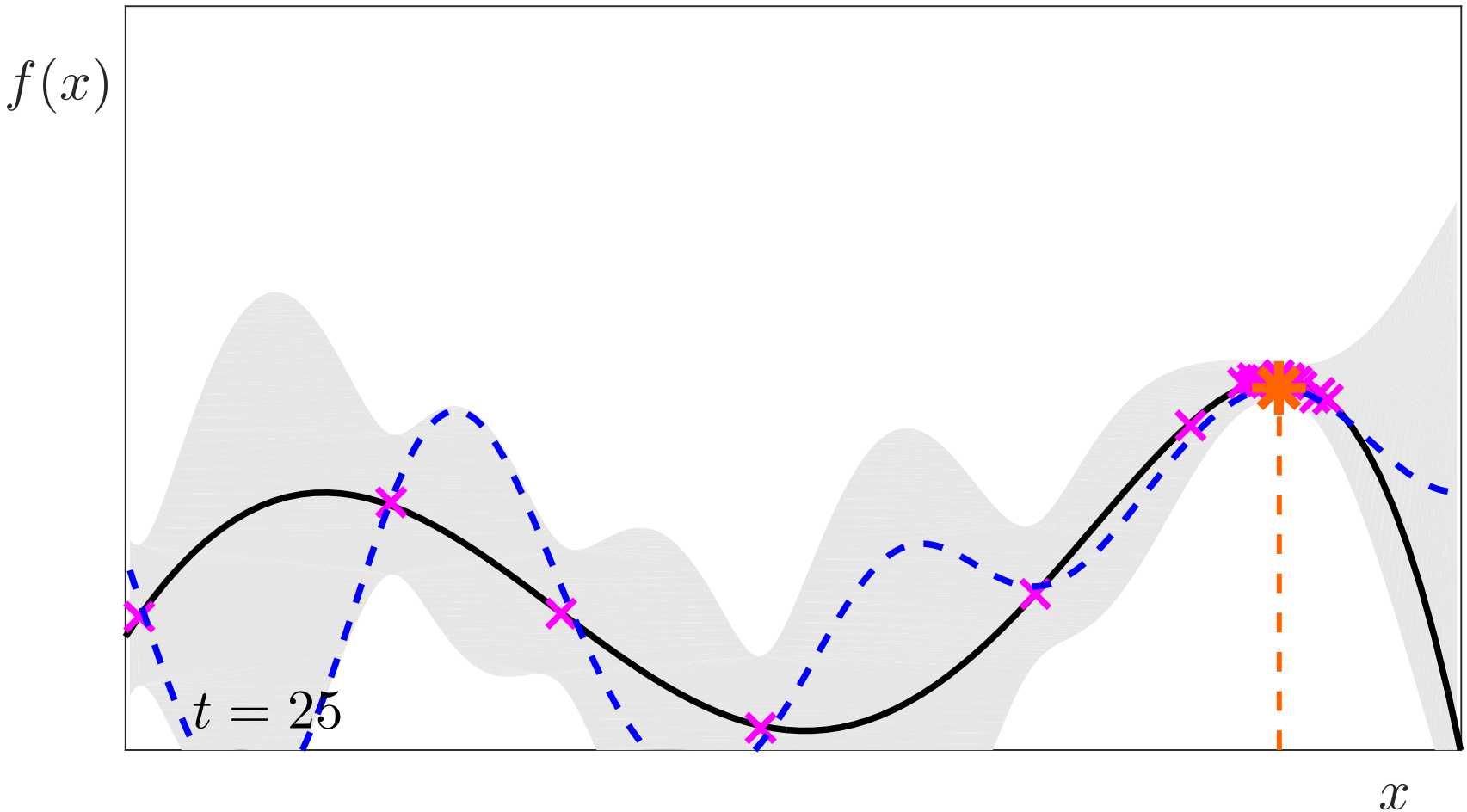

Black-box Optimisation in the Bayesian Paradigm

Other criteria for selecting x_t:

- Upper Confidence Bounds (Srinivas et al. 2010)
- Expected improvement (Jones et al. 1998)
- Probability of improvement (Kushner et al. 1964)
- Entropy search (Hernández-Lobato et al. 2014, Wang et al. 2017)
- . . . and a few more.

Bayesian models for f:

- Gaussian Processes (most popular)
- Neural networks (Snoek et al. 2015)
- Random forests (Hutter 2009)

Off-the-shelf models: general, but can be inefficient.

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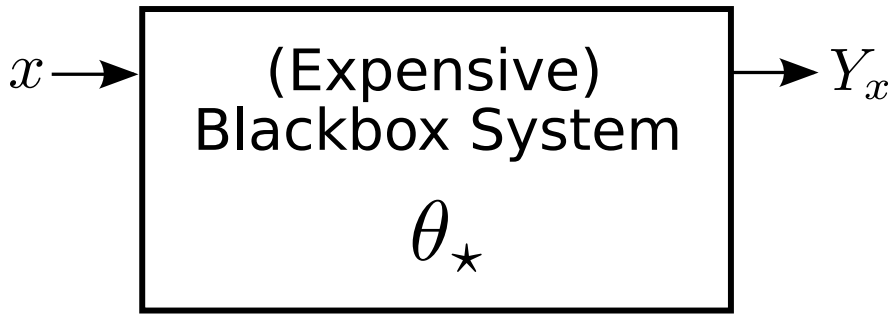

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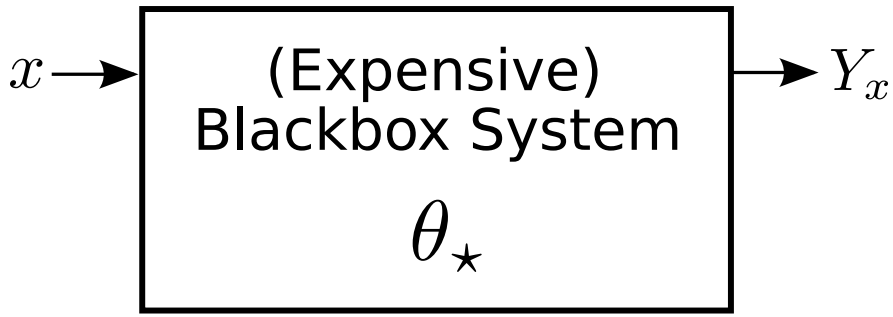

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Desiderata for a General Framework:

- Flexibility to capture custom/complex relations for $X \to Y_X$.
  - Incorporate domain expertise into models.
- Ability to achieve any desired goal.

Formalism for "goal-oriented" DOE

System:

- A true parameter $\theta_\star \in \Theta$ that completely specifies the system.
- $\Theta \leftarrow$ a parameter space.

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- We wish to achieve small $\lambda(\theta_\star, D_n)$ after n experiments.

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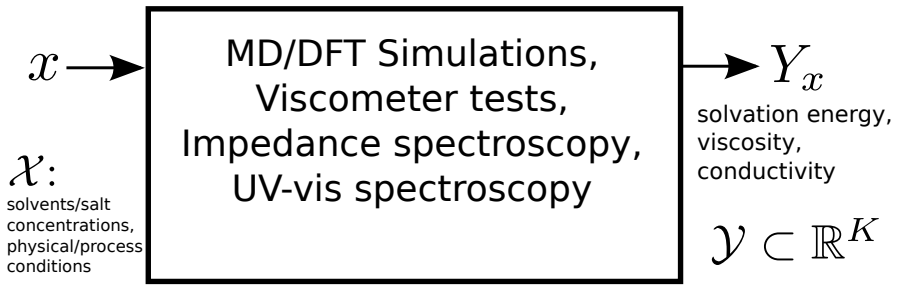
Bayesian Models:

- A prior for $\theta_\star$: $\mathbb{P}(\theta_\star)$.
- A discriminative model for observations $y|x, \theta$: $\mathbb{P}(y|x, \theta)$.

Incorporating Domain Expertise via Bayesian Models
An example in Electrolyte Design



Three control variables:

Q: EC-EMC fraction, S: molarity of salt $LiPF_6$, T: temperature.

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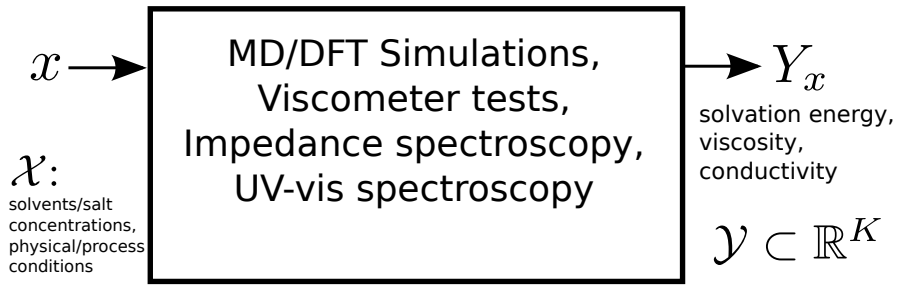

Three control variables:
Q: EC-EMC fraction, S: molarity of salt $LiPF_6$, T: temperature.

$f_{\text{vis}}(Q, S, T) = \exp(-aT + bS) \cdot g_{\text{vis}}(Q)$. (Reynolds model)
$f_{\text{dissol}}(Q, S, T) = cT \cdot \frac{1}{1+\exp(dS)} \cdot g_{\text{dissolv}}(Q)$.

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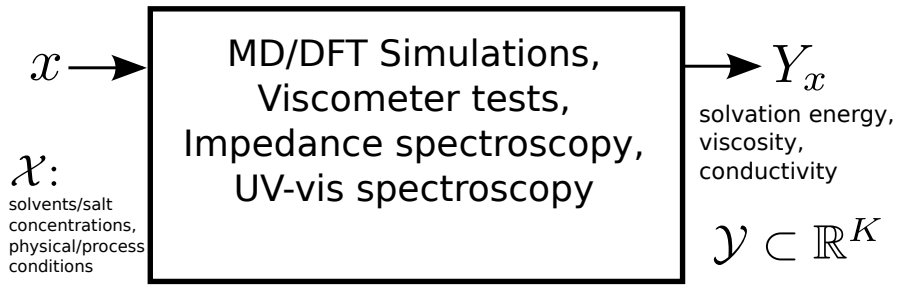

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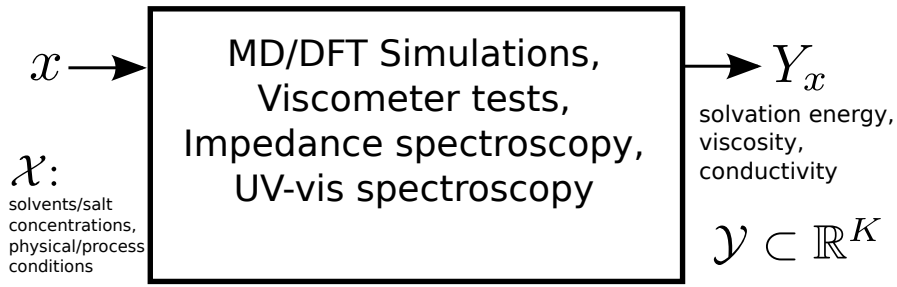
$f_{\text{dissol}}(Q, S, T) = cT \cdot \frac{1}{1+\exp(dS)} \cdot g_{\text{dissolv}}(Q)$.

Observations: $y_{\text{visc}}|x, \theta \sim \mathcal{N}(f_{\text{vis}}(Q, S, T), \eta^2)$.
$y_{\text{dissol}}|x, \theta \sim \mathcal{N}(f_{\text{dissol}}(Q, S, T), \sigma^2)$.

Incorporating Domain Expertise via Bayesian Models
An example in Electrolyte Design



Three control variables:
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Unknown parameters: $\theta = (a, b, c, d, g_{\text{vis}}, g_{\text{dissolv}}) \in \Theta$.
True parameter $\theta_\star = (a_\star, b_\star, c_\star, d_\star, g_{\text{vis}\star}, g_{\text{dissolv}\star})$.
Use prior $\mathbb{P}(\theta_\star)$ to specify plausible values for $\theta_\star$.

Specifying the goal via a Penalty Function

Practitioner specifies goal of the experiment via $\lambda(\theta, D_n)$.

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Example 2: Active Learning
Estimate some parameter $\tau_\star = \tau(\theta_\star)$ of the system.

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Will look at more examples shortly.

MPS: Myopic Posterior Sampling for DOE

Expected look-ahead penalty at x if θ was the true parameter and we have already collected data D:

$$\lambda^+(\theta, D, x) \;=\; \mathbb{E}_{Y_x \sim \mathbb{P}(Y|x,\theta)}\Big[\lambda\big(\theta,\; D \cup \{(x, Y_x)\}\big)\Big].$$

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Algorithm: MPS $(\pi^{\mathrm{PS}}_{\mathrm{M}})$

- Set $D_0 \leftarrow$ initial data.
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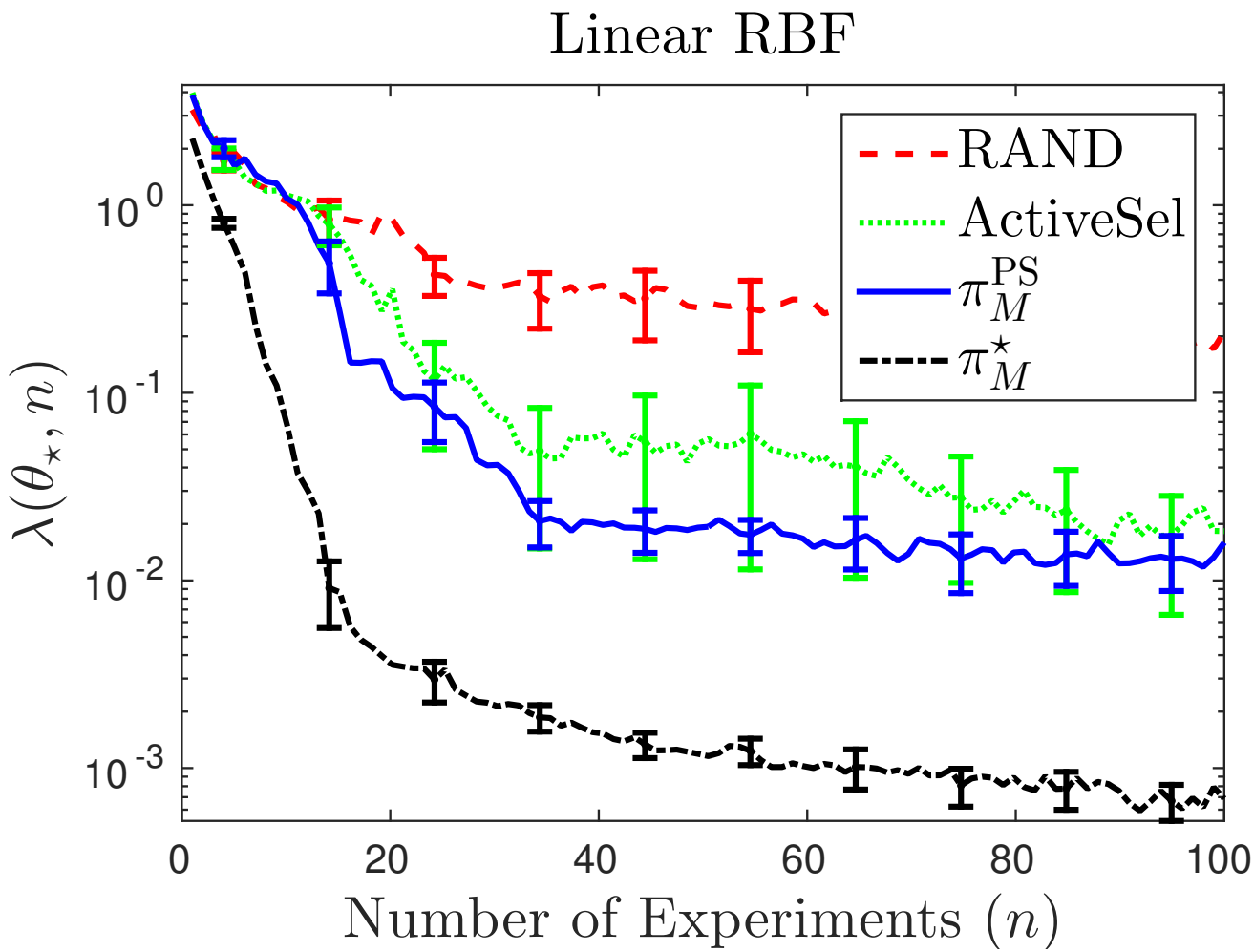
N.B: When the goal is optimisation, this reduces to exactly Thompson sampling.

Experiment: Active Learning

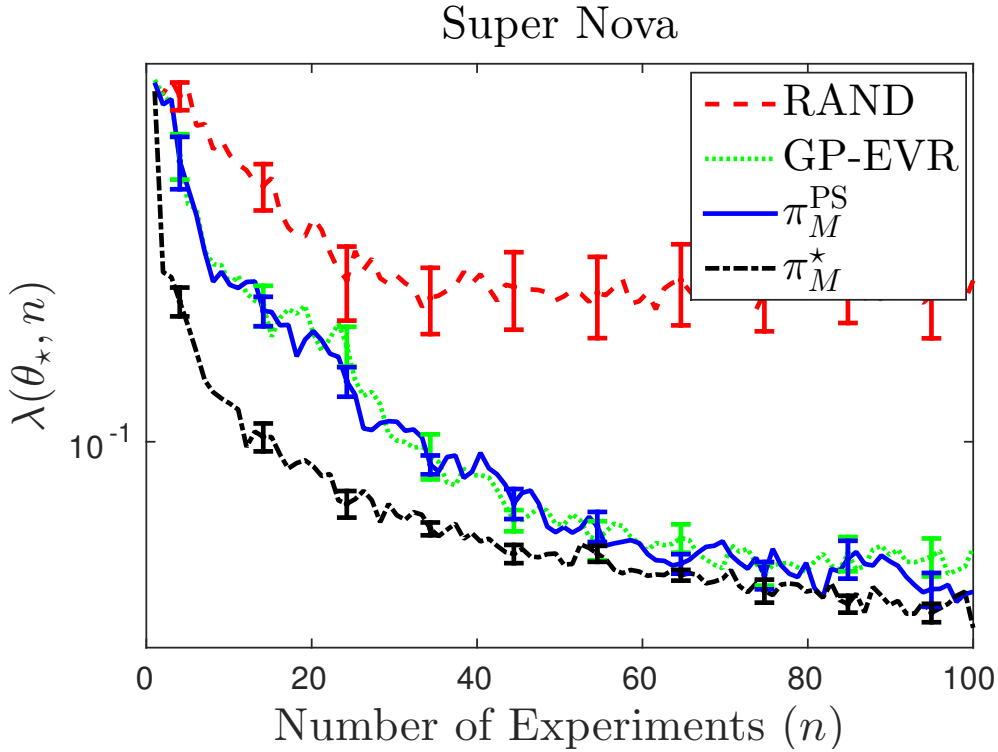


ActiveSel: (Chaudhuri et al. 2015)

Experiment: Posterior Estimation in Astrophysics

Astrophysicist defines prior on Hubble constant, and dark matter fraction and dark energy fraction. Computer posterior distrbution given Type Ia supernova data Q. Likelihood computed using the Robertson-Walker metric.

$$\lambda(\theta_\star, D_n) = \|p(\tau(\theta_\star)|Q) - \hat{p}(\tau(\theta_\star)|Q)\|_2$$



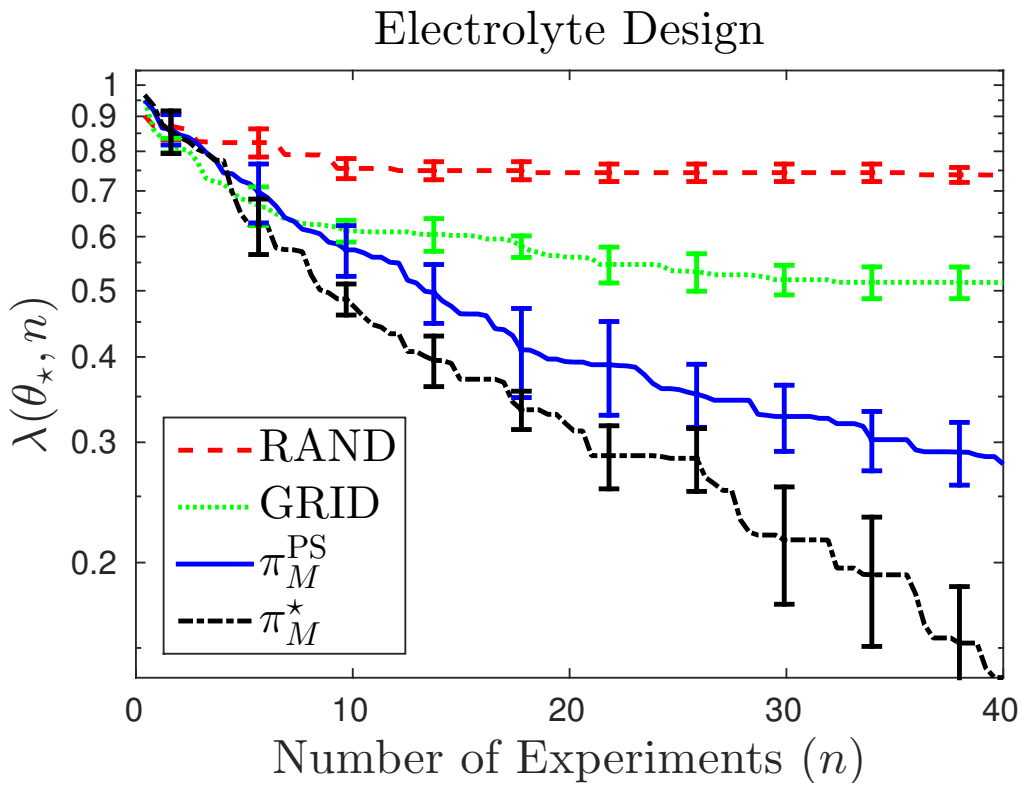
GP-EVR: (Kandasamy et al. IJCAI 2015)

Experiment: Custom goal in Electrolyte Design

An experiment measures solubility, viscosity and conductivity of an electrolyte design.

Goal: Optimise conductivity while learning solubility and viscosity.

$$\lambda(\theta_\star, D_n) = \|f_{\text{dissol}} - \hat{f}_{\text{dissol}}(D_n)\|^2 + \|f_{\text{vis}} - \hat{f}_{\text{vis}}(D_n)\|^2 + (\max f_{\text{con}} - \max_{X_t, t \le n} f_{\text{con}}(X_t)),$$



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We use ideas/conditions from

- Adaptive Submodularity
- Re-inforcement Learning
- Bandits

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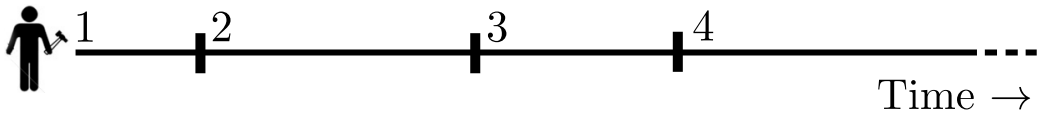
Part 3.1: Parallel Experiments

Sequential experiments with one worker



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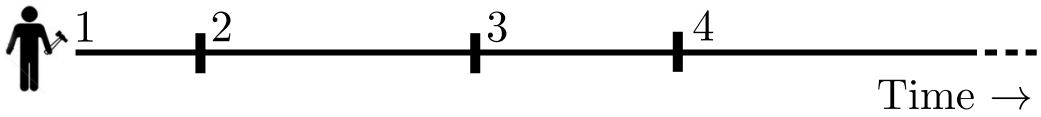
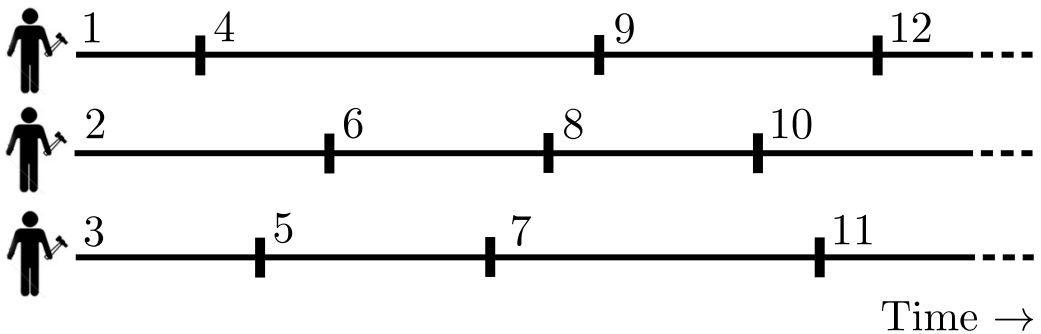


Parallel experiments with M workers (Asynchronous)



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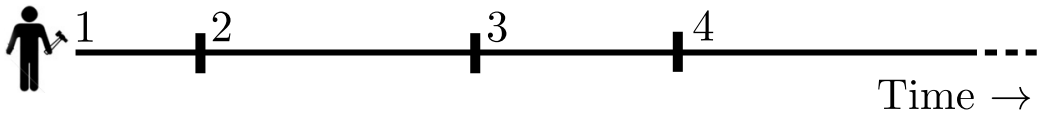

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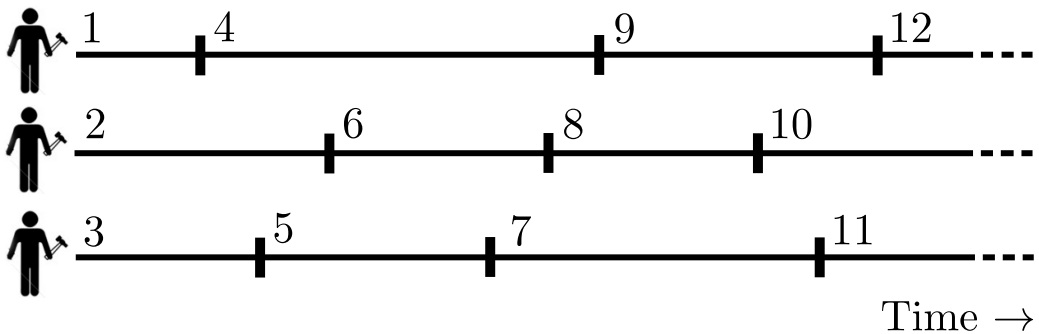
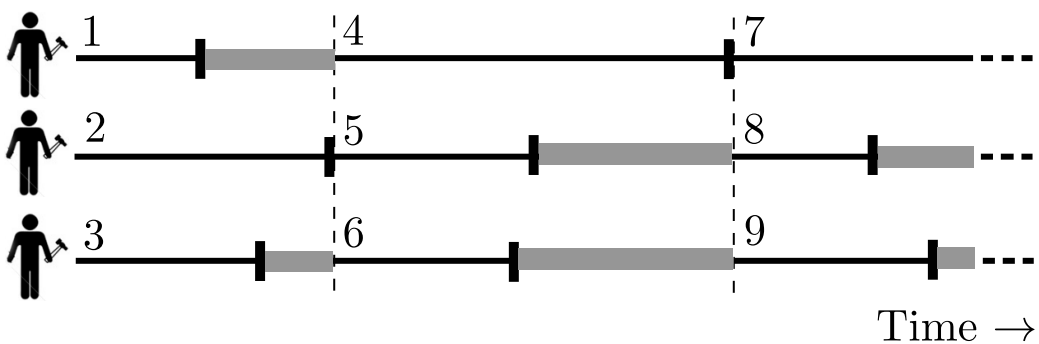


Parallel experiments with M workers (Synchronous)

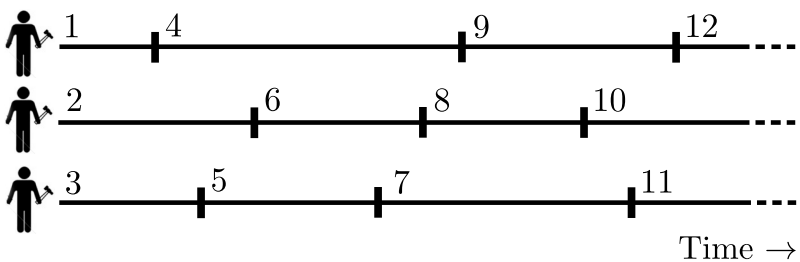


Parallelised DOE via Posterior Sampling

Asynchronous:

At any given time,

1. $(x', y') \leftarrow$ Wait for a worker to finish.
2. Update posterior for $\theta_\star$.
3. Draw a sample $\theta \sim \mathbb{P}(\theta_\star | D_t)$.
4. Re-deploy worker at $\operatorname{argmin} \lambda^+(\theta, D_t, x)$.



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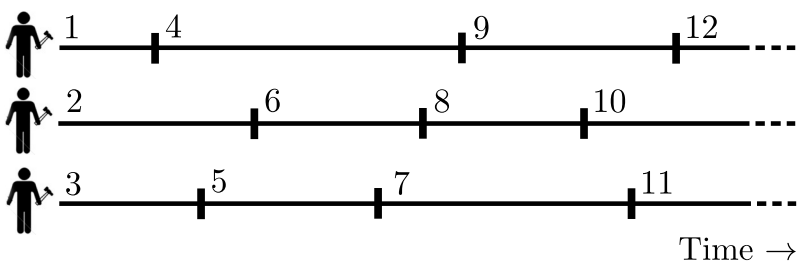
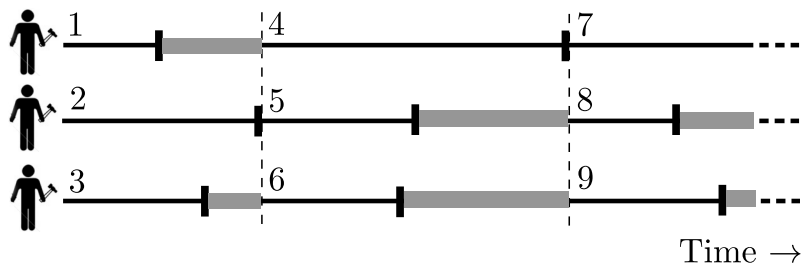


Synchronous:

At any given time,

1. $\{(x'_m, y'_m)\}_{m=1}^M \leftarrow$ Wait for all workers to finish.
2. Update posterior for $\theta_\star$.
3. Draw M samples $\theta_m \sim \mathbb{P}(\theta_\star | D_t)$, $\forall m$.
4. Re-deploy worker m at $\operatorname{argmin} \lambda^+(\theta_m, D_t, x)$.



Theory: parallel DOE via posterior sampling

Conjecture: For synchronous & asynchronous parallel DOE via posterior sampling

$$\mathbb{E}[\lambda(\theta_\star, D_n)] \lesssim \frac{M \log(M)}{n} + \text{sequential result}$$

Theorem: For parallelised Thompson samping (Black-box Optimisation) (Kandasamy et al. AISTATS 2018)

$$\mathbb{E}[f(x_\star) - \max_{t \leq n} f(x_t)] \lesssim \frac{M \log(M)}{n} + \frac{C}{\sqrt{n}}$$

Can also quantify difference between synchronous and asynchronous settings. (Kandasamy et al. AISTATS 2018)

- If evaluation times are the same, synchronous is slightly better.
- When there is high variability in evaluation times, asynchronous is much better than synchronous.

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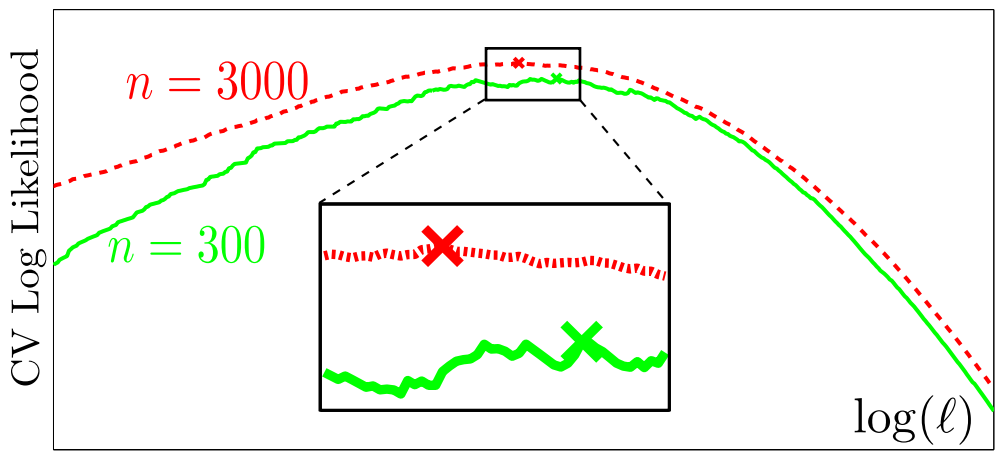
Part 2.2: Multi-fidelity Experiments

Motivating question:
What if we have cheap approximations to an experimentation?

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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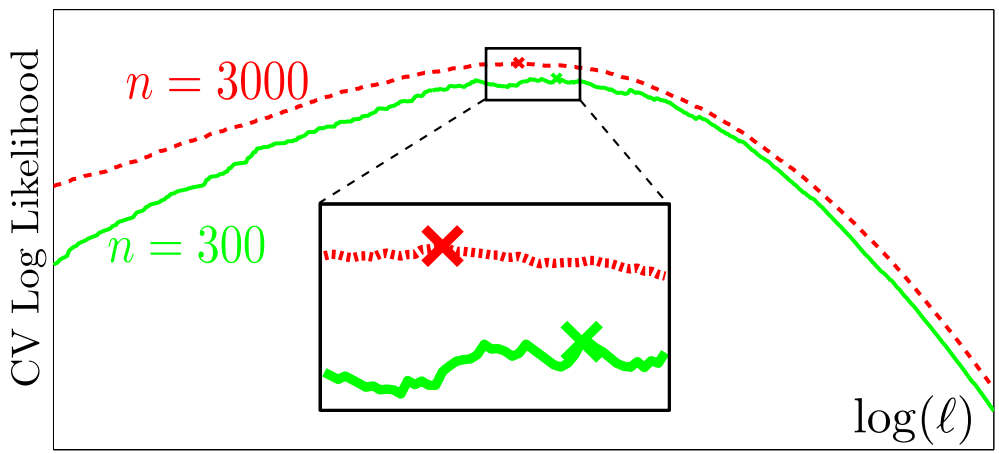
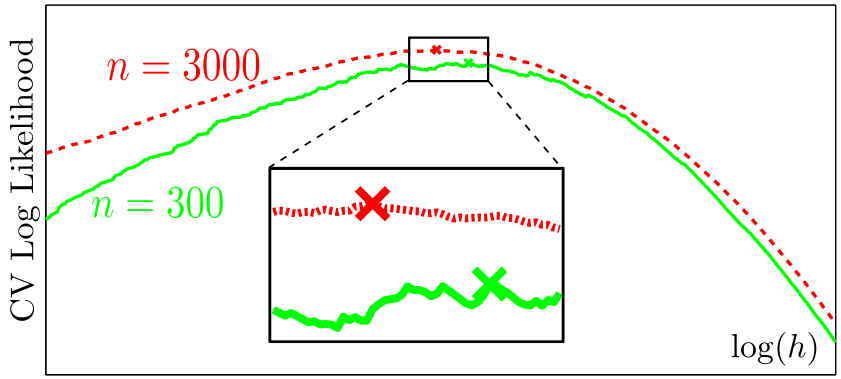


2. Computational astrophysics: cosmological simulations and numerical computations with less granularity.

3. In many applications: real world experiment vs simulation.

Multi-fidelity Hyper-parameter tuning



E.g. Train an ML model with $N_\bullet$ data and $T_\bullet$ iterations.

- But use $N < N_\bullet$ data and $T < T_\bullet$ iterations to approximate cross validation performance at $(N_\bullet, T_\bullet)$.

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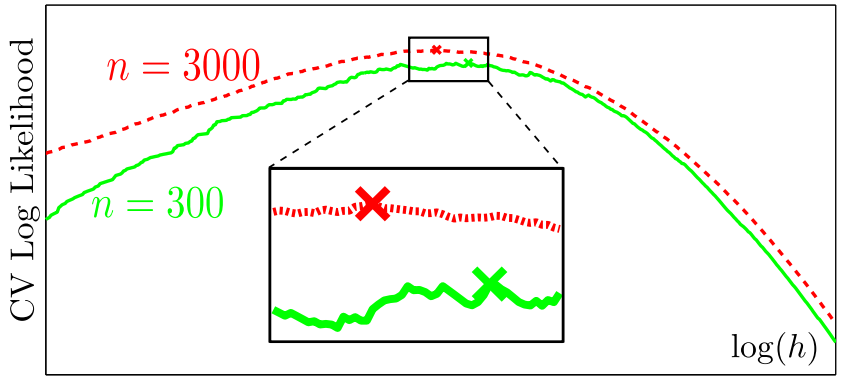

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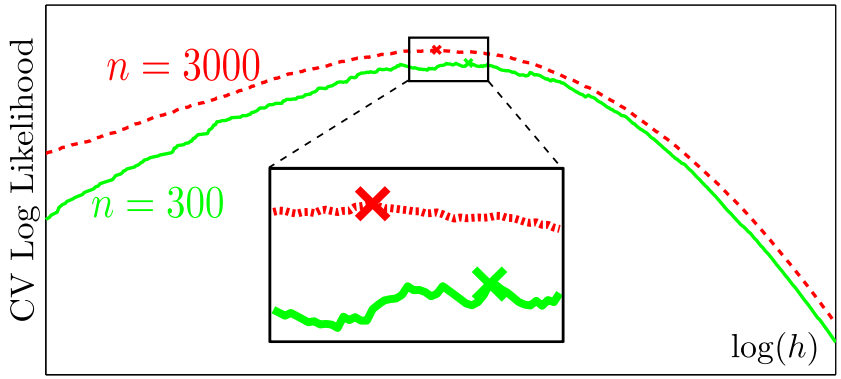

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Multi-fidelity Black-box optimisation using GPs:

(Kandasamy et al. NIPS 2016a&b, Kandasamy et al. ICML 2017,
Sen, Kandasamy et al. ICML 2018)

Multi-fidelity Optimisation

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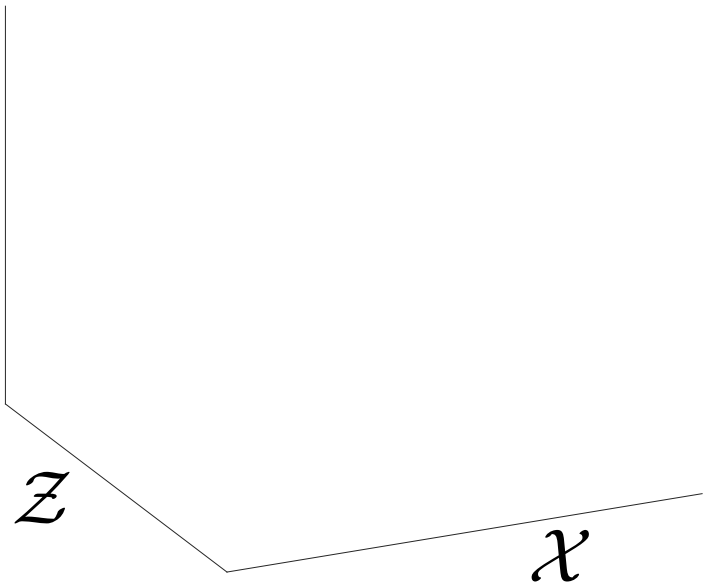

A fidelity space $\mathcal{Z}$ and domain $\mathcal{X}$

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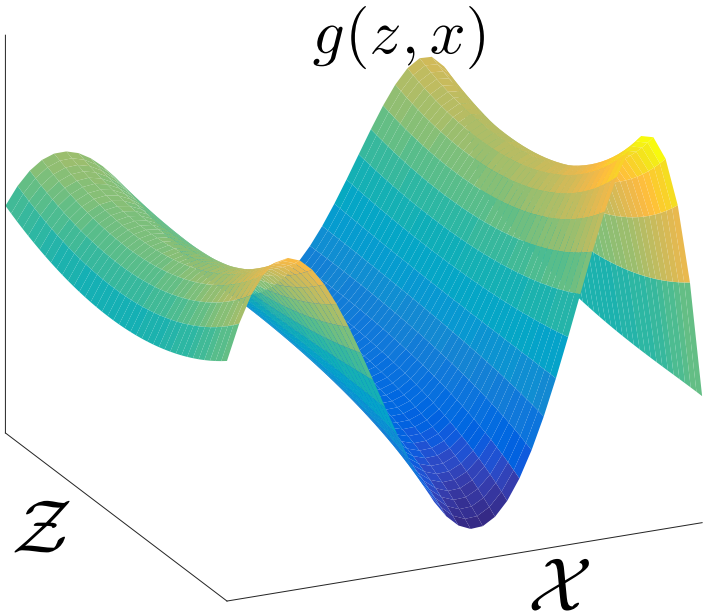

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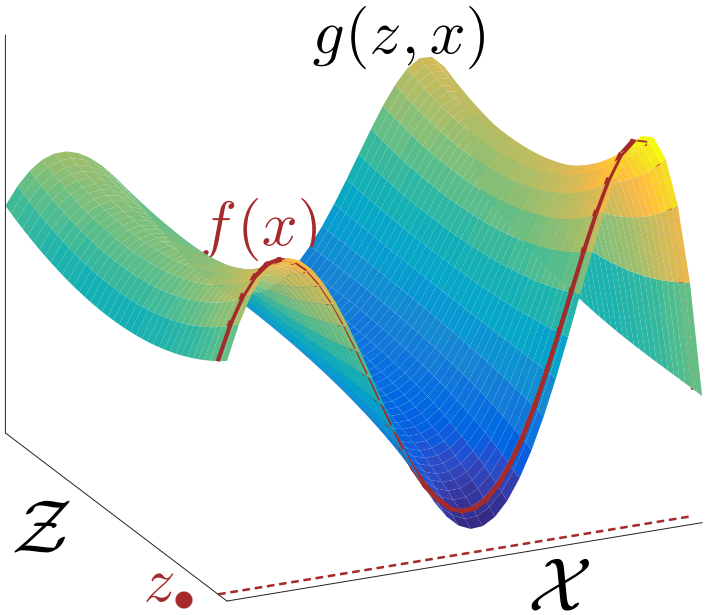

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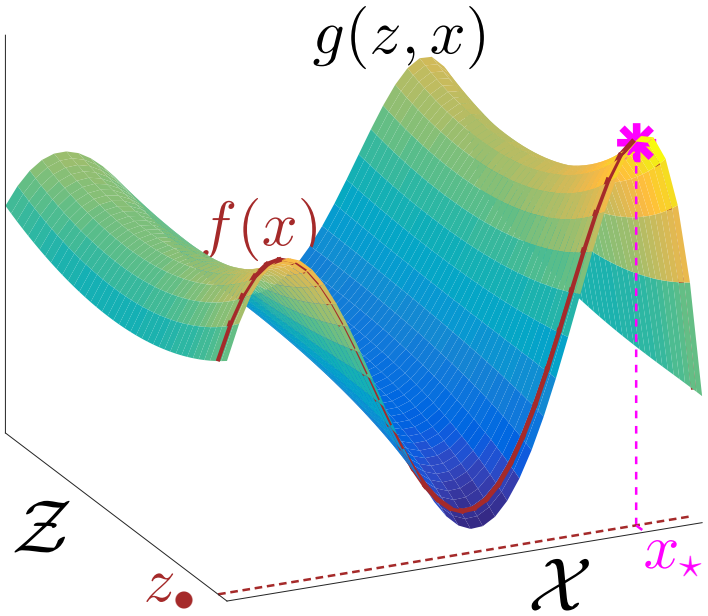

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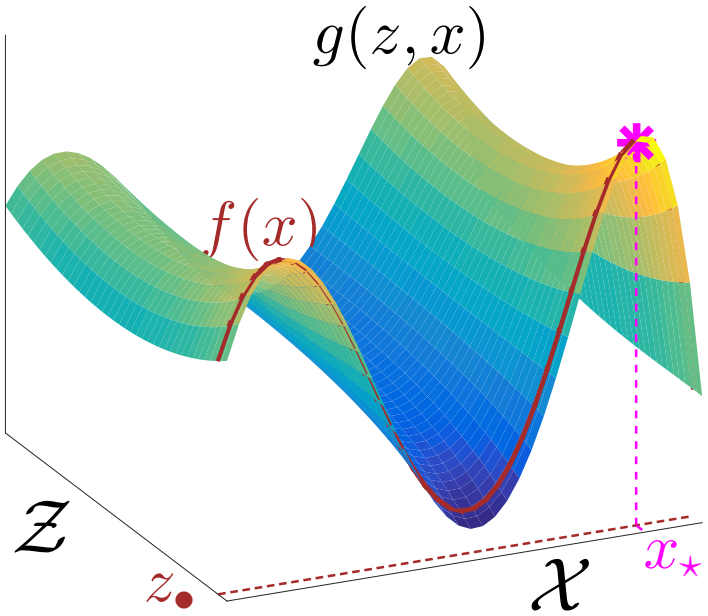

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A cost function, $\gamma : \mathcal{Z} \rightarrow \mathbb{R}_+$. $\gamma(z) = \gamma(N, T) = \mathcal{O}(N^2 T)$ (say).

Algorithms

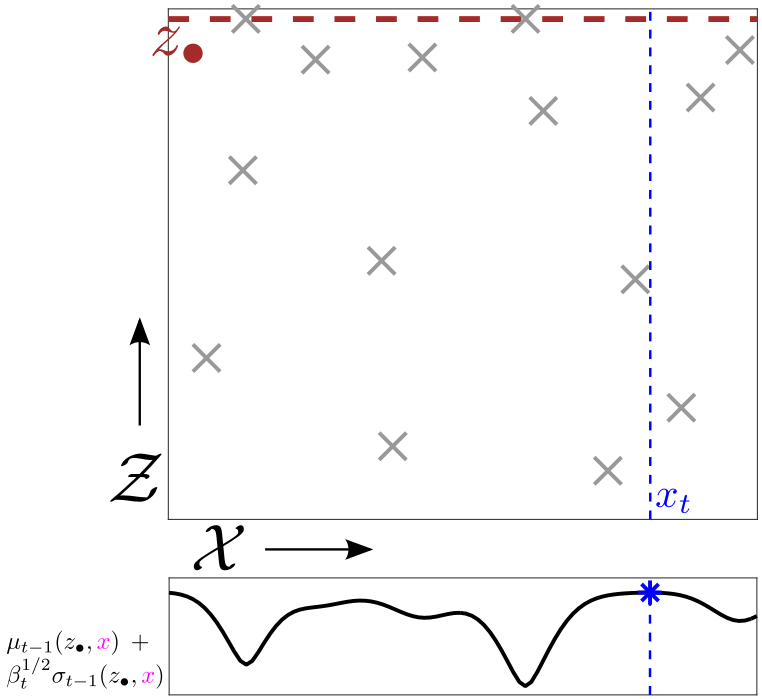
- Finite number of approximations: MF-GP-UCB
  (Kandasamy et al. NIPS 2016b)
- Continuous approximations: BOCA
  (Kandasamy et al. ICML 2017)

Key intuition in both algorithms

- By default, will evaluate at the low (cheap) fidelities.
- Proceed to higher (expensive) fidelities when there is a good information to cost trade-off.

Algorithm: BOCA

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

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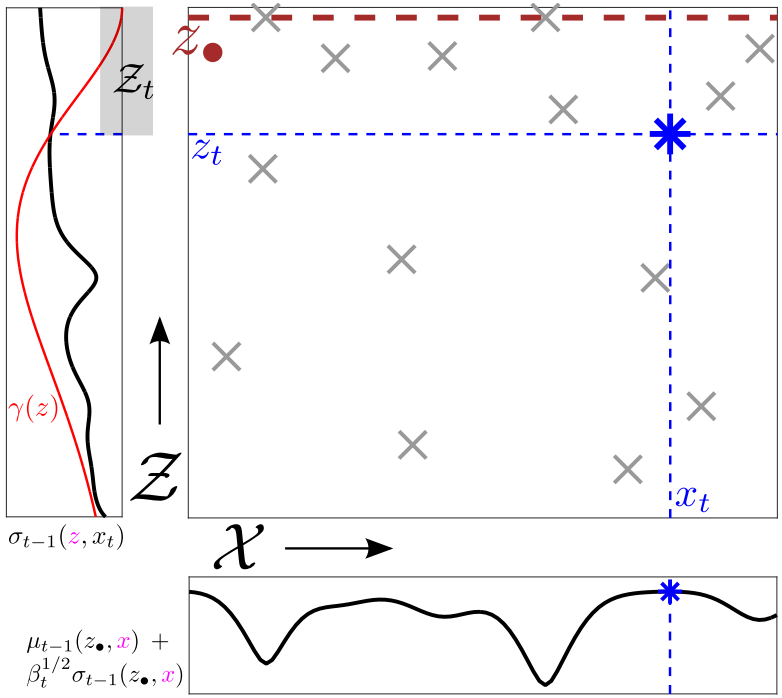

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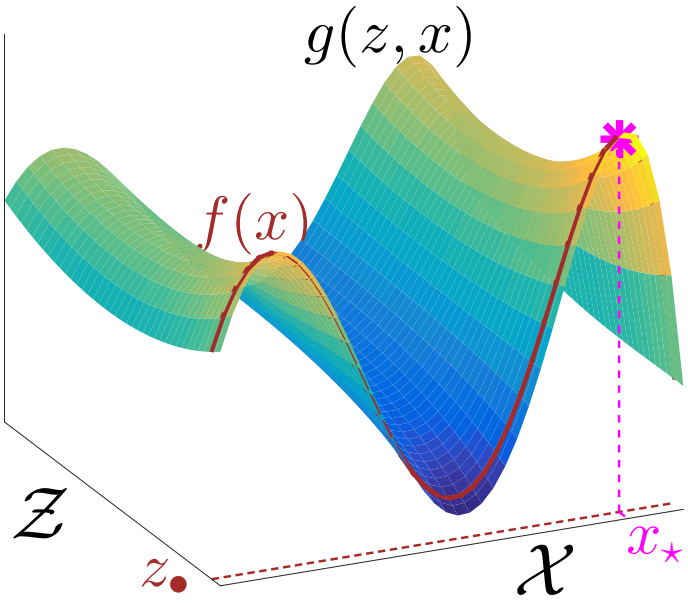
$$x_t = \operatorname*{argmax}_{x \in \mathcal{X}} \mu_{t-1}(z_\bullet, x) + \beta_t^{1/2}\sigma_{t-1}(z_\bullet, x)$$

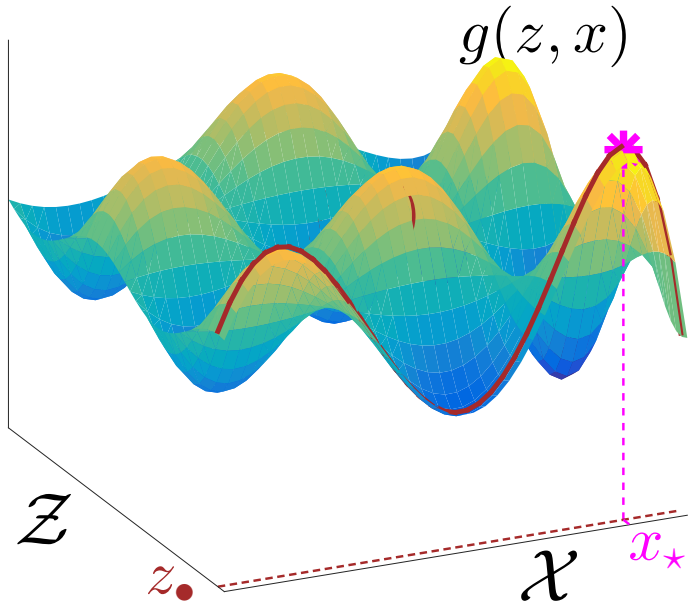
(2) $$\mathcal{Z}_t \approx \{z_\bullet\} \cup \left\{ z : \sigma_{t-1}(z, x_t) \geq \gamma(z) = \left(\frac{\gamma(z)}{\gamma(z_\bullet)}\right)^q \xi(z) \right\}$$

(3) $$z_t = \operatorname*{argmin}_{z \in \mathcal{Z}_t} \gamma(z) \qquad \text{(cheapest } z \text{ in } \mathcal{Z}_t\text{)}$$

Theoretical Results for BOCA



"good"



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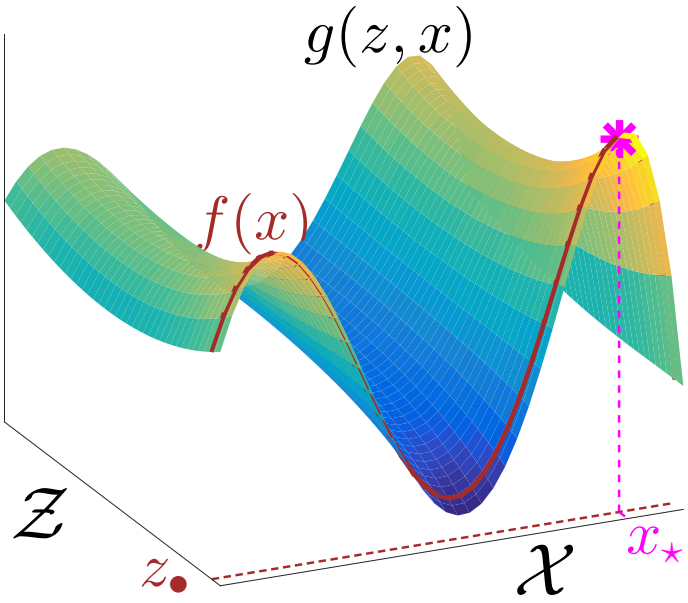

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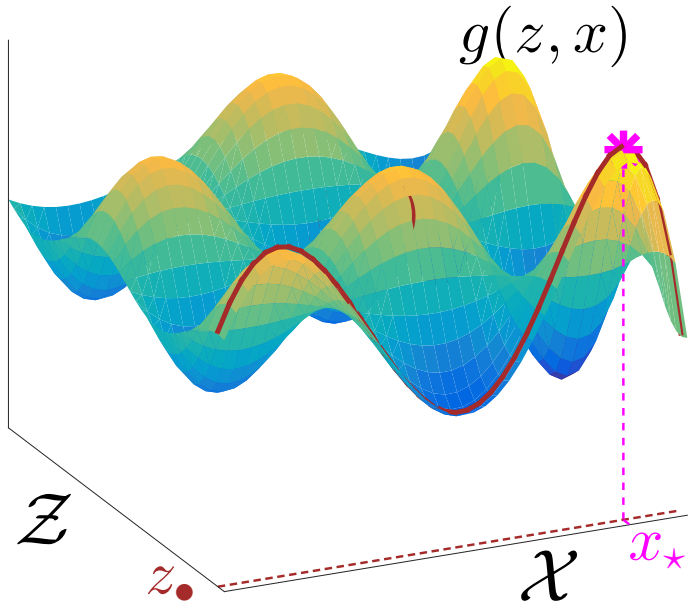

"bad"

Theorem: (Informal) (Kandasamy et al. ICML 2017)
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).

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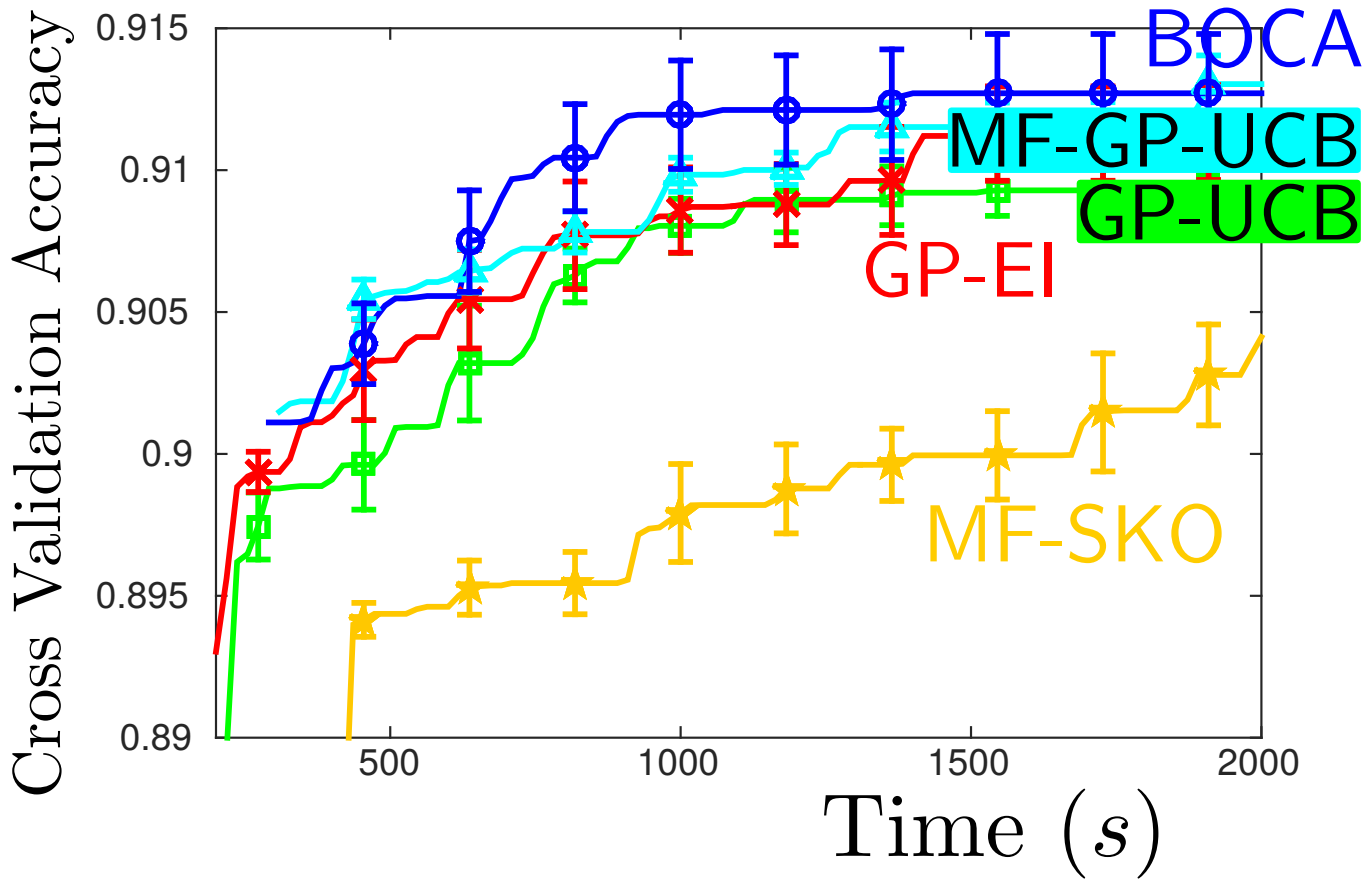

Experiment: Cosmological inference on Type-1a supernovae data

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 $G_\bullet = 10^6$.
Approximate with $N \in [50, 192]$ or $G \in [10^2, 10^6]$ (2D fidelity space).

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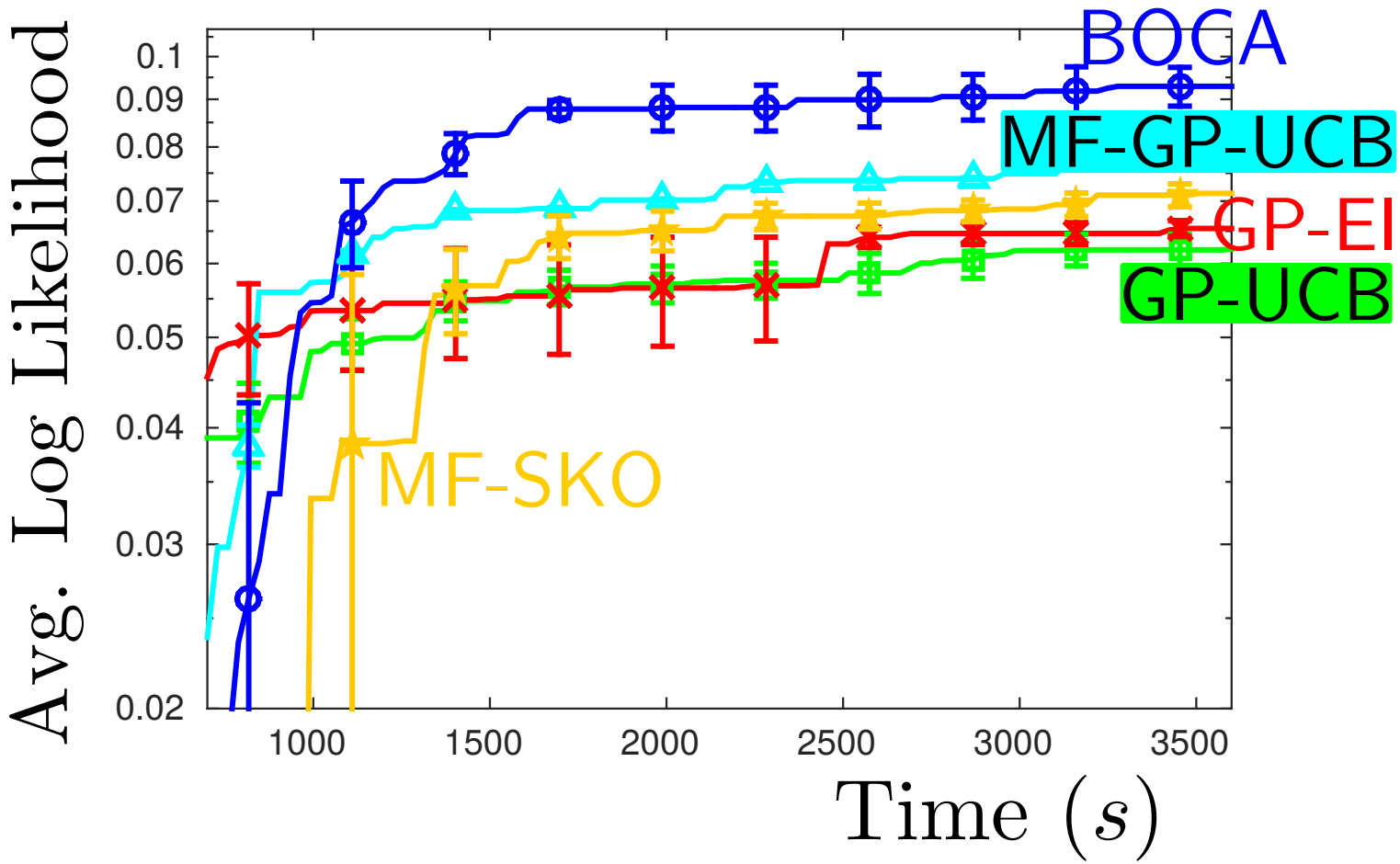

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E.g. Tuning a machine learning model with several hyper-parameters

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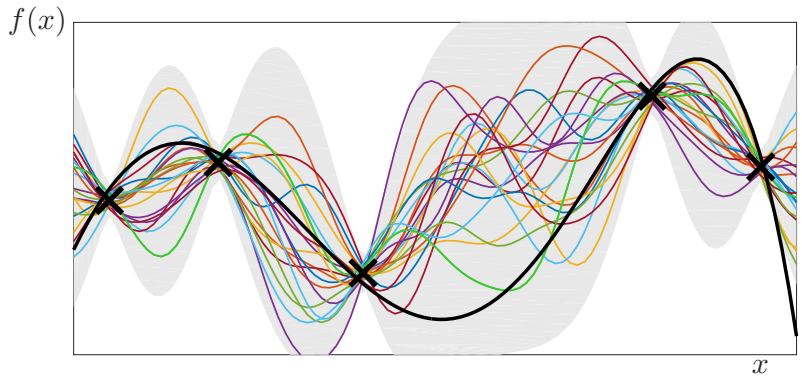

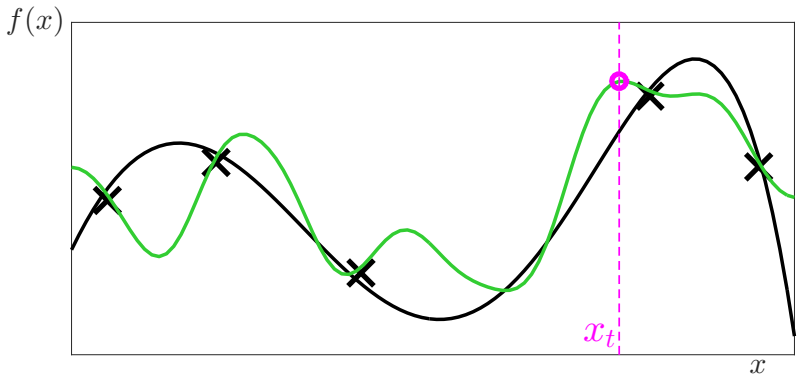

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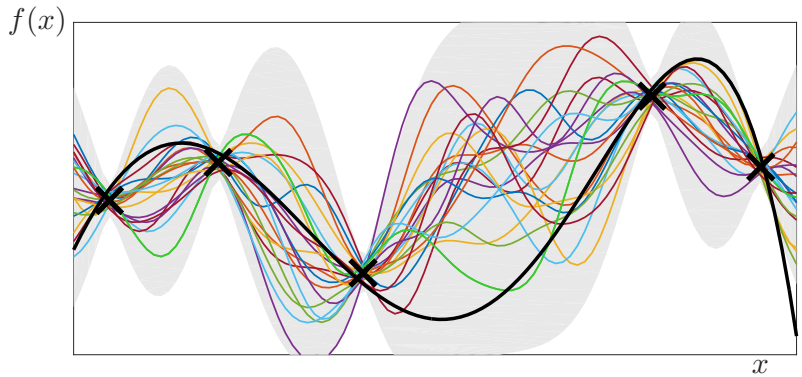

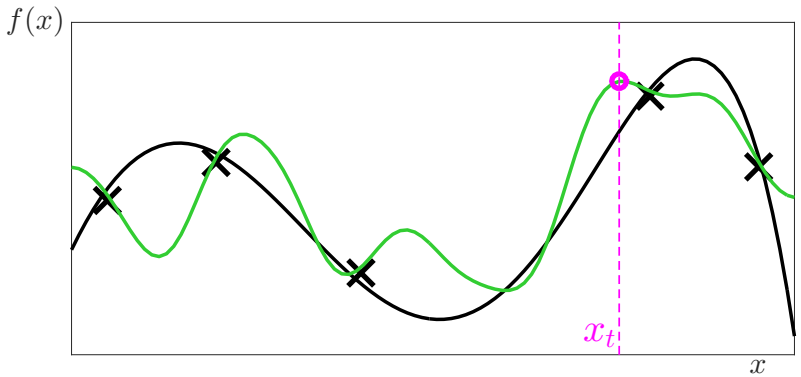

1. **Statistical Difficulty:** estimating a high dimensional GP.
2. **Computational Difficulty:** maximising a high dimensional acquisition (e.g. sample or UCB) φ_t.

Additive Models for High Dimensional BO

(Kandasamy et al. ICML 2015)

Structural assumption:

$$f(x) = f^{(1)}(x^{(1)}) + f^{(2)}(x^{(2)}) + \ldots + f^{(M)}(x^{(M)}).$$

$x^{(j)} \in \mathcal{X}^{(j)} = [0,1]^p, \qquad p \ll d, \qquad x^{(i)} \cap x^{(j)} = \varnothing.$

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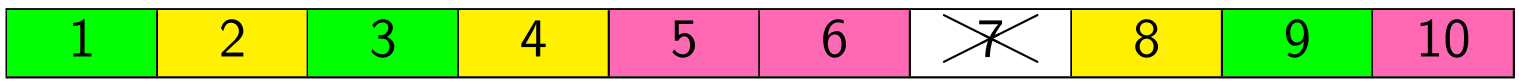
E.g. $f(x_{\{1,\ldots,10\}}) = f^{(1)}(x_{\{1,3,9\}}) + f^{(2)}(x_{\{2,4,8\}}) + f^{(3)}(x_{\{5,6,10\}})$.



Call $\{\mathcal{X}^{(j)}{}_{j=1}^{M}\} = \{(1,3,9),(2,4,8),(5,6,10)\}$ the "decomposition".

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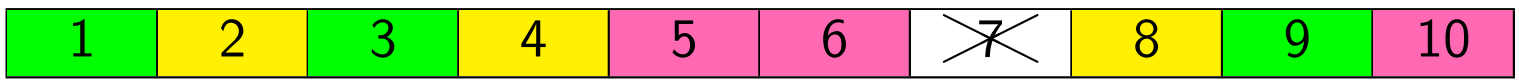

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Advantages:

- Statistical: Better bias-variance trade-offs in high dimensions.
- Computational: Easy to maximise acquisition and choose x_t.

Add-GP-UCB

(Kandasamy et al. ICML 2015)

Upper Confidence Bound:

$$\varphi_t(x) = \sum_{j=1}^{M} \underbrace{\mu_{t-1}^{(j)}(x^{(j)}) + \beta_t^{1/2}\sigma_{t-1}^{(j)}(x^{(j)})}_{\widetilde{\varphi}_t^{(j)}(x^{(j)})}.$$

Maximise each $\widetilde{\varphi}_t^{(j)}$ separately.

Requires only $\mathcal{O}(\mathrm{poly}(d)\epsilon^{-p})$ effort (vs $\mathcal{O}(\epsilon^{-d})$ for GP-UCB).

Additive models can still be useful in non-additive settings

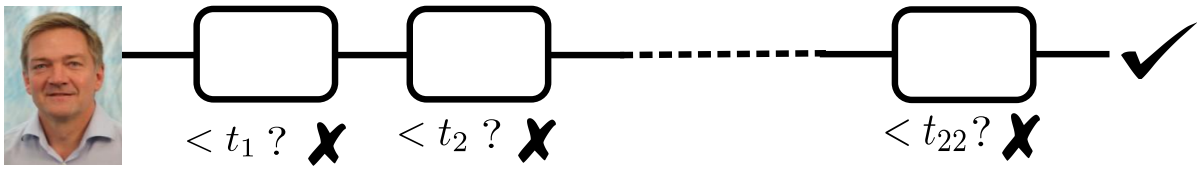
- Additive models common in high dimensional regression.
  E.g.: Backfitting, MARS, COSSO, RODEO, SpAM etc.
  (Friedman '91, Lin et al. '06, Lafferty et al '05, Ravikumar et al. '09)
- Additive models are *statistically* simpler $\implies$ worse bias, but much better variance in low sample regime.
- In bandit applications queries are *expensive*. So we usually cannot afford many queries.

- **Observation:**
  Add-GP-UCB does well even when f is not additive.
  - Better bias/ variance trade-off in estimating the GP.
  - Easy to maximise upper confidence bound.

Experiment: Viola & Jones Face Detection

A cascade of 22 weak classifiers.

Image classified negative if the score $<$ threshold at any stage.



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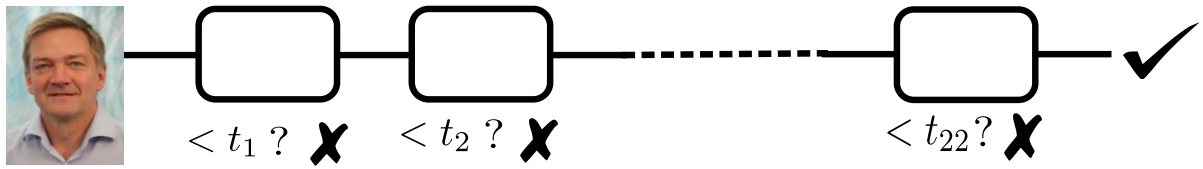

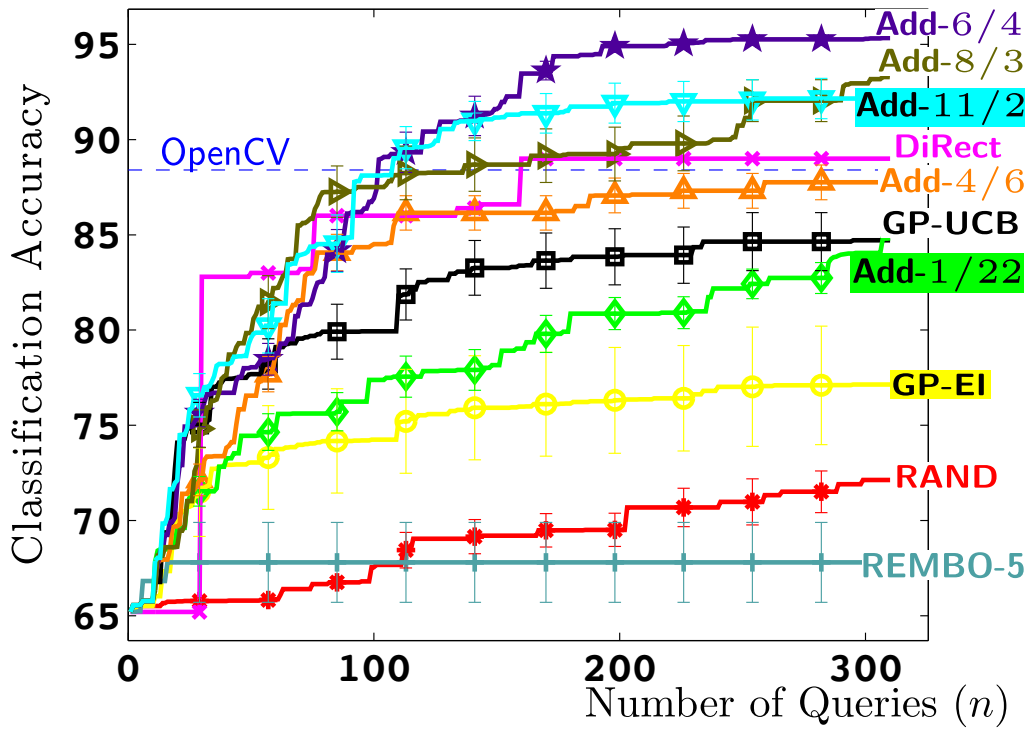

In the paper we go up to $>$ 100 dimensions.

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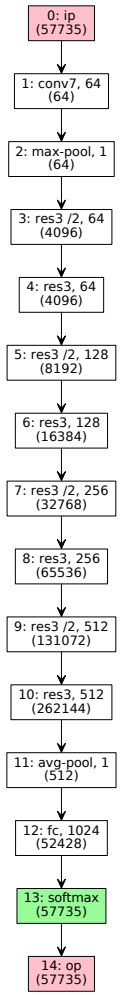
Part 3.4: Tuning Neural Network Architectures



Feedforward network

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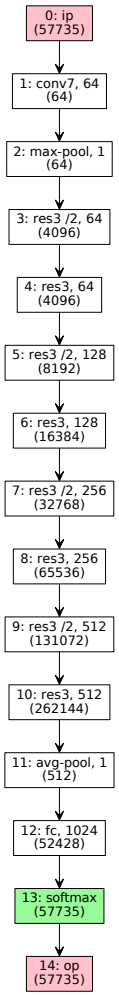

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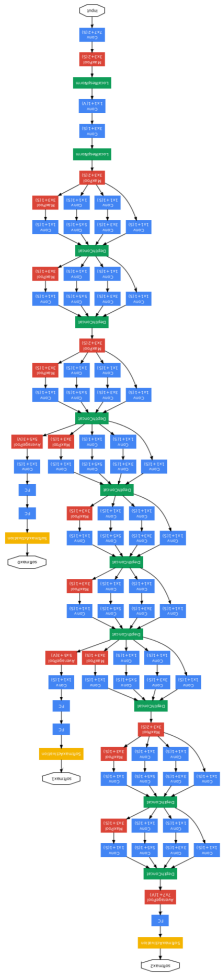

GoogLeNet

(Szegedy et al. 2015)

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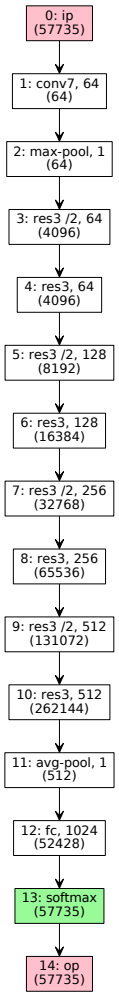

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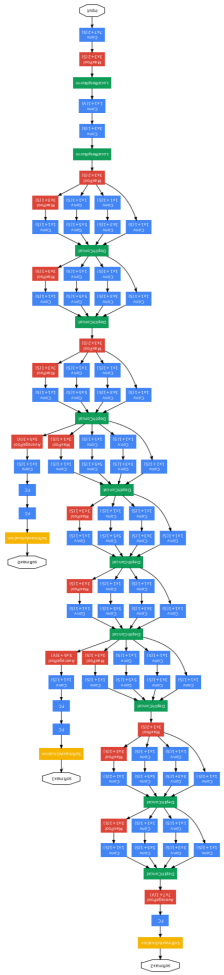

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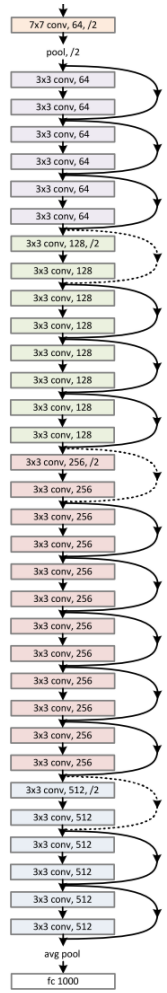

ResNet (He et al. 2016)

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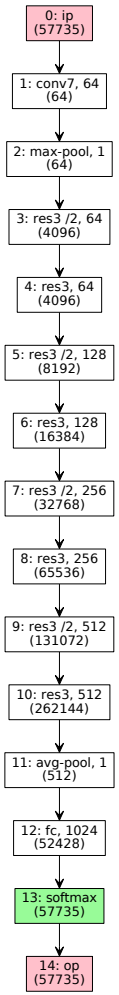

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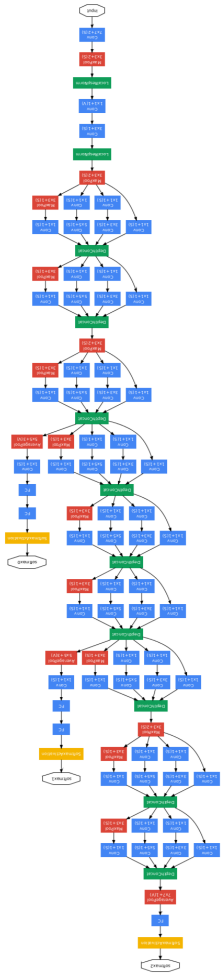

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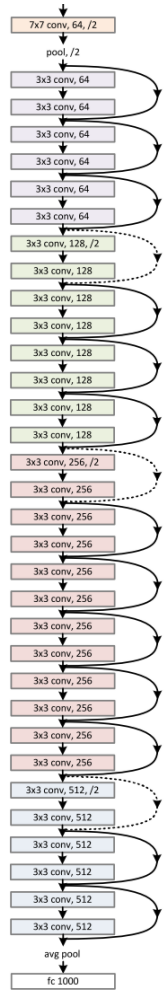

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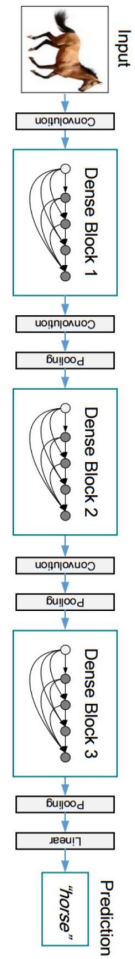

DenseNet (Huang et al. 2017)

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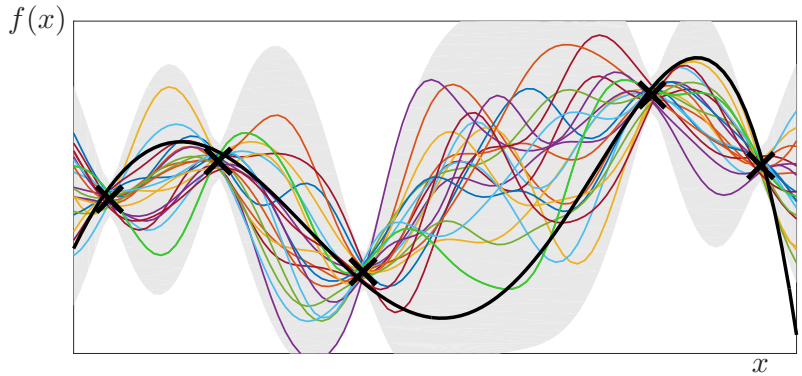
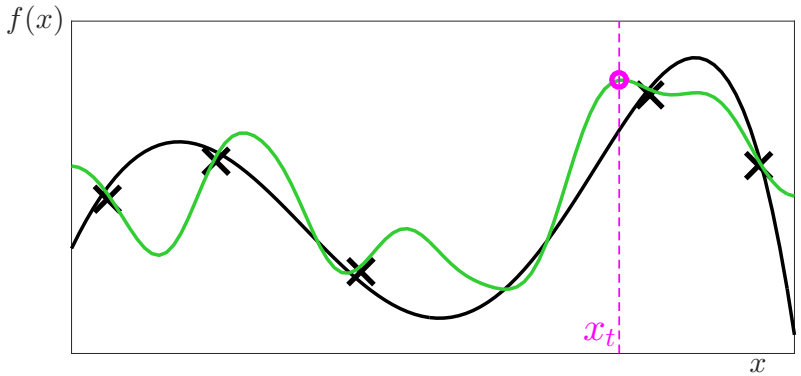
At each time step





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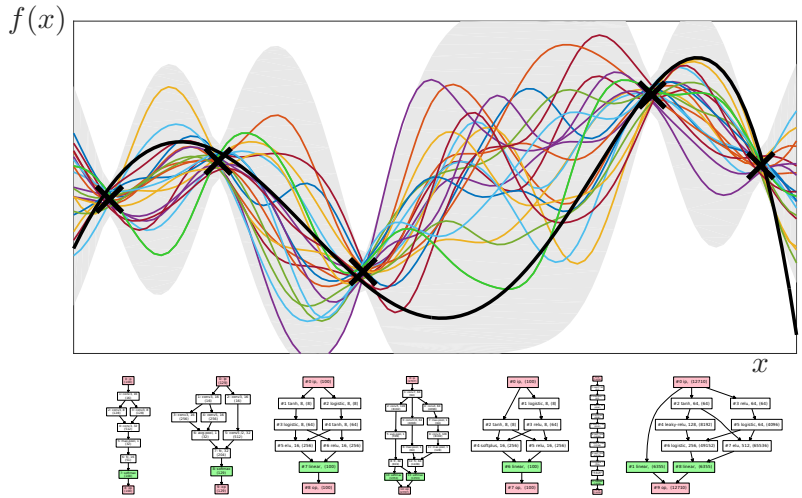

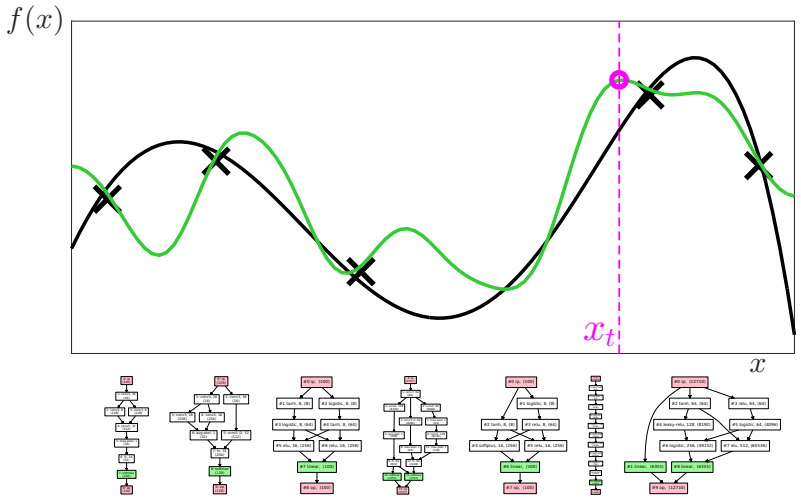

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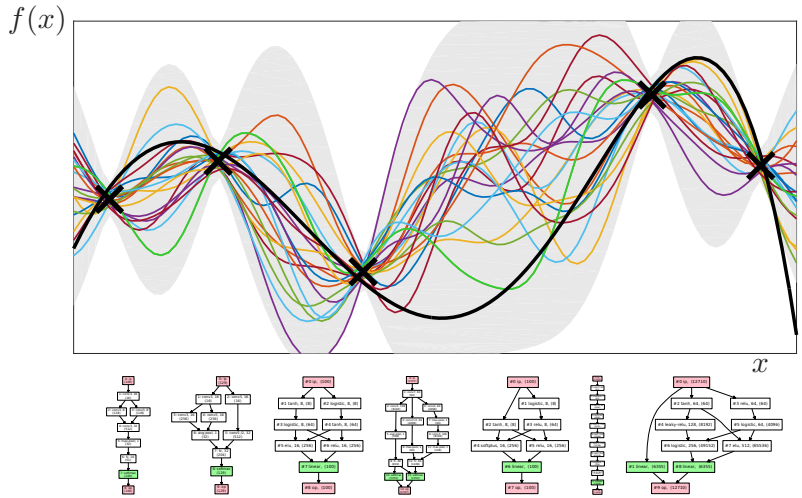
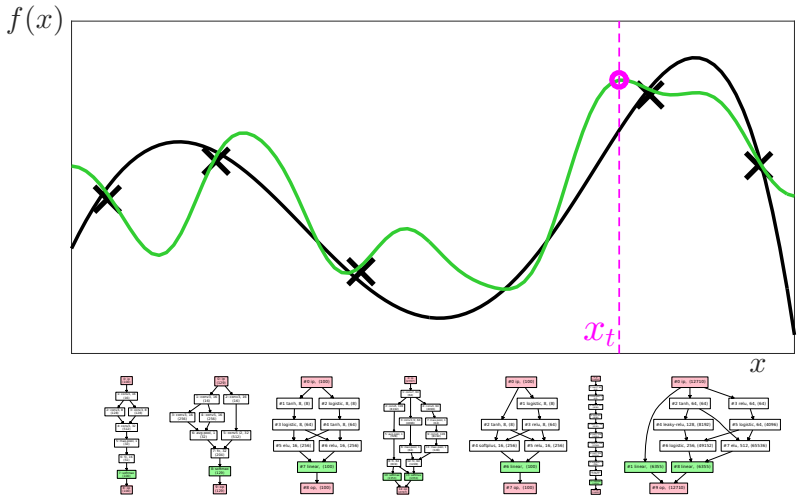




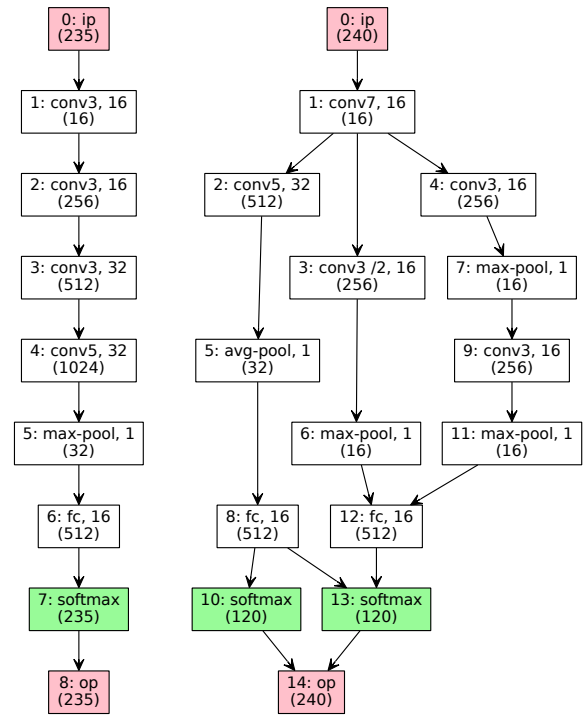
Main challenges

- Define a distance between neural network architectures.
- Optimise φ_t on the space of neural networks.

OTMANN: A distance between Neural Architectures

(Kandasamy et al. Arxiv 2018)

Key idea: To compute distance between architectures G_1, G_2, match computation in layers in G_1 to G_2.



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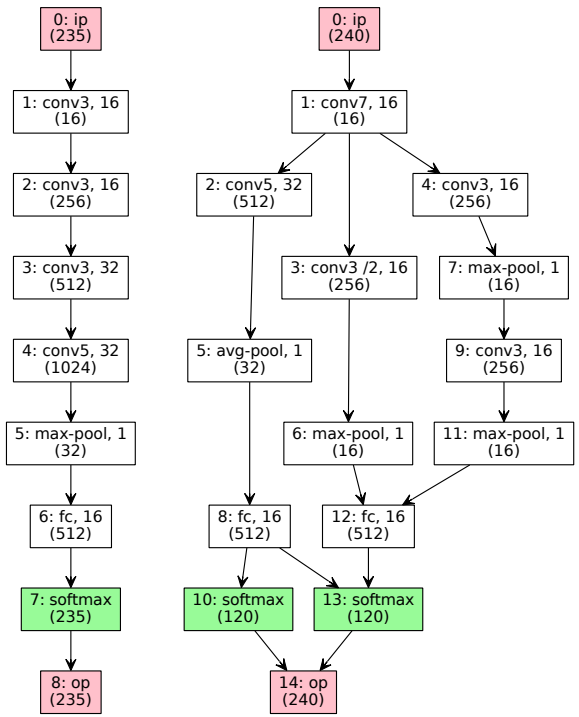

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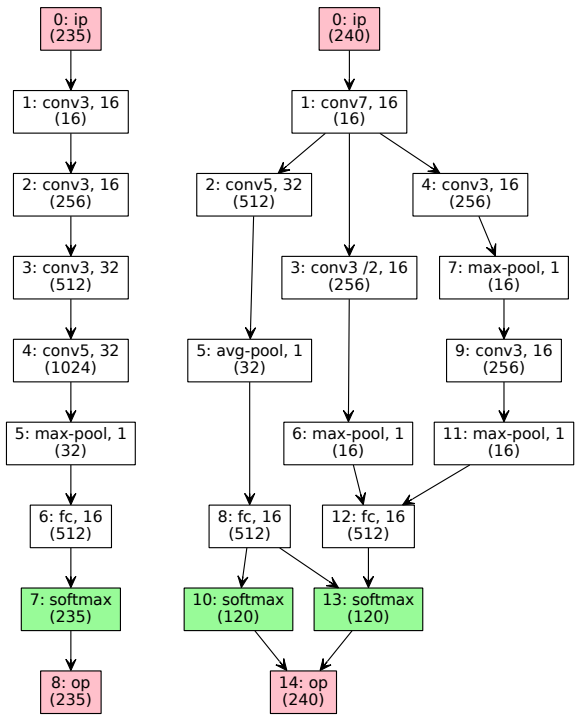
Minimise $\quad \phi_{\text{lmm}}(Z) + \phi_{\text{str}}(Z) + \phi_{\text{nas}}(Z)$

$\phi_{\text{lmm}}(Z)$: label mismatch penalty

$\phi_{\text{str}}(Z)$: structural penalty

$\phi_{\text{nas}}(Z)$: non-assignment penalty



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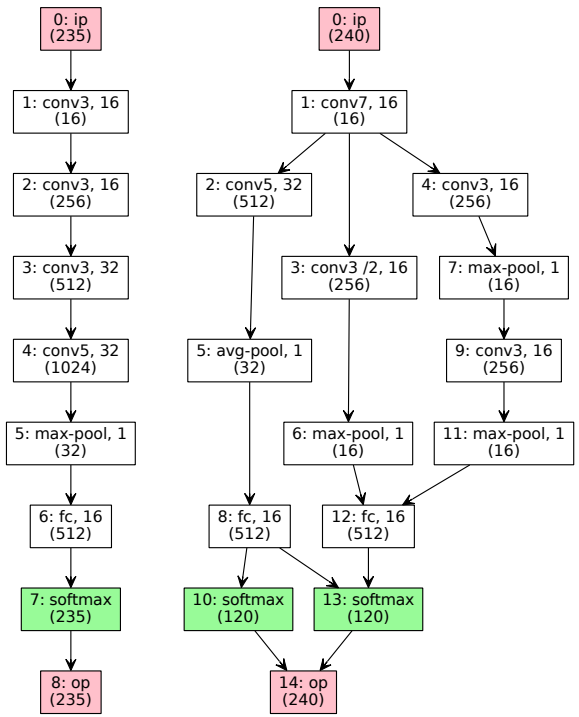

Can prove that the solution is a distance.

Optimising the sample from the posterior

Via an evolutionary algorithm.

Operation	Description
dec_single	Pick a layer at random and decrease the number of units by $1/8$.
dec_en_masse	Pick several layers at random in topological order and decrease the number of units by $1/8$ for all of them.
inc_single	Pick a layer at random and increase the number of units by $1/8$.
inc_en_masse	Pick several layers at random in topological order and increase the number of units by $1/8$ for all of them.
dup_path	Pick a random path $u_1, u_2, \ldots, u_{k-1}, u_k$, duplicate layers $u_2, \ldots, u_{k-1}$ and connect them to u_1 and u_k.
remove_layer	Pick a layer at random and remove it. Connect the layer's parents to its children if necessary.
skip	Randomly pick layers u, v where u is topologically before v. Add (u, v) to $\mathcal{E}$.
swap_label	Randomly pick a layer and change its label.
wedge_layer	Randomly remove an edge (u, v) from $\mathcal{E}$. Create a new layer w and add $(u, w), (w, v)$ to $\mathcal{E}$.

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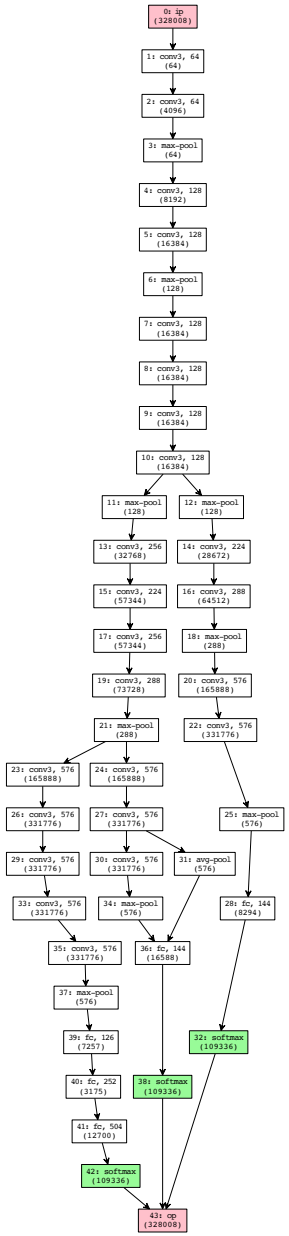
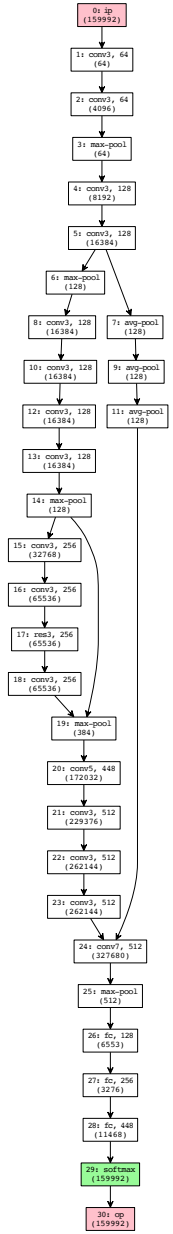
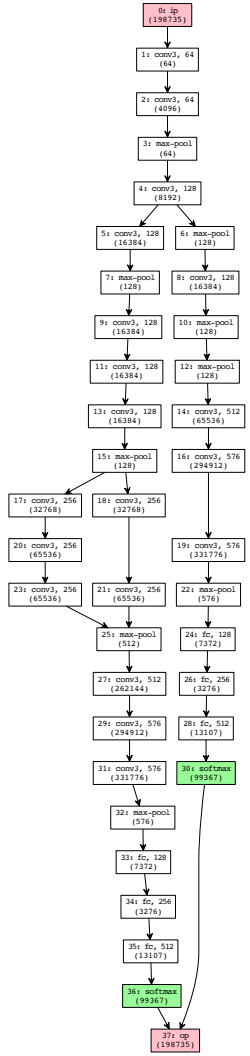
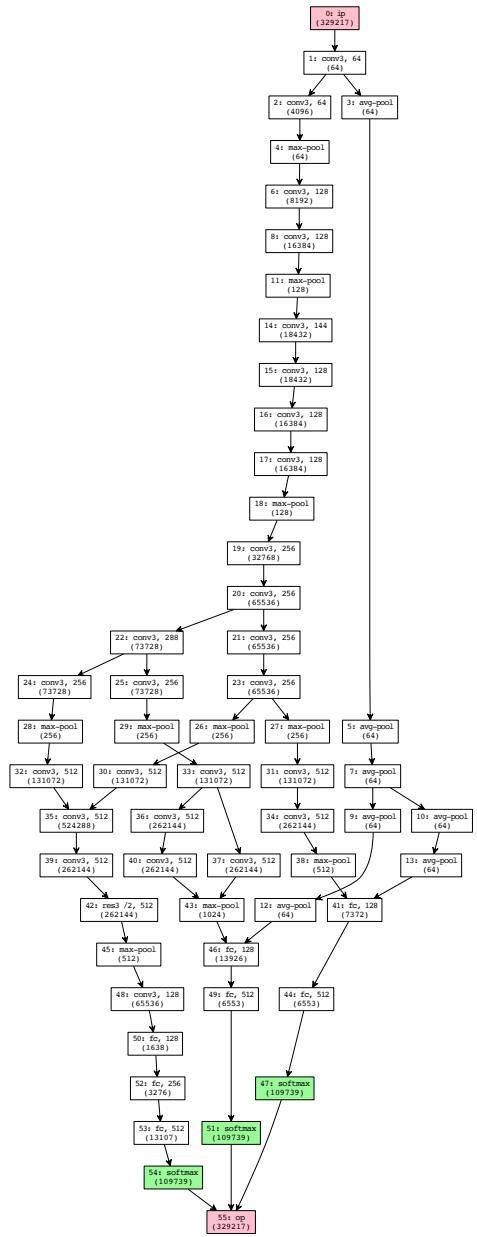
Resulting procedure: NASBOT
Neural Architecture Search with Bayesian Optimisation and Optimal Transport (Kandasamy et al. Arxiv 2018)

Architectures found on Cifar10

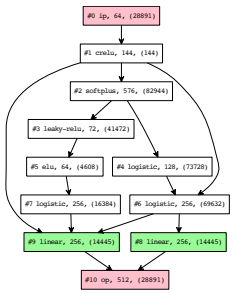


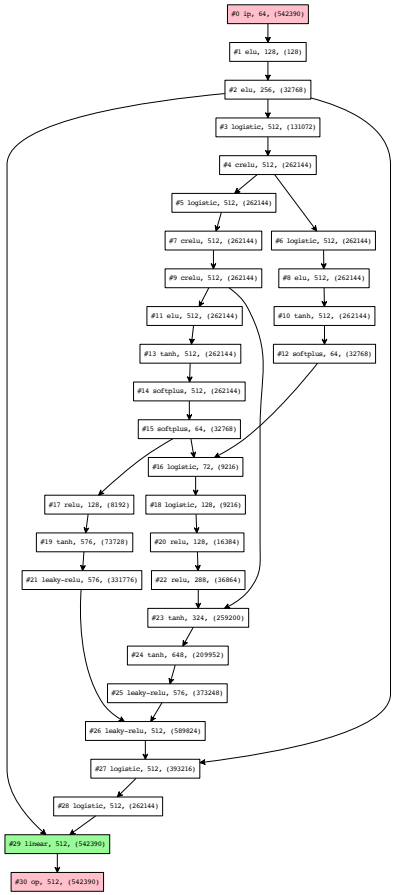


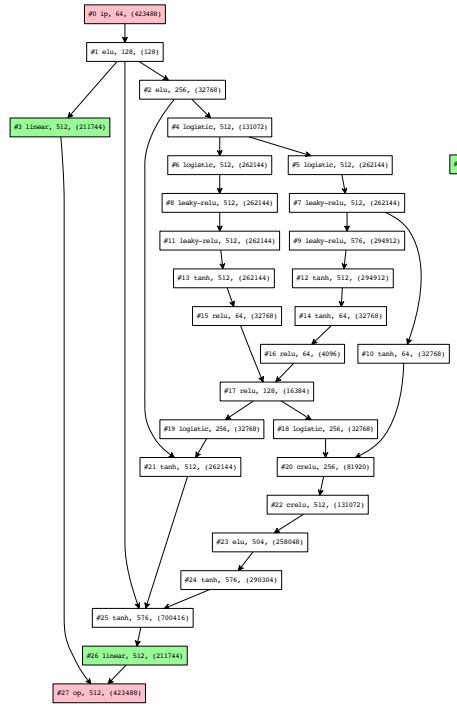


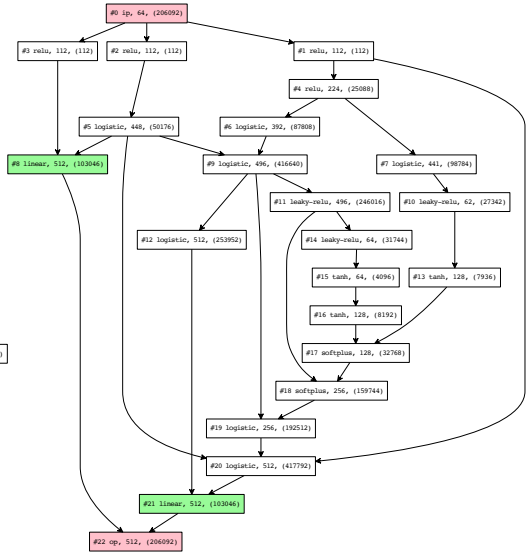


Architectures found on Indoor Location

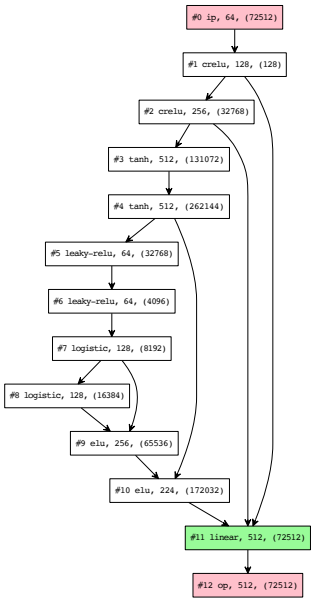


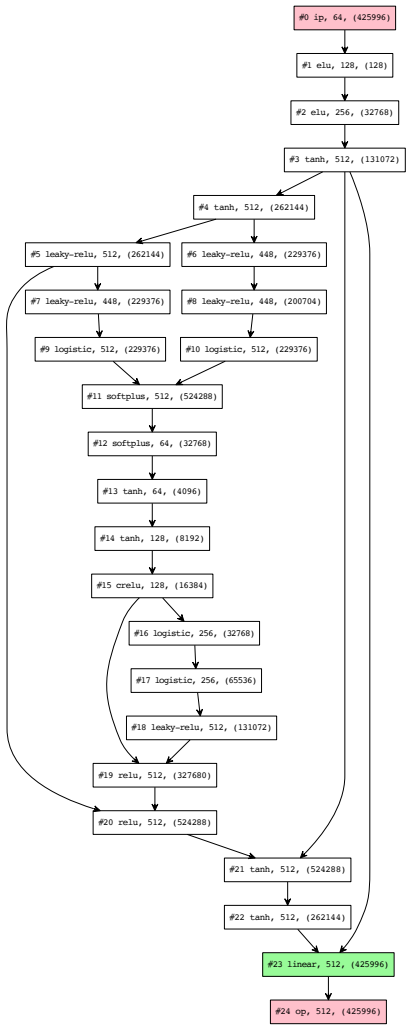


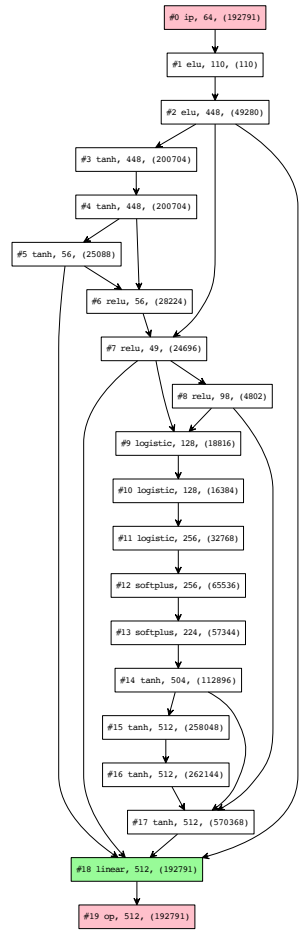


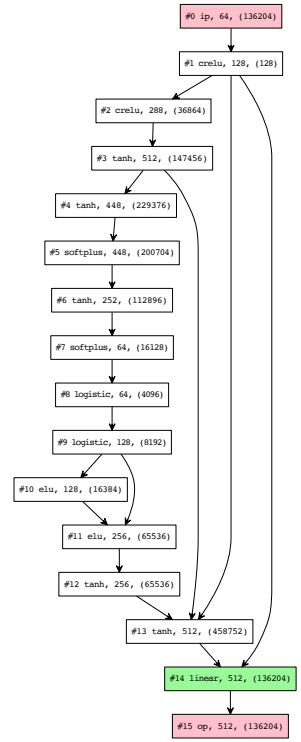


Architectures found on Slice Localisation



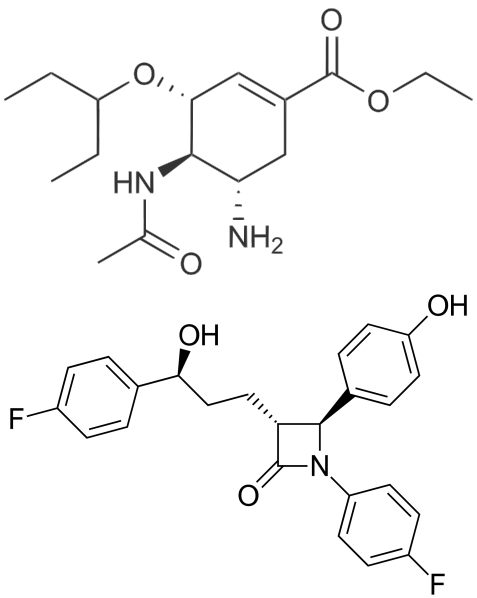




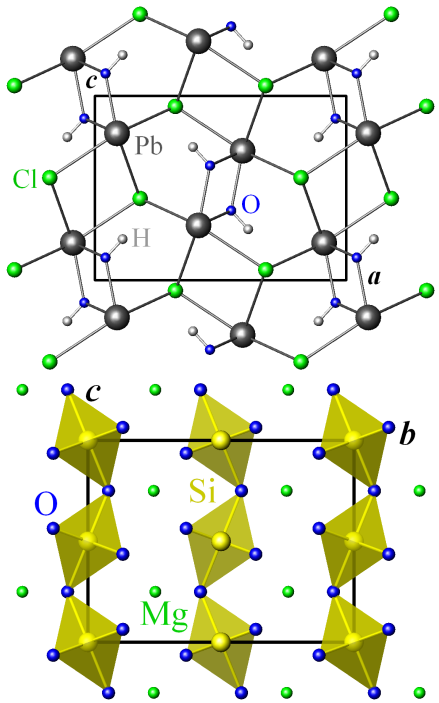


DOE on other (graphical) structures

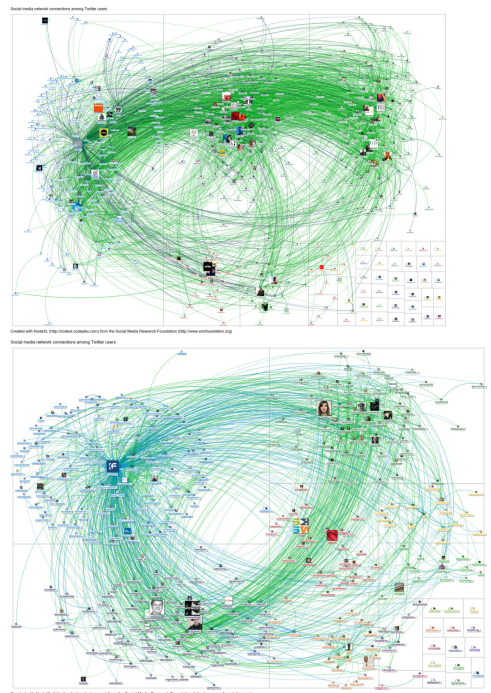
Drug Discovery with Small molecules



Crystal Structures



Social networks & viral marketing



Summary

- A framework for "goal oriented" DOE.
  - General: can achieve any desired goal.
  - Flexible: can incorporate domain expertise.
- Myopic Posterior Sampling (MPS): An algorithm for DOE inspired by Thompson sampling.
- Can be trivially parallelised.

Summary

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Scaling up DOE

- Multi-fidelity experimentation: Use cheap approximations to a an expensive experiment to speed things up.
- High dimensional DOE: Additive models have favourable statistical and computational properties.
- DOE in "complex" domains.

Outline

- Part I: Preliminaries (Black-box Optimisation)
  1. Bayesian Models
  2. Black-box Optimisation via Thompson Sampling
- Part II: DOE via posterior sampling
- Part III: Scaling up DOE (back to Black-box Optimisation)
  1. Parallelising experiments
  2. Multi-fidelity experimentation
  3. High dimensional input spaces
  4. Beyond Euclidean/categorical domains
- Part IV: ExperiML & Collaborations with LBL

What is an experiment?

An experiment is any action that has an opportunity cost attached to it.

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Examples:

1. Experiments to design/discover new materials/drugs.
2. Experiments to optimise and industrial process.
3. Personalised (contextual) experiments: online advertising, search etc.

Currently companies have to choose between two bad alternatives

Exhaustive search over restricted design space

Manual tuning by experts

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- \+ Automated.
- – Expensive testing on many poor designs.
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Value proposition: Faster & Better.
Our technology enables searching over large design spaces and identifies better designs in 10-100 times fewer trials than exhaustive search and expert tuning with significantly less effort from experts.

What we need for a collaboration

A well defined DOE problem. This includes,

- **Design variables** that can be tuned in the given problem and the constraints on each variable.
- **Experimental results.** E.g: how well did a design do on the criteria you care.
- **Goal:** What is the goal of conducting these experiments?
- **Means to experiment:** For each design, a means to conduct the experiment and obtain feedback, either in simulation or in a real system.

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In addition ...

- **Domain expertise:** Explicit models, tacit knowledge etc.
- **Past data:** Data from past experiments on this or relevant tasks.

In return, we will ...

- Execute our methods on the data/problem given.
- . . . and recommend new experiments(s) to conduct.

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- Execute our methods on the data/problem given.
- . . . and recommend new experiments(s) to conduct.
- If there is a simulation, we can run it ourselves. Otherwise, we will need your help to run experiments.


Akshay


Barnabás


Biswajit

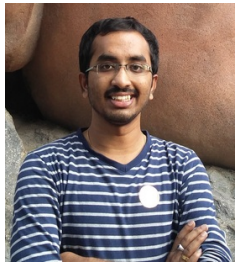

Chun-liang


Eric

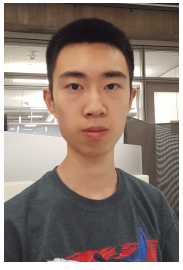

Gautam


Jeff


Junier


Karun


Rajat


Reed


Sanjay


Shalom


Shuli


Willie

CMU, University of Massachusetts Amherst, Rice University,
University of Texas Austin, Microsoft Research, ExperiML

Thank You