CSCI 699 - ProbGen

Probabilistic and Generative Models

Willie Neiswanger

Lecture 12 - Predictive UQ, Active Learning, and Bayesian Optimization

Today

Today

Lecture: Using predictive UQ models for active learning and sequential decision making, including Bayesian optimization and optimal experimental design.

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- Finish: deep uncertainty quantification.

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- Decision making under uncertainty.
- Active learning.
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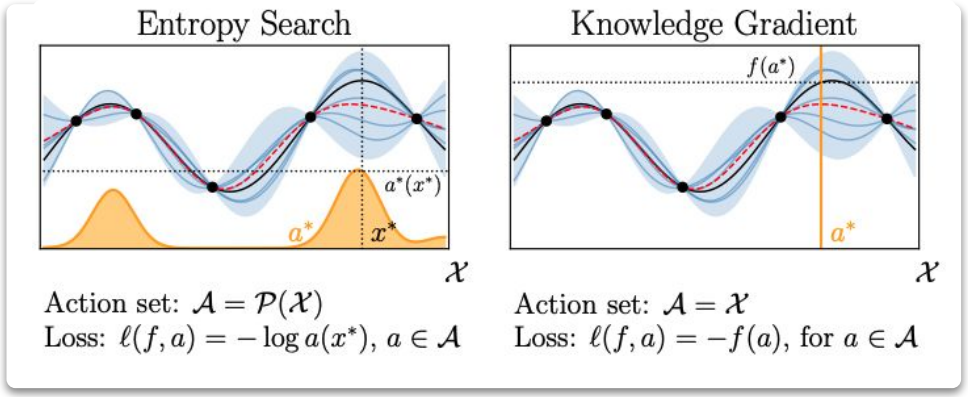
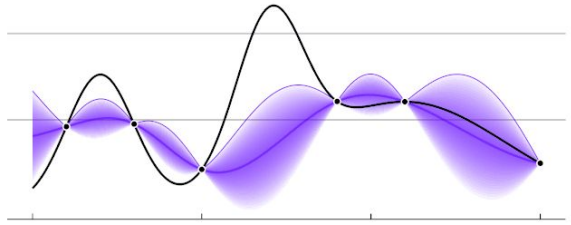
- *E.g.*, UCB, PI, EI, KG, ES, etc.



"Generalizing Bayesian Optimization with Decision-theoretic Entropies", 2022



Bayesian Optimization, Wikipedia

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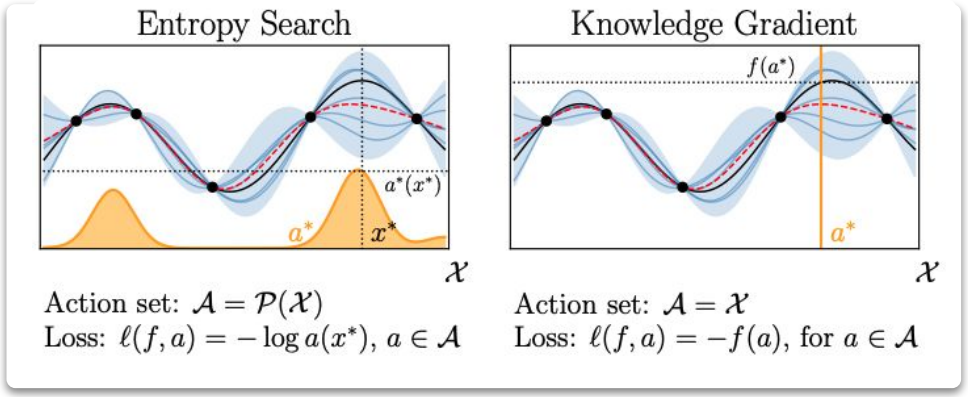

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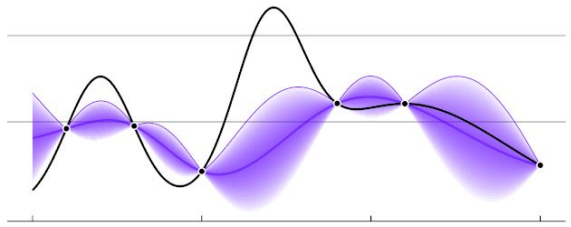
After:

- Paper presentations from students.



Bayesian Optimization, Wikipedia

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TextGrad: Automatic "Differentiation" via Text

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Federico Bianchi[1*] FEDE@STANFORD.EDU
Joseph Boen[2*] TBOEN@STANFORD.EDU
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Repository and Tutorials

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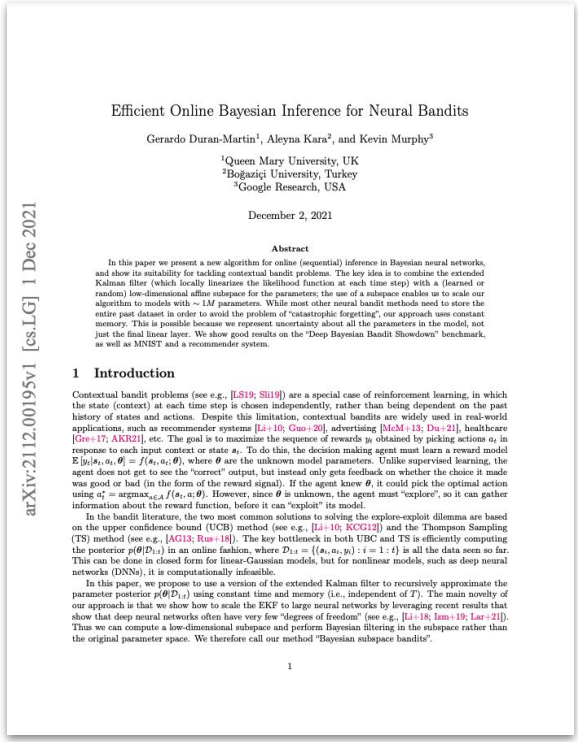

Efficient Online Bayesian Inference for Neural Bandits

Gerardo Duran-Martin[1], Aleyna Kara[2], and Kevin Murphy[3]
[1]Queen Mary University, UK
[2]Boğaziçi University, Turkey
[3]Google Research, USA

December 2, 2021

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In this paper we present a new algorithm for online (sequential) inference in Bayesian neural networks, and show its suitability for tackling contextual bandit problems. The key idea is to combine the extended Kalman filter (which locally linearizes the likelihood function at each time step) with a (learned or random) low-dimensional affine subspace for the parameters; the use of a subspace enables us to scale our algorithm to models with $\sim 1M$ parameters. While most other neural bandit methods need to store the entire past dataset in order to avoid the problem of "catastrophic forgetting", our approach uses constant memory. This is possible because we represent uncertainty about all the parameters in the model, not just the final linear layer. We show good results on the "Deep Bayesian Bandit Showdown" benchmark, as well as MNIST and a recommender system.

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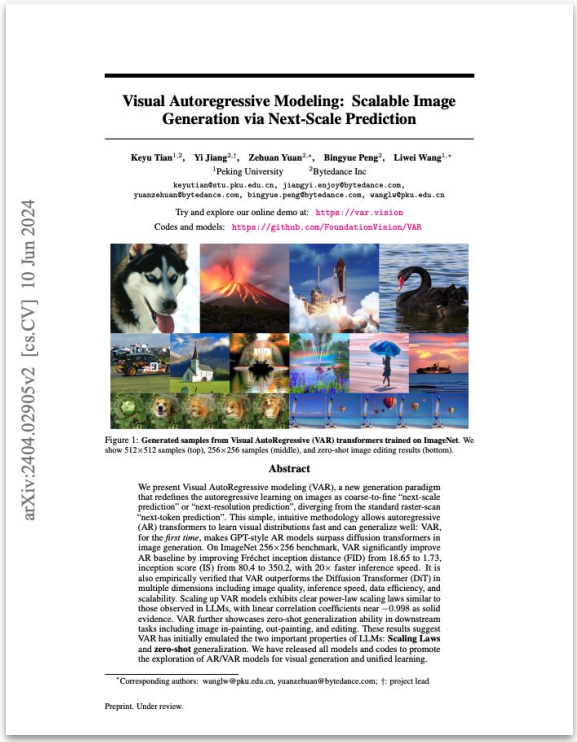

Visual Autoregressive Modeling: Scalable Image Generation via Next-Scale Prediction

Keyu Tian[1,2], Yi Jiang[2,†], Zehuan Yuan[2,*], Bingyue Peng[2], Liwei Wang[1,*]
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Try and explore our online demo at: https://var.vision
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Figure 1: **Generated samples from Visual AutoRegressive (VAR) transformers trained on ImageNet**. We show 512×512 samples (top), 256×256 samples (middle), and zero-shot image editing results (bottom).

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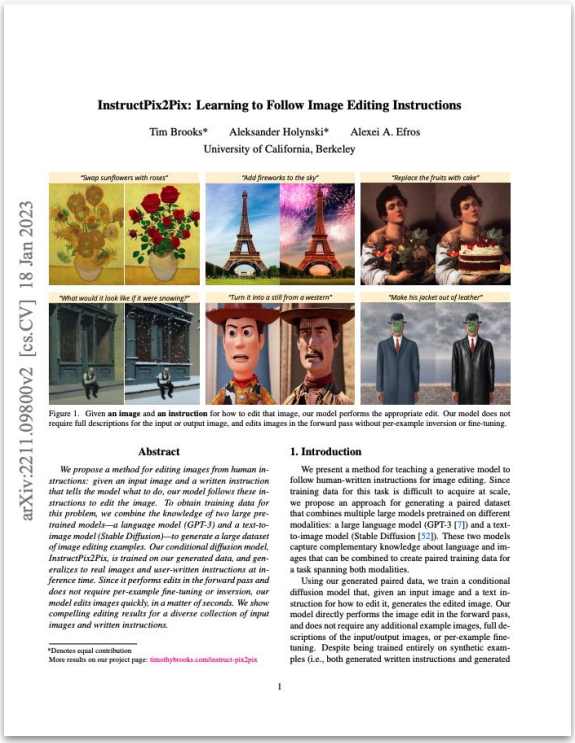
*Corresponding authors: wanglw@pku.edu.cn, yuanzehuan@bytedance.com; †: project lead

Preprint. Under review.



InstructPix2Pix: Learning to Follow Image Editing Instructions

Tim Brooks* Aleksander Holynski* Alexei A. Efros
University of California, Berkeley

Figure 1. Given **an image** and **an instruction** for how to edit that image, our model performs the appropriate edit. Our model does not require full descriptions for the input or output image, and edits images in the forward pass without per-example inversion or fine-tuning.

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We propose a method for editing images from human instructions: given an input image and a written instruction that tells the model what to do, our model follows these instructions to edit the image. To obtain training data for this problem, we combine the knowledge of two large pre-trained models—a language model (GPT-3) and a text-to-image model (Stable Diffusion)—to generate a large dataset of image editing examples. Our conditional diffusion model, InstructPix2Pix, is trained on our generated data, and generalizes to real images and user-written instructions at inference time. Since it performs edits in the forward pass and does not require per-example fine-tuning or inversion, our model edits images quickly, in a matter of seconds. We show compelling editing results for a diverse collection of input images and written instructions.

*Denotes equal contribution
More results on our project page: timothybrooks.com/instruct-pix2pix

I. Introduction

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arXiv:2406.07496v1 [cs.CL] 11 Jun 2024

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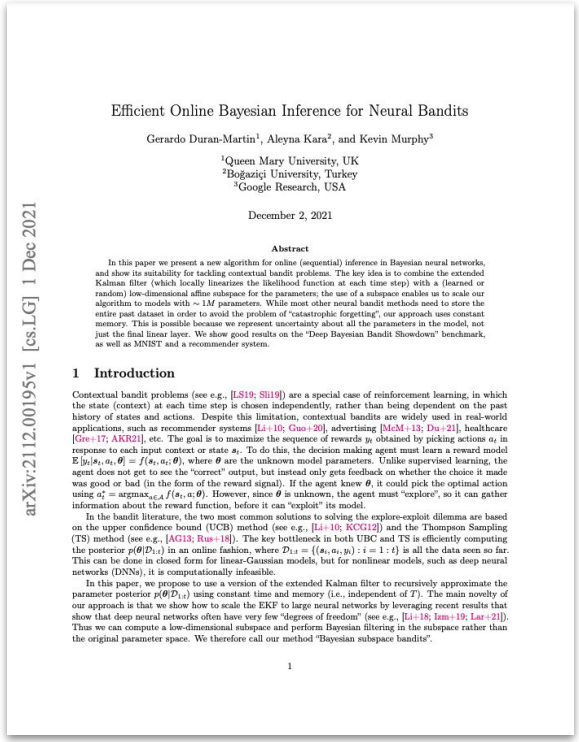

arXiv:2112.00195v1 [cs.LG] 1 Dec 2021

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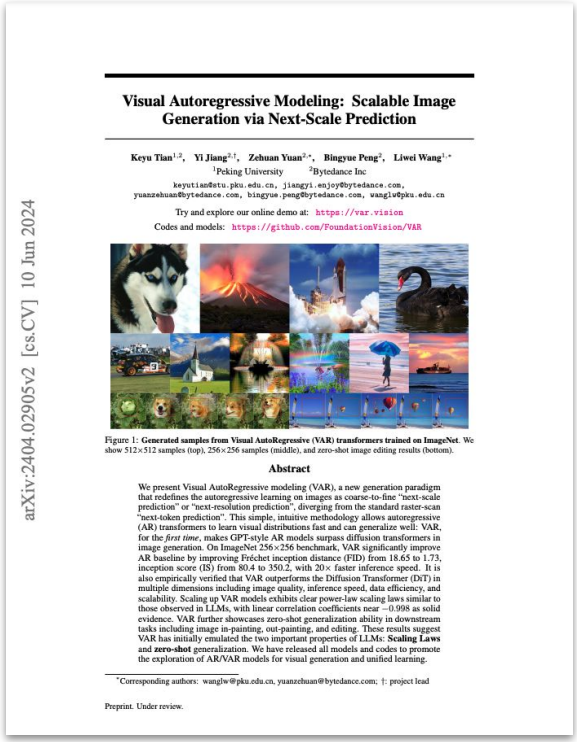

arXiv:2404.02905v2 [cs.CV] 10 Jun 2024

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Keyu Tian[1,2], Yi Jiang[2,†], Zehuan Yuan[2,*], Bingyue Peng[2], Liwei Wang[1,*]
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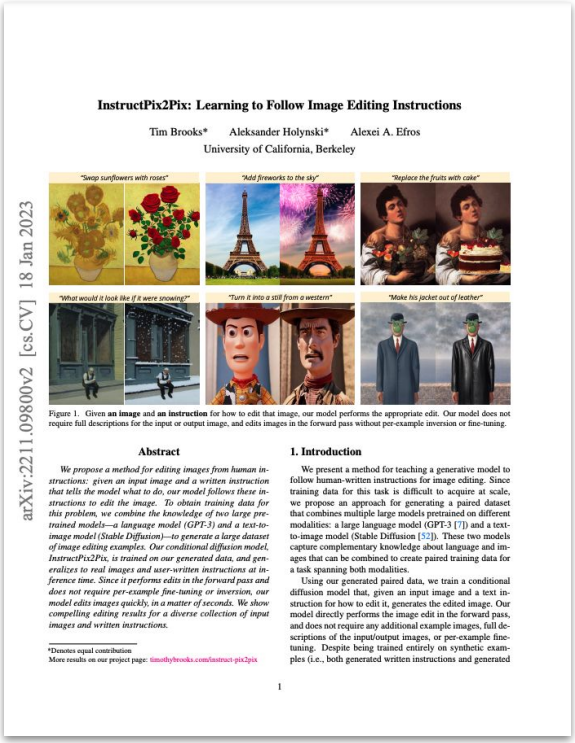

arXiv:2211.09800v2 [cs.CV] 18 Jan 2023

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arXiv:2406.07496v1 [cs.CL] 11 Jun 2024

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[1]Department of Computer Science, Stanford University
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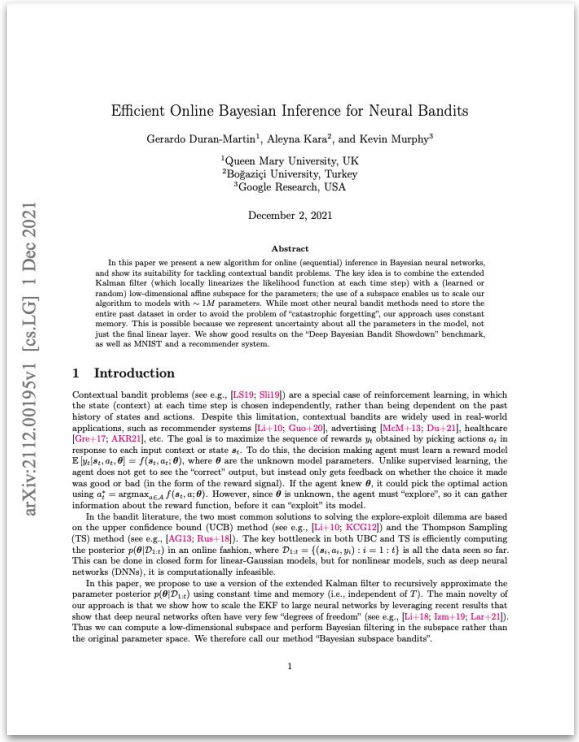

arXiv:2112.00195v1 [cs.LG] 1 Dec 2021

Efficient Online Bayesian Inference for Neural Bandits

Gerardo Duran-Martin[1], Aleyna Kara[2], and Kevin Murphy[3]
[1]Queen Mary University, UK
[2]Boğaziçi University, Turkey
[3]Google Research, USA

December 2, 2021

Abstract

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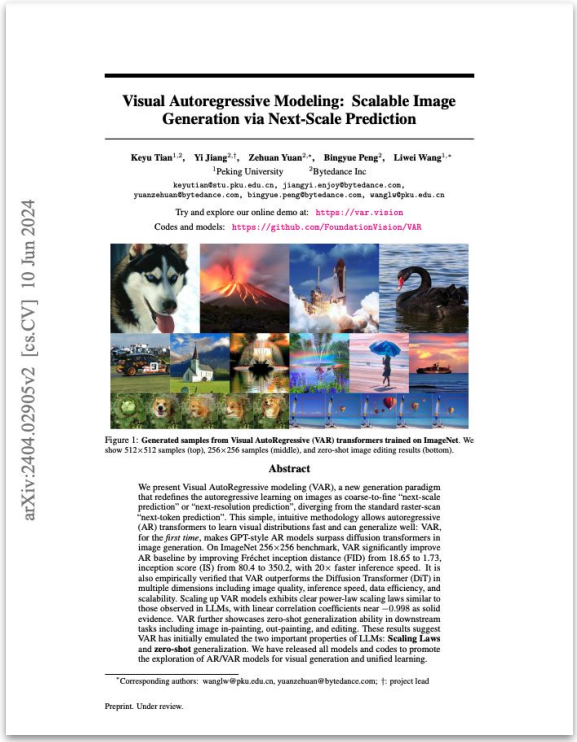

arXiv:2404.02905v2 [cs.CV] 10 Jun 2024

Visual Autoregressive Modeling: Scalable Image Generation via Next-Scale Prediction

Keyu Tian[1,2], Yi Jiang[2,†], Zehuan Yuan[2,*], Bingyue Peng[2], Liwei Wang[1,*]
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Try and explore our online demo at: https://var.vision

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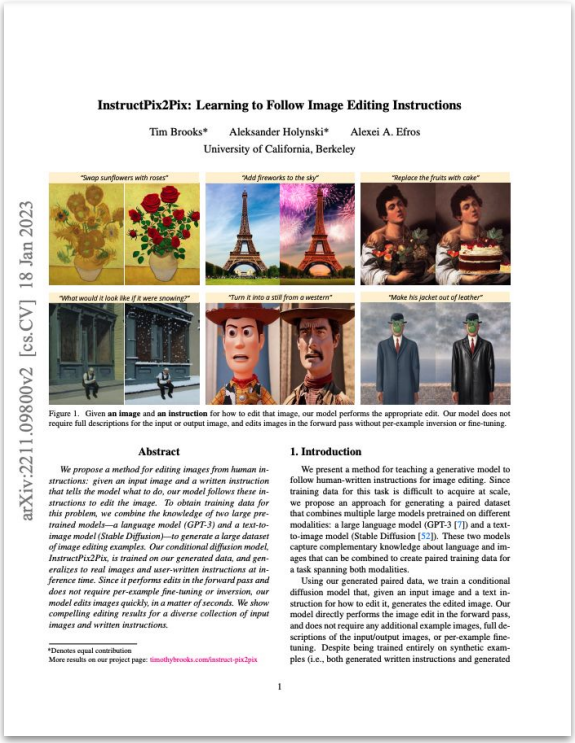
Preprint. Under review.



arXiv:2211.09800v2 [cs.CV] 18 Jan 2023

InstructPix2Pix: Learning to Follow Image Editing Instructions

Tim Brooks* Aleksander Holynski* Alexei A. Efros
University of California, Berkeley

Figure 1. Given **an image** and **an instruction** for how to edit that image, our model performs the appropriate edit. Our model does not require full descriptions for the input or output image, and edits images in the forward pass without per-example inversion or fine-tuning.

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Today

After: Next batch of four **paper presentations**.

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Repository and Tutorials

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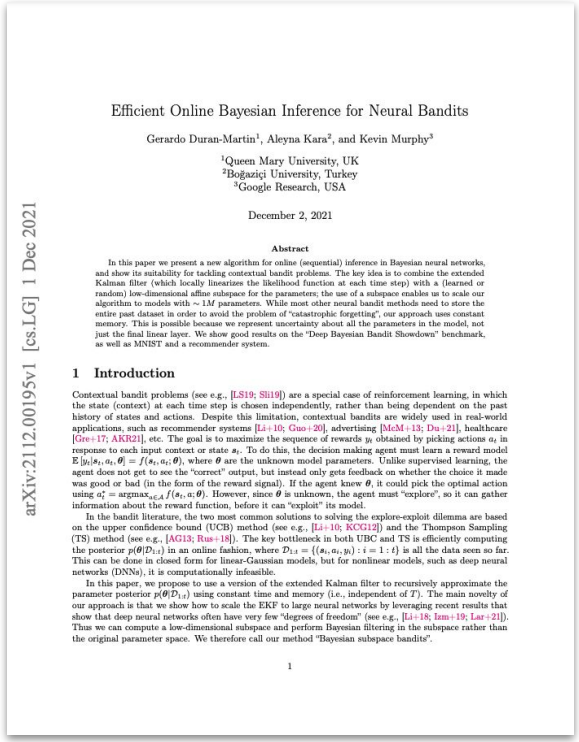
arXiv:2406.07496v1 [cs.CL] 11 Jun 2024



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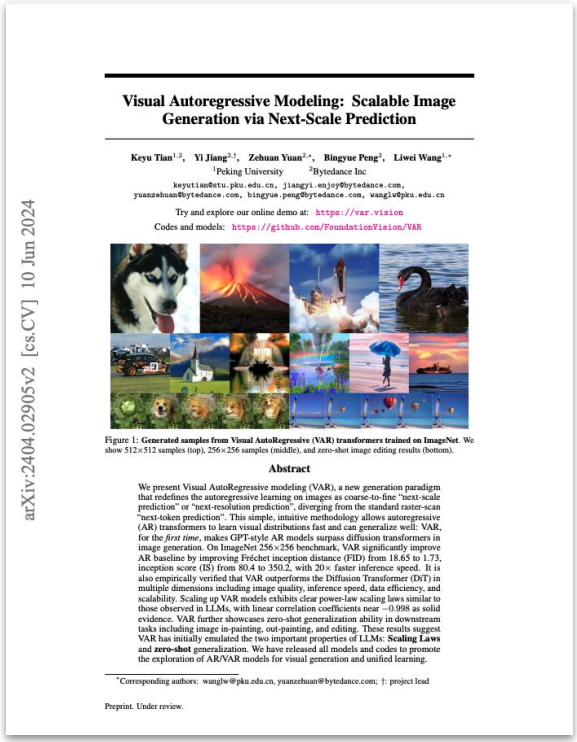

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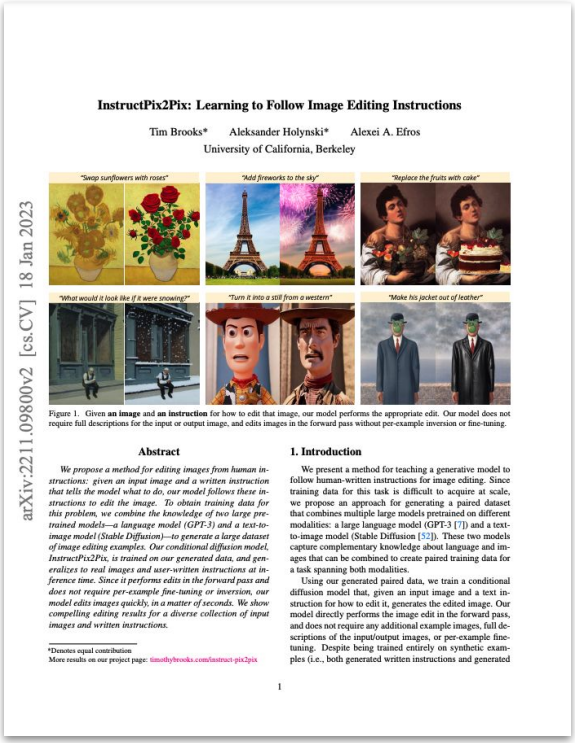

InstructPix2Pix: Learning to Follow Image Editing Instructions

Tim Brooks* Aleksander Holynski* Alexei A. Efros
University of California, Berkeley

"Swap sunflowers with roses" "Add fireworks to the sky" "Replace the fruits with cake"
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arXiv:2211.09800v2 [cs.CV] 18 Jan 2023

VAR: image generation via autoregressive models

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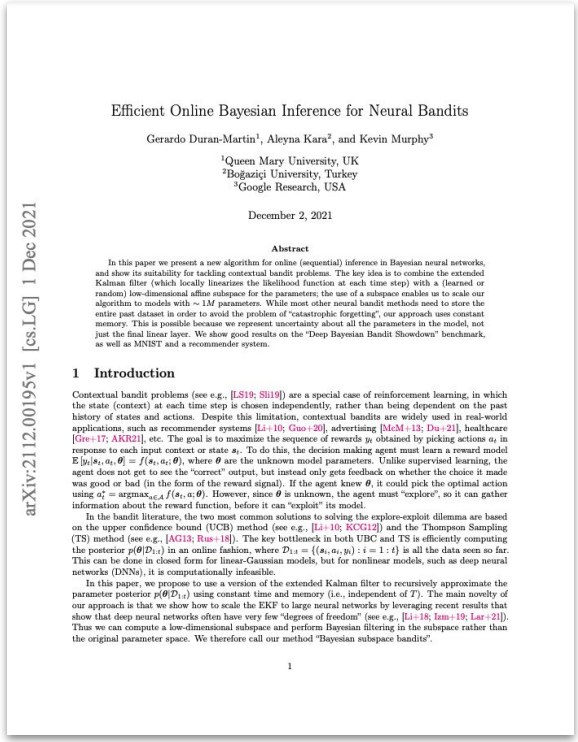

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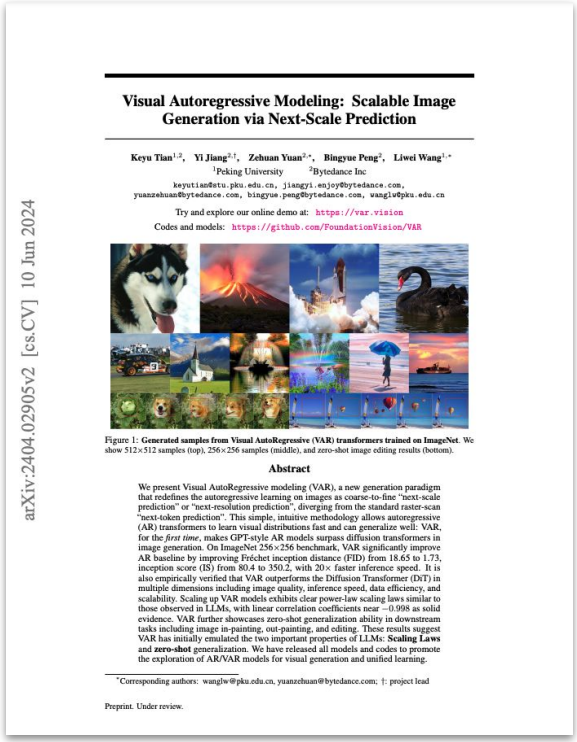

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Try and explore our online demo at: https://var.vision
Codes and models: https://github.com/FoundationVision/VAR

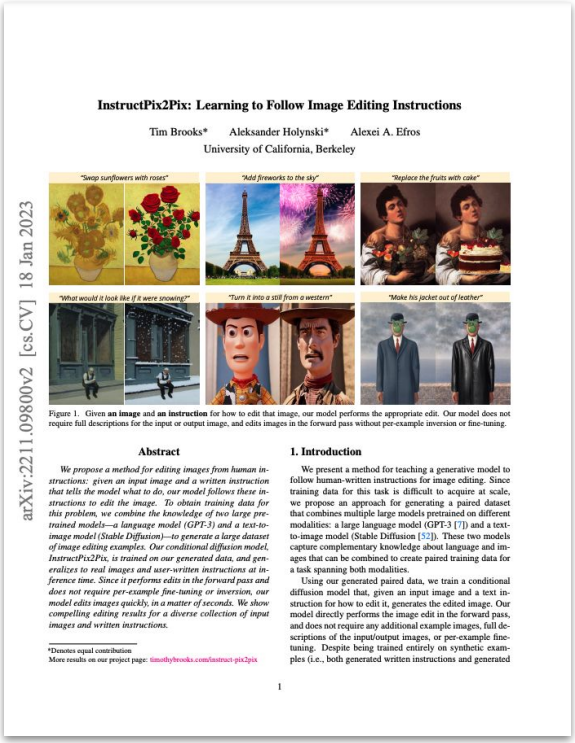
Figure 1: **Generated samples from Visual AutoRegressive (VAR) transformers trained on ImageNet**. We show 512×512 samples (top), 256×256 samples (middle), and zero-shot image editing results (bottom).

Abstract

We present Visual AutoRegressive modeling (VAR), a new generation paradigm that redefines the autoregressive learning on images as coarse-to-fine "next-scale prediction" or "next-resolution prediction", diverging from the standard raster-scan "next-token prediction". This simple, intuitive methodology allows autoregressive (AR) transformers to learn visual distributions fast and can generalize well: VAR, for the *first time*, makes GPT-style AR models surpass diffusion transformers in image generation. On ImageNet 256×256 benchmark, VAR significantly improve AR baseline by improving Fréchet inception distance (FID) from 18.65 to 1.73, inception score (IS) from 80.4 to 350.2, with 20× faster inference speed. It is also empirically verified that VAR outperforms the Diffusion Transformer (DiT) in multiple dimensions including image quality, inference speed, data efficiency, and scalability. Scaling up VAR models exhibits clear power-law scaling laws similar to those observed in LLMs, with linear correlation coefficients near −0.998 as solid evidence. VAR further showcases zero-shot generalization ability in downstream tasks including image in-painting, out-painting, and editing. These results suggest VAR has initially emulated the two important properties of LLMs: **Scaling Laws** and **zero-shot** generalization. We have released all models and codes to promote the exploration of AR/VAR models for visual generation and unified learning.

*Corresponding authors: wanglw@pku.edu.cn, yuanzehuan@bytedance.com; †: project lead

Preprint. Under review.



InstructPix2Pix: Learning to Follow Image Editing Instructions

Tim Brooks* Aleksander Holynski* Alexei A. Efros
University of California, Berkeley

Figure 1. Given **an image** and **an instruction** for how to edit that image, our model performs the appropriate edit. Our model does not require full descriptions for the input or output image, and edits images in the forward pass without per-example inversion or fine-tuning.

Abstract

We propose a method for editing images from human instructions: given an input image and a written instruction that tells the model what to do, our model follows these instructions to edit the image. To obtain training data for this problem, we combine the knowledge of two large pre-trained models—a language model (GPT-3) and a text-to-image model (Stable Diffusion)—to generate a large dataset of image editing examples. Our conditional diffusion model, InstructPix2Pix, is trained on our generated data, and generalizes to real images and user-written instructions at inference time. Since it performs edits in the forward pass and does not require per-example fine-tuning or inversion, our model edits images quickly, in a matter of seconds. We show compelling editing results for a diverse collection of input images and written instructions.

*Denotes equal contribution
More results on our project page: timothybrooks.com/instruct-pix2pix

I. Introduction

We present a method for teaching a generative model to follow human-written instructions for image editing. Since training data for this task is difficult to acquire at scale, we propose an approach for generating a paired dataset that combines multiple large models pretrained on different modalities: a large language model (GPT-3 [7]) and a text-to-image model (Stable Diffusion [52]). These two models capture complementary knowledge about language and images that can be combined to create paired training data for a task spanning both modalities.

Using our generated paired data, we train a conditional diffusion model that, given an input image and a text instruction for how to edit it, generates the edited image. Our model directly performs the image edit in the forward pass, and does not require any additional example images, full descriptions of the input/output images, or per-example fine-tuning. Despite being trained entirely on synthetic examples (i.e., both generated written instructions and generated

1

InstructPix2Pix: model to perform edits on images

Quick Aside

Midway Reports and Grading:

- We (Oliver and I) finished reviewing through and grading all midway reports.
  - Everyone did a nice job :D!
- We have a few light comments on each report — which could be useful for final report.
  - We will likely send these via our group message threads on slack.
- And will also upload grades on Brightspace.

Quick Aside

Reminder — Final Course Project Timeline

- Final Presentations (30 mins long)
  - **April 25** - Groups 1-5.
  - **May 02** - Groups 6-9.

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- Final Presentations (30 mins long)
  - **April 25** - Groups 1-5.
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- Final Report (8-10 pages, extended version of midway report)
  - (LaTeX template will be provided soon).
  - **Due May 9, EOD**

Review: Predictive UQ and Gaussian Processes

Review — Gaussian Processes

Review — Gaussian Processes

Intuitively, a *GP* is a probabilistic model, which can be viewed as a distribution over functions.

Review — Gaussian Processes

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But it uses a (multivariate) **Gaussian distribution** to model these functions 🤯!

Review — Gaussian Processes

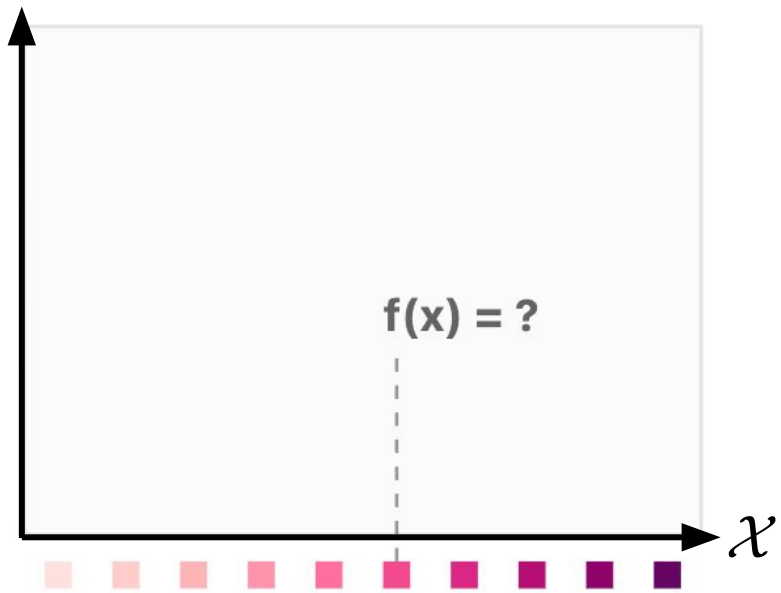
Intuitively, a *GP* is a probabilistic model, which can be viewed as a distribution over functions.

But it uses a (multivariate) **Gaussian distribution** to model these functions 🤯!

Let’s visualize this…

Review — Gaussian Processes

Suppose we pick a set of *d=10* points on the *x*-axis, and want to define a **function** (or set of functions) over these points:



Source: A Visual Exploration of Gaussian Processes

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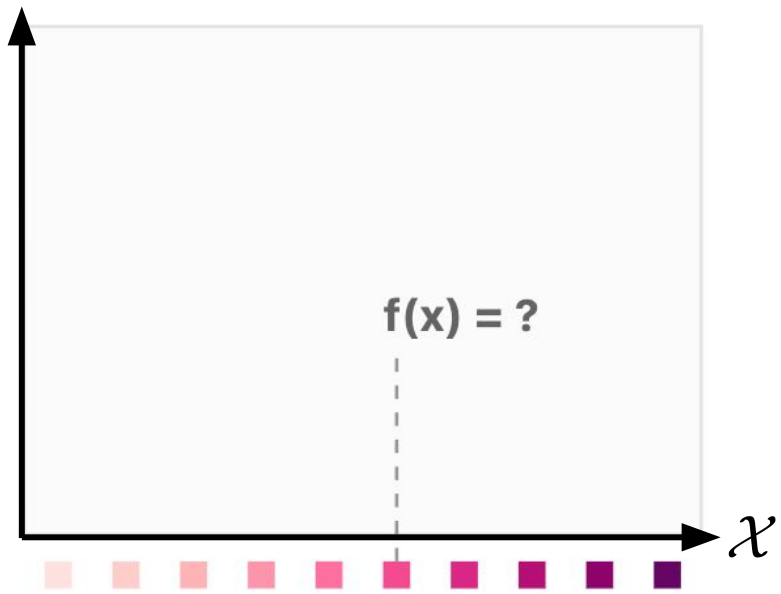

10 points are denoted by different colors

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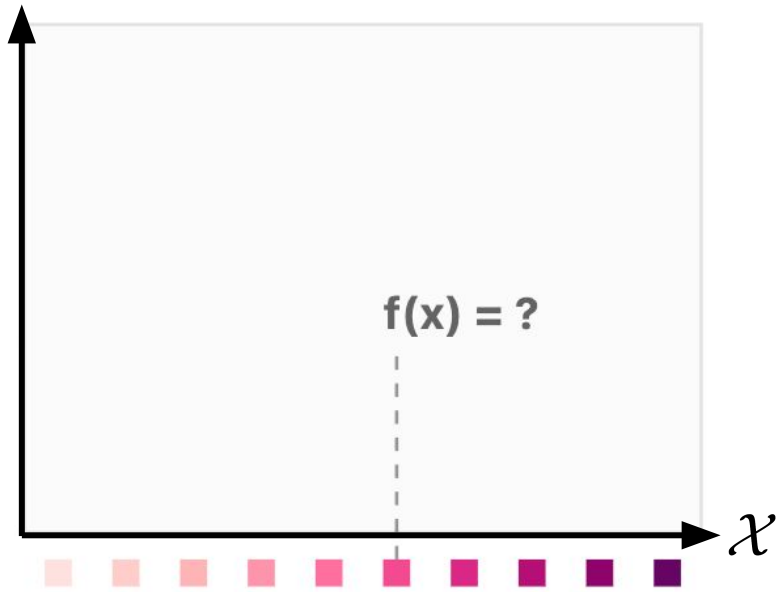


10 points are denoted by different colors

We can define a *distribution of functions*, defined on these 10 points, in the following way…

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Processes

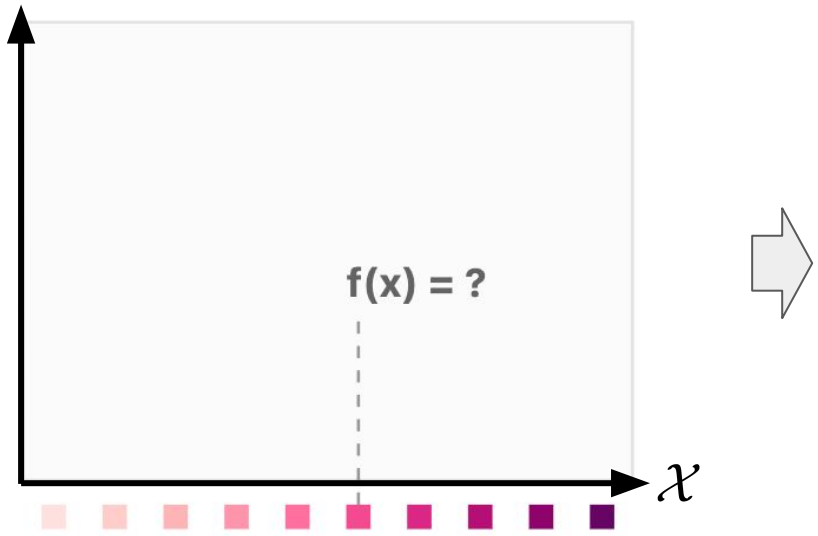
We define a MVN of ***d* dimensions**, with a mean and covariance matrix parameter.

Mean parameter $\mu \in \mathbb{R}^d$ — assume we set this to ***0*** for now.

Covariance matrix $\sum \in \mathbb{R}^{d \times d}$ — define using a *kernel function* based on distance between input points (next slide).

Review — Gaussian Processes

For these 10 points:



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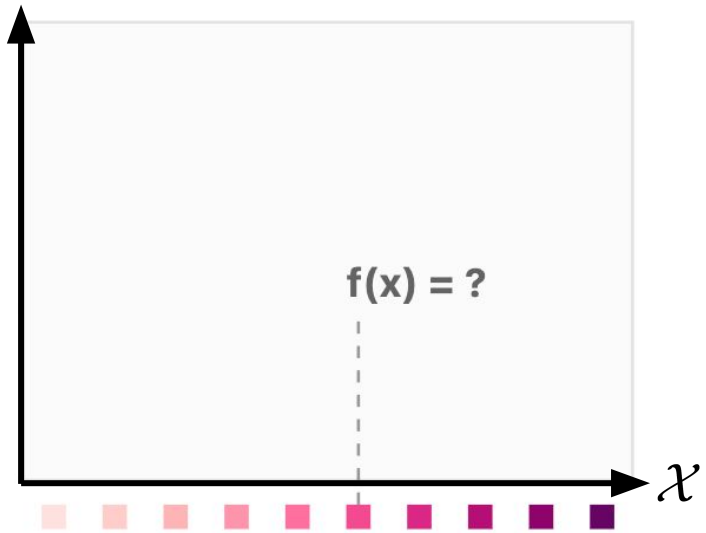
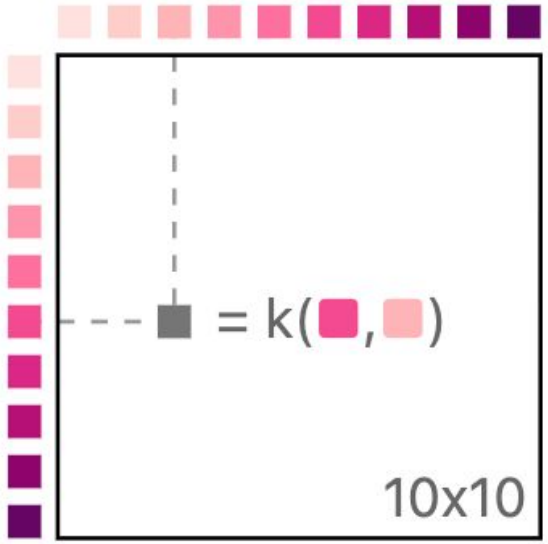


Covariance matrix:



Define covariance between any pair of inputs using kernel function $k(\cdot, \cdot)$.

One example: *RBF kernel*,

$$k(x_1, x_2) = \sigma^2 \left(-\frac{\|x_1 - x_2\|^2}{2\ell^2} \right)$$

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Review — Gaussian Processes

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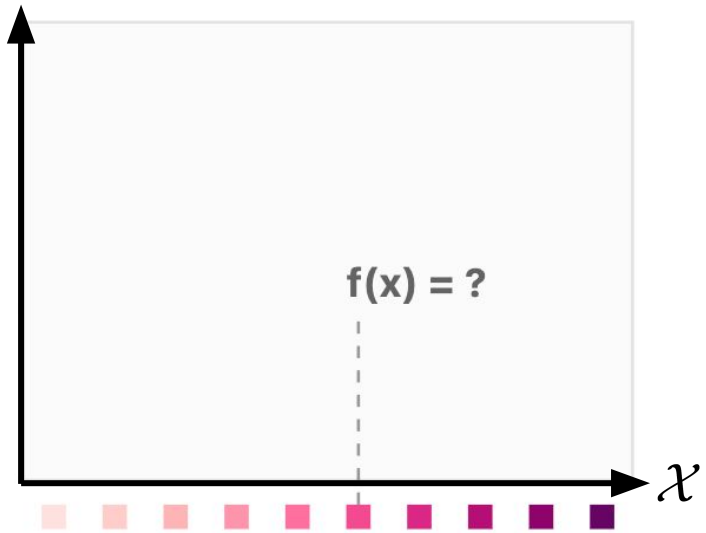

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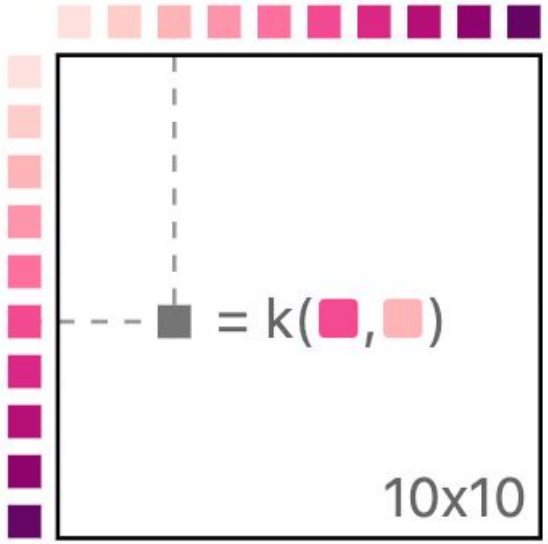

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One example: *RBF kernel*,

$$k(x_1, x_2) = \sigma^2 \left(-\frac{\|x_1 - x_2\|^2}{2\ell^2} \right)$$

Highest when $x_1 = x_2$, lowest when x_2 very different from x_2.

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Processes

This yields a MVN, where samples give function values for the *d* input points:

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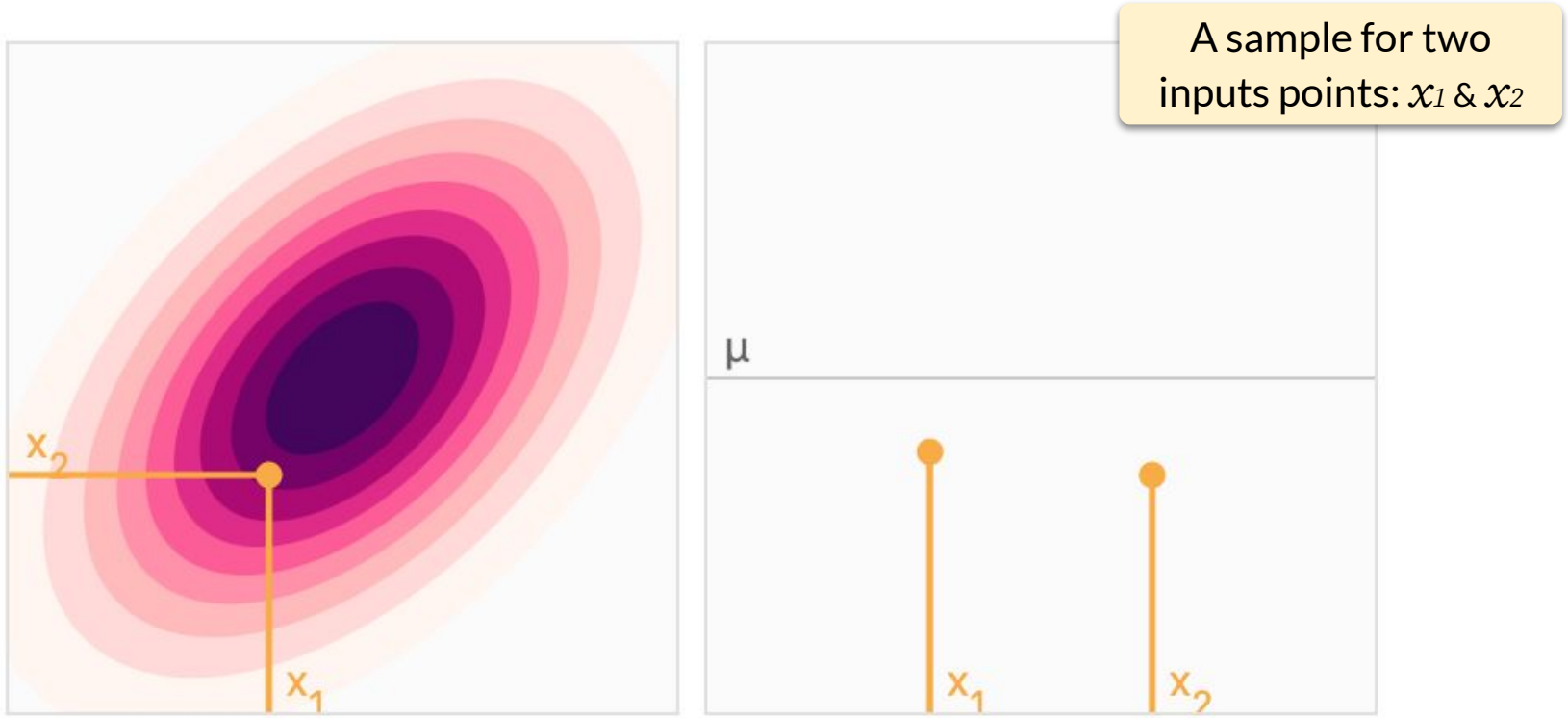

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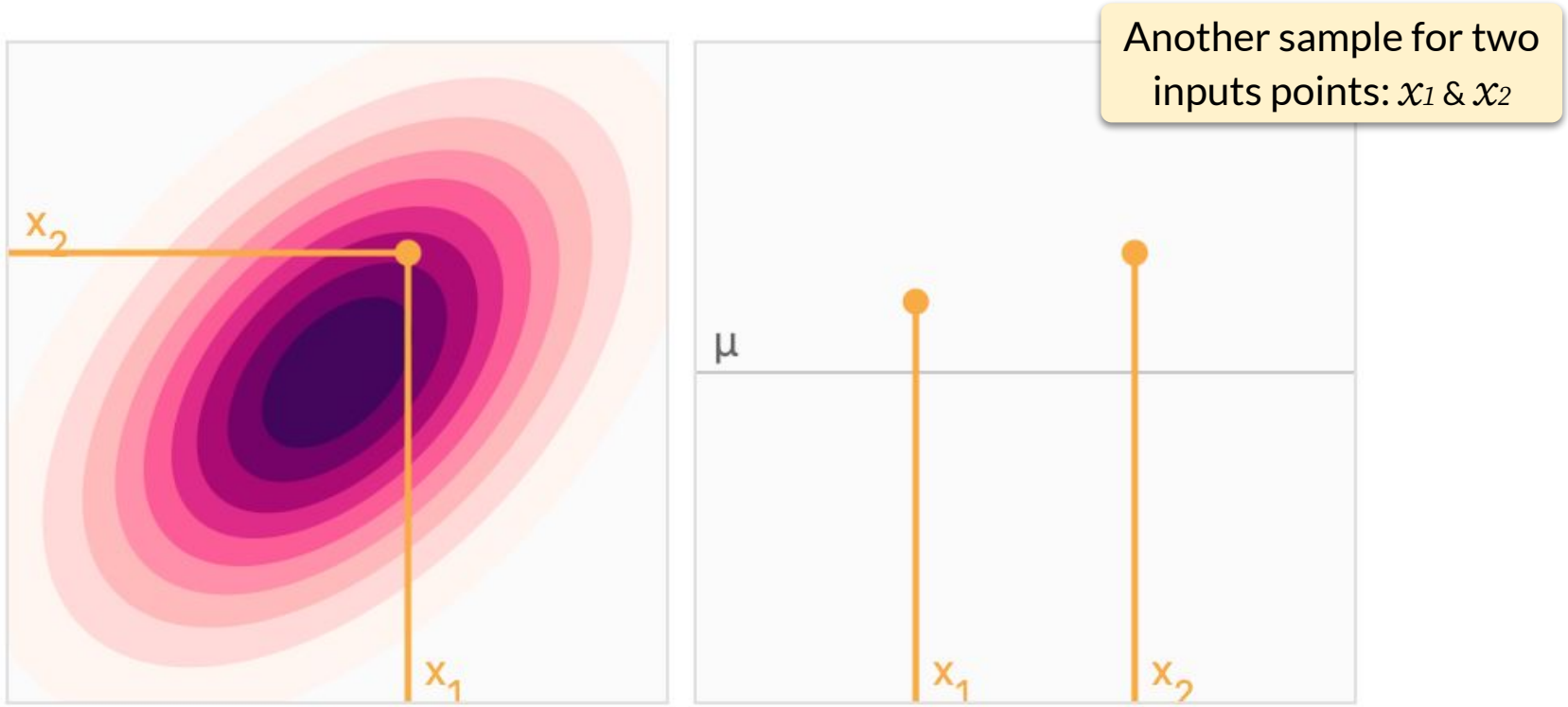

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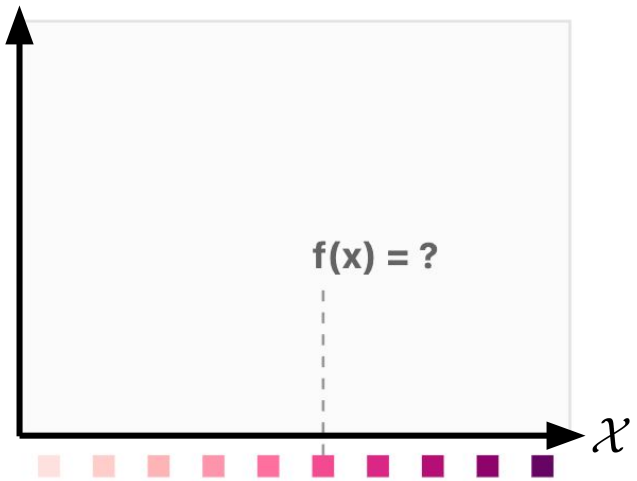

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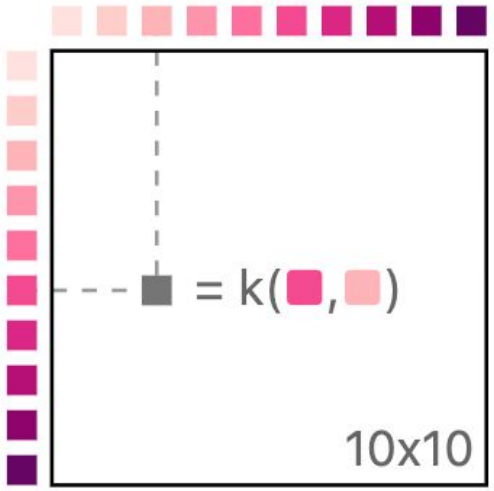
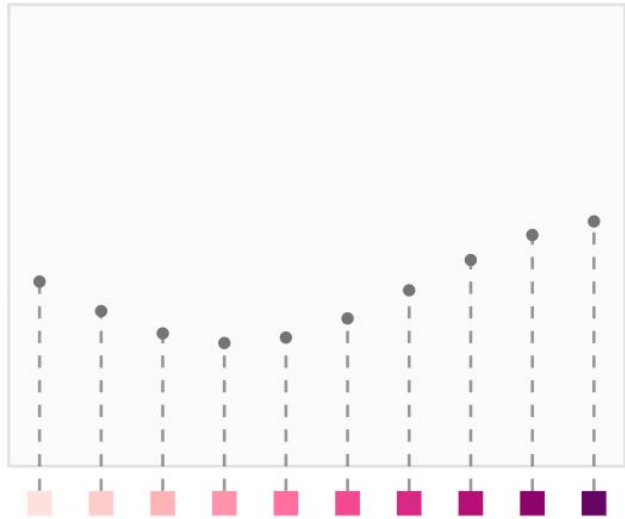


Sampled function values



Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Processes

We define a **Gaussian Process (GP)** as a distribution over functions, parameterized by a *mean function* $m(\cdot)$ and *covariance kernel function* $k(\cdot, \cdot)$, written

$$f \sim \mathrm{GP}(m(\cdot), k(\cdot, \cdot))$$

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$$f \sim \mathrm{GP}(m(\cdot), k(\cdot, \cdot))$$

Where, for any finite collection of *d* input points, we can:

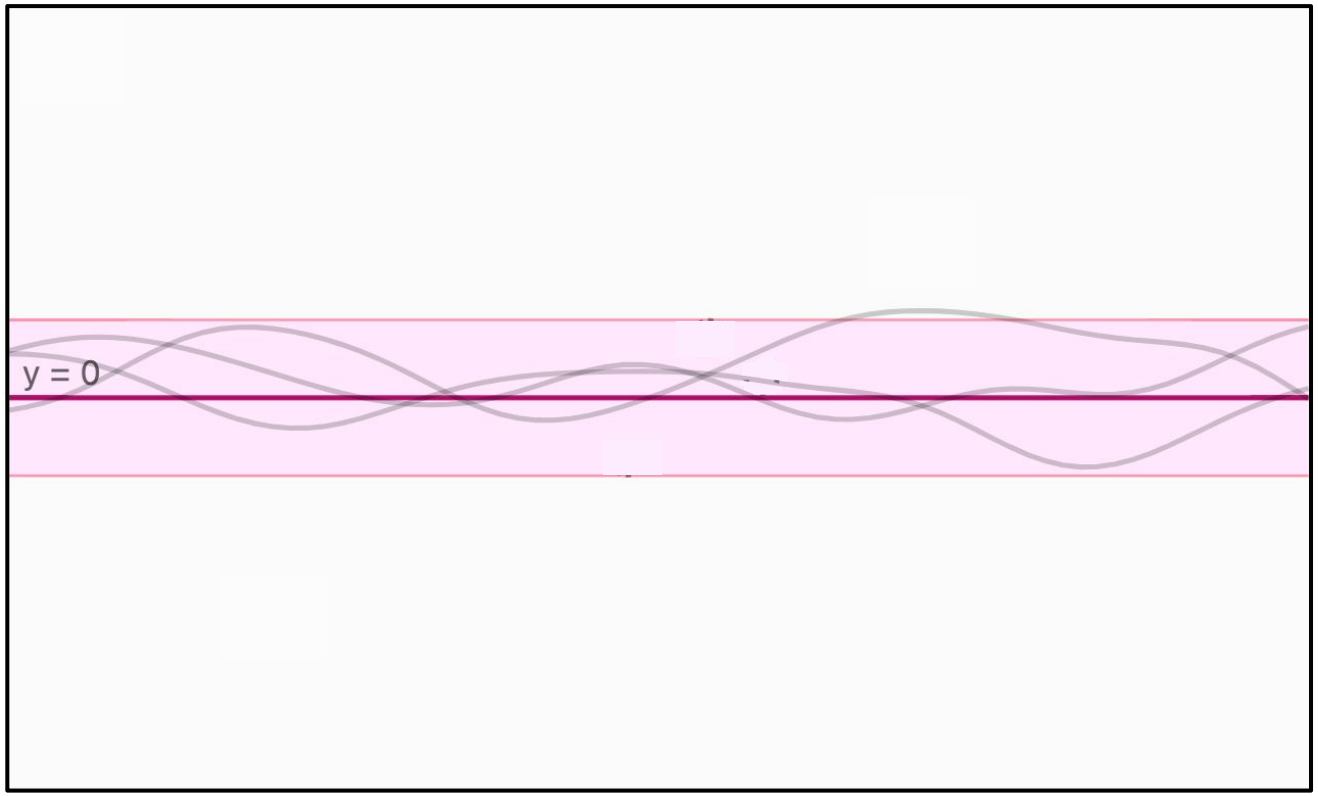
- Define a MVN *on these d points*, using the mean/kernel functions to define a mean parameter and covariance matrix.
- And this MVN yields a distribution over function values.

Review — Gaussian Processes

What does this distribution look like?

Review — Gaussian Processes

What does this distribution look like? → **often drawn like this:**



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Review — Gaussian Processes

Called a *Sausage Plot* because it looks like a sausage

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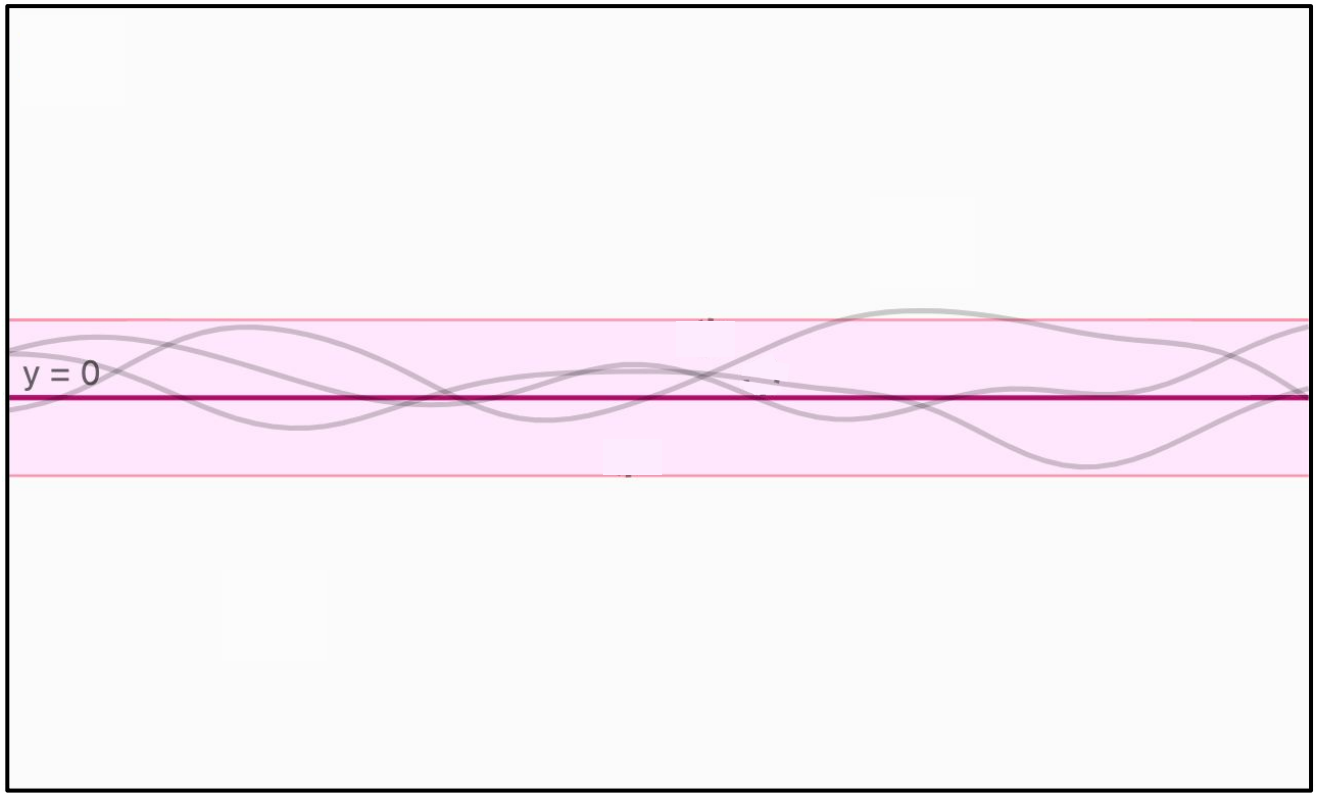

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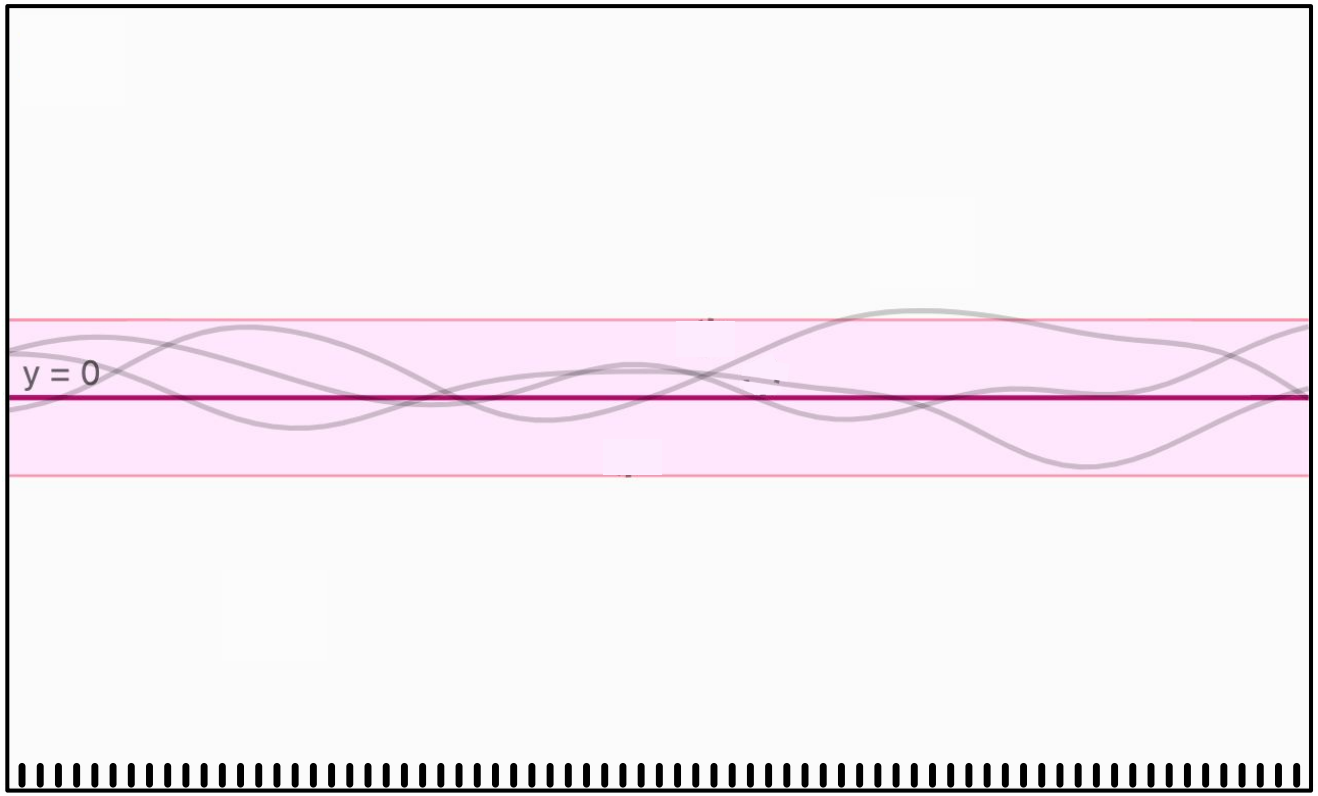

This plot depicts a MVN defined on a large set of grid points

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Review — Gaussian Processes

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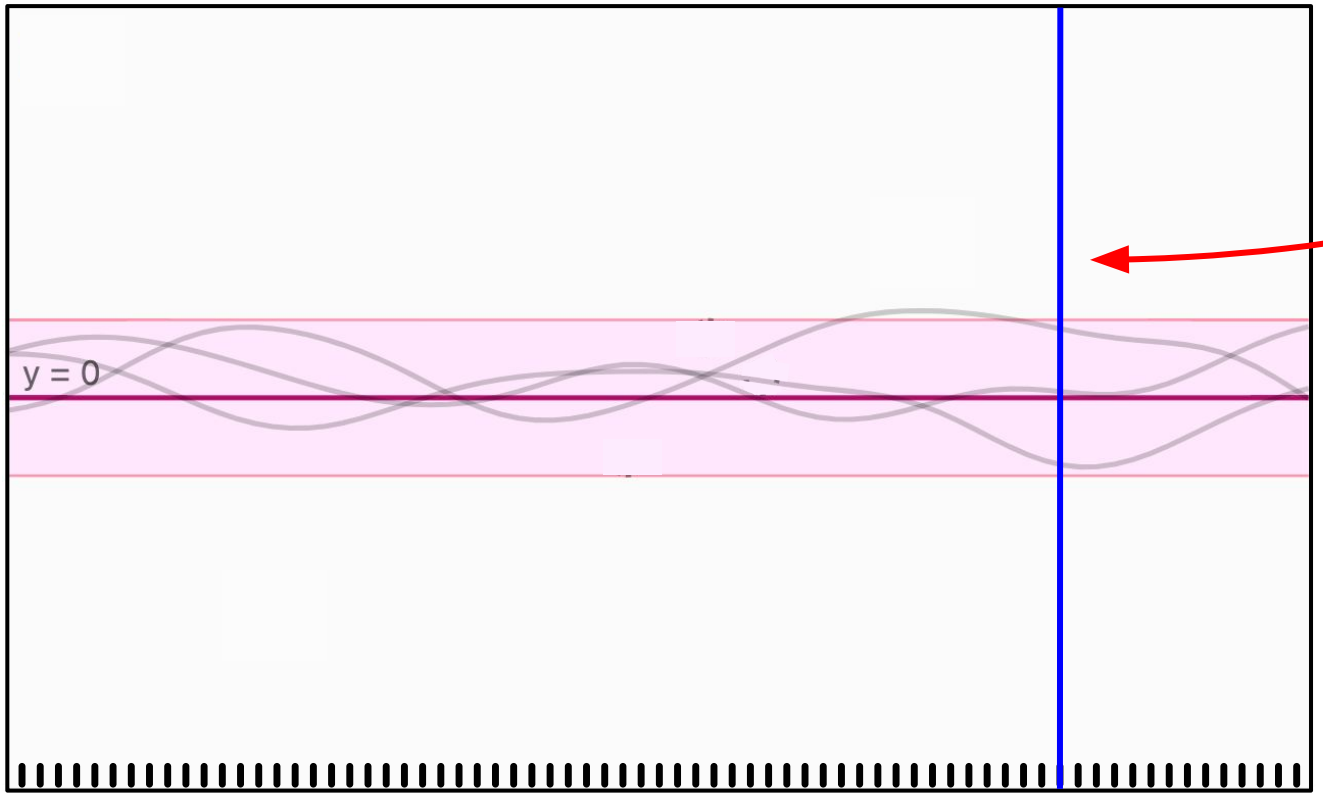

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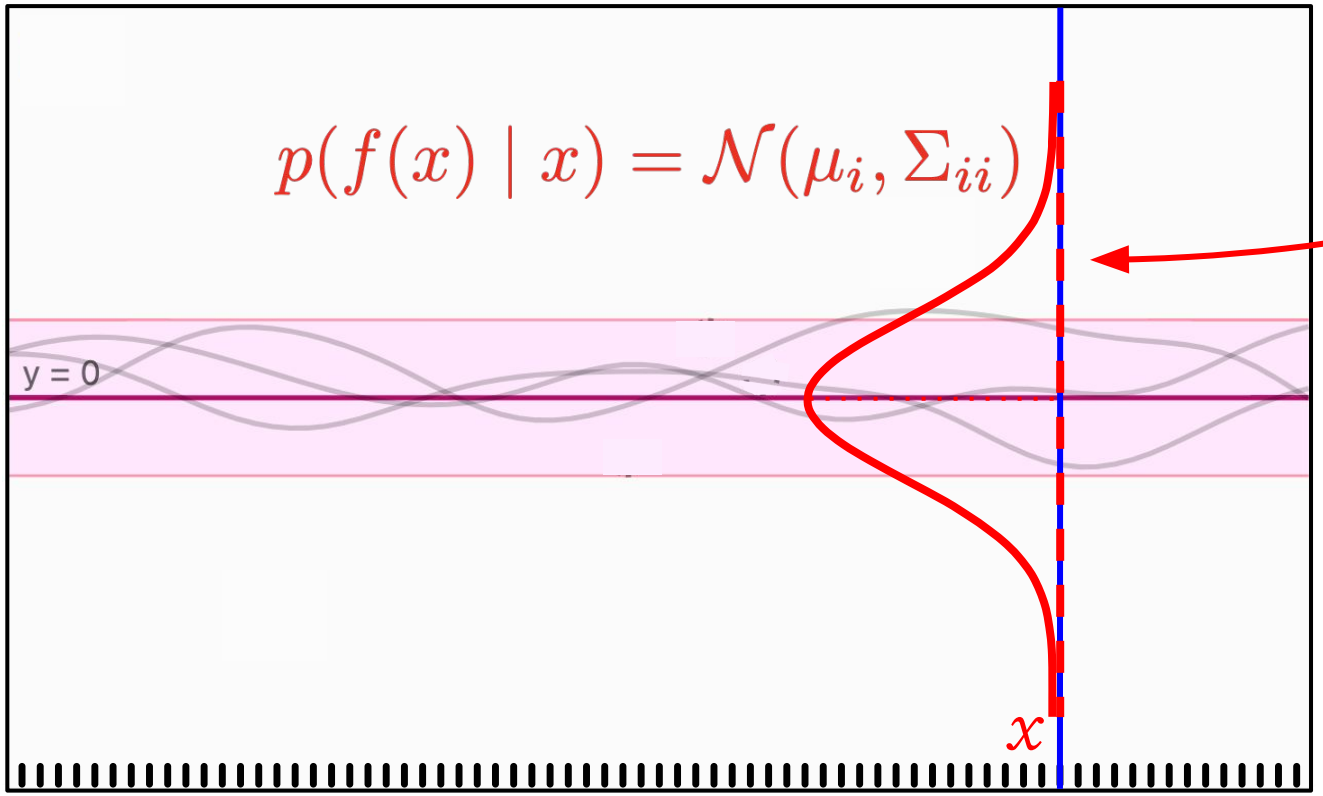

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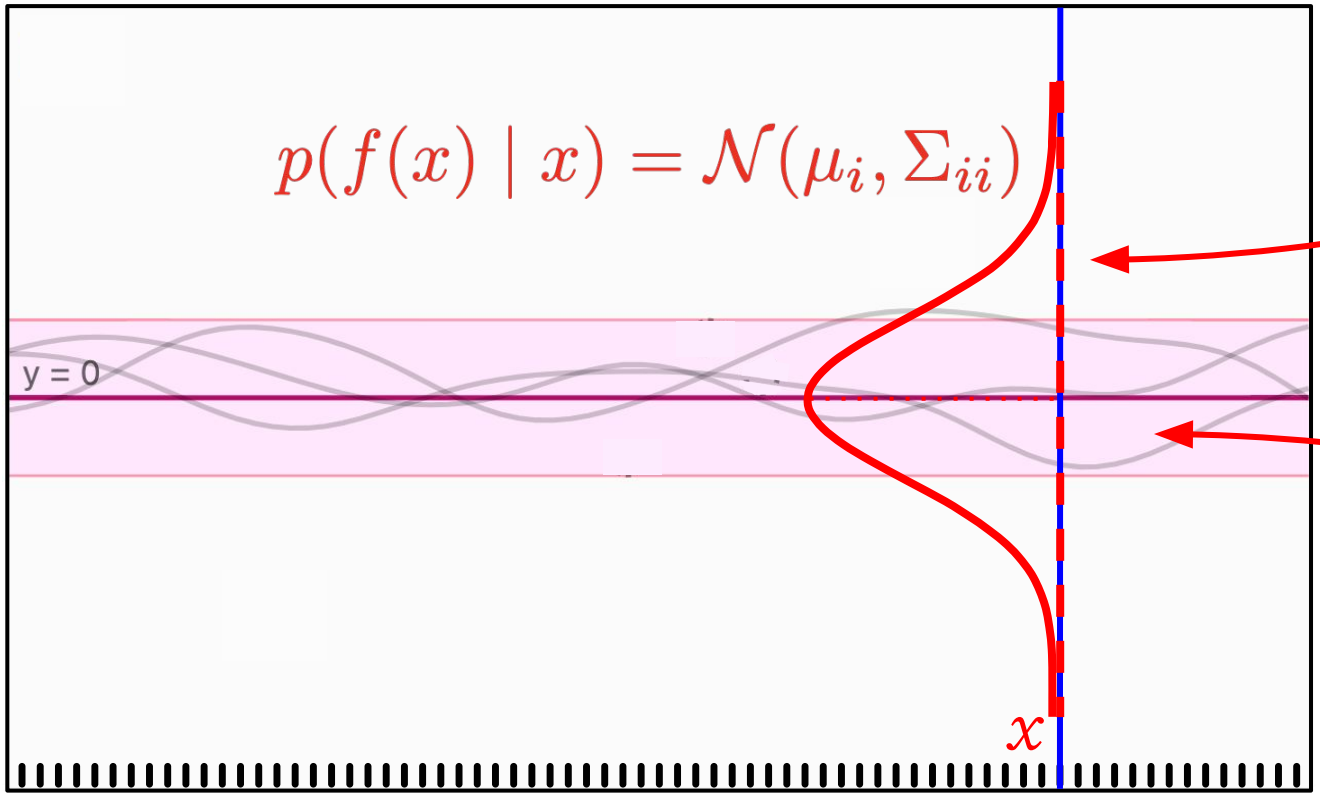

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Samples from the MVN are shown in grey (appear as functions!)

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Process Posterior

How do we use a GP as a predictive uncertainty model?

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Review — Gaussian Process Posterior

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In particular, we will:

- Use a GP to define a prior over functions.
- Observe a set of (x, y) pairs.
- Compute a posterior GP over functions.

Review — Gaussian Process Posterior

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⇒ Use it as a prior distribution and do Bayesian inference!

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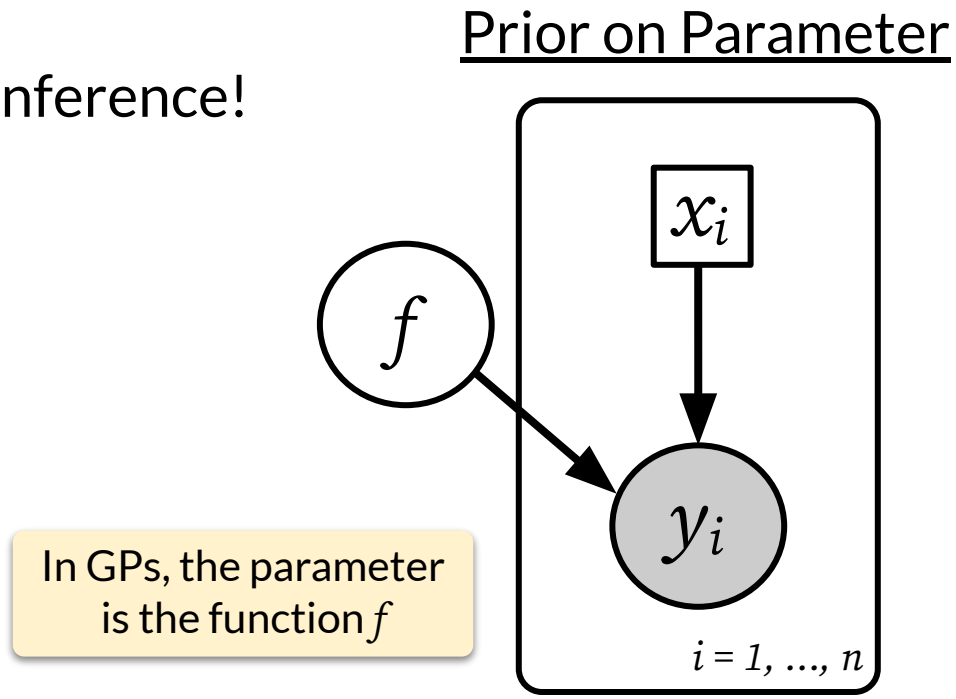

Review — Gaussian Process Posterior

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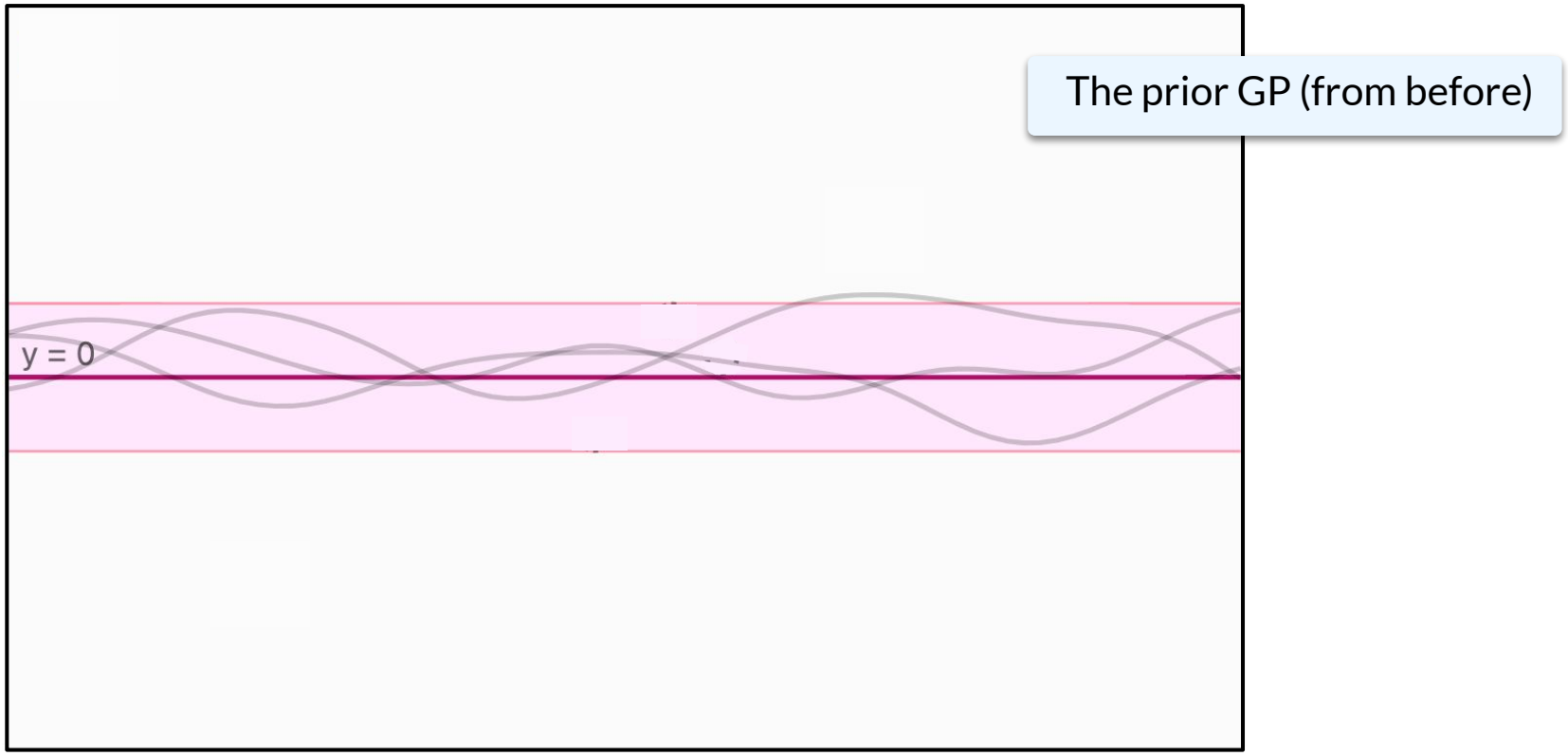
- ⇒ Posterior is *(essentially)* also a multivariate normal distribution.

Posterior is technically a **posterior Gaussian process**, so it's another GP with a mean function and covariance kernel parameters

⇒ which can be computed in closed form.

Review — Gaussian Process Posterior

Visualizing this:



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Review — Gaussian Process Posterior

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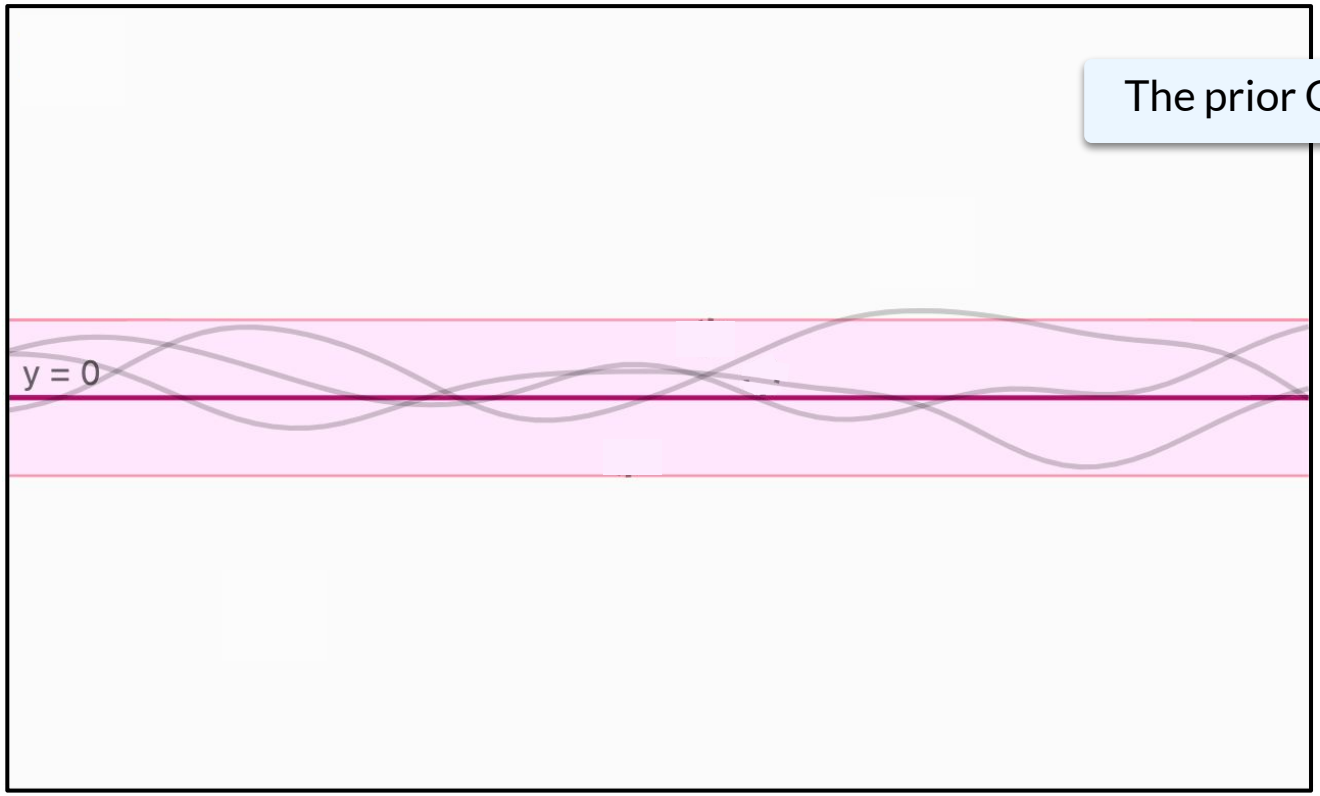

The prior GP (from before)

Mean function is constant **0** function

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Process Posterior

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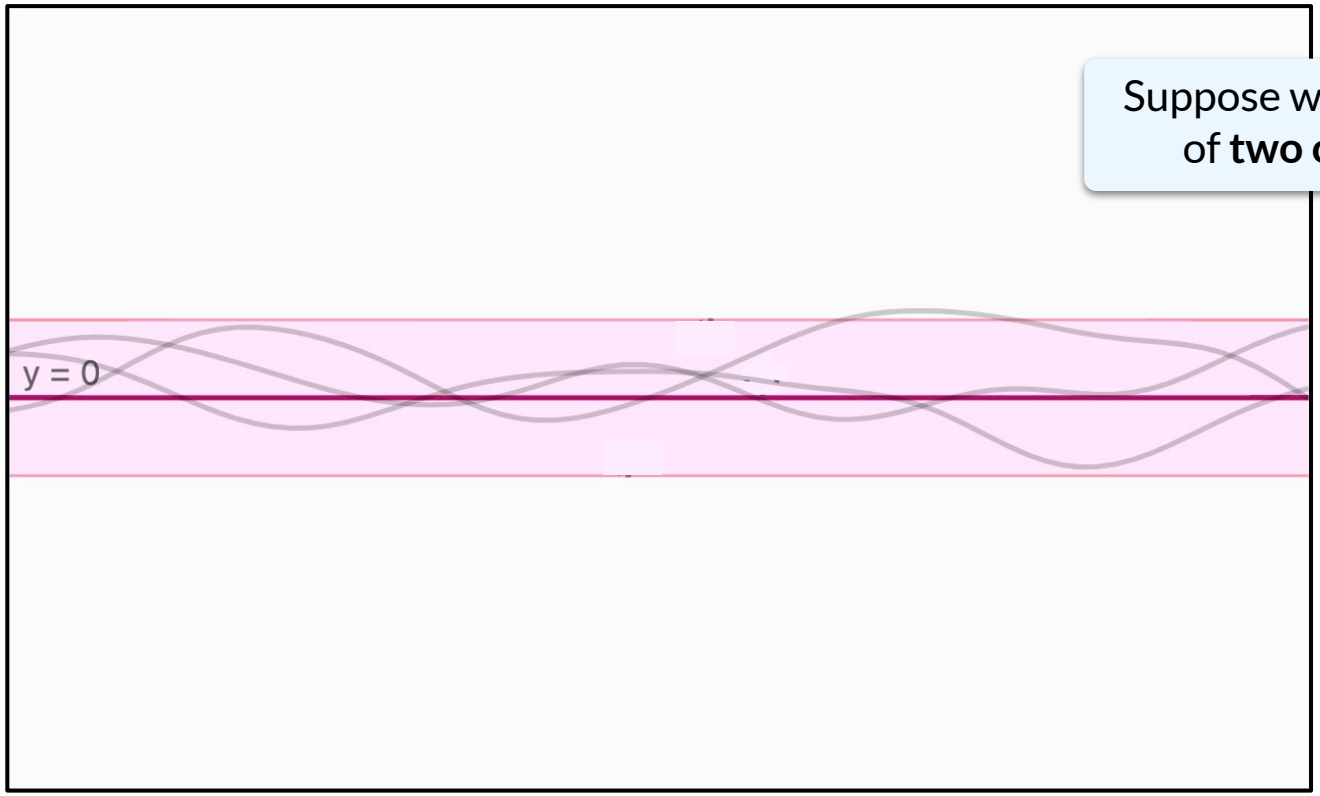

Suppose we have a dataset of **two observations**

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Process Posterior

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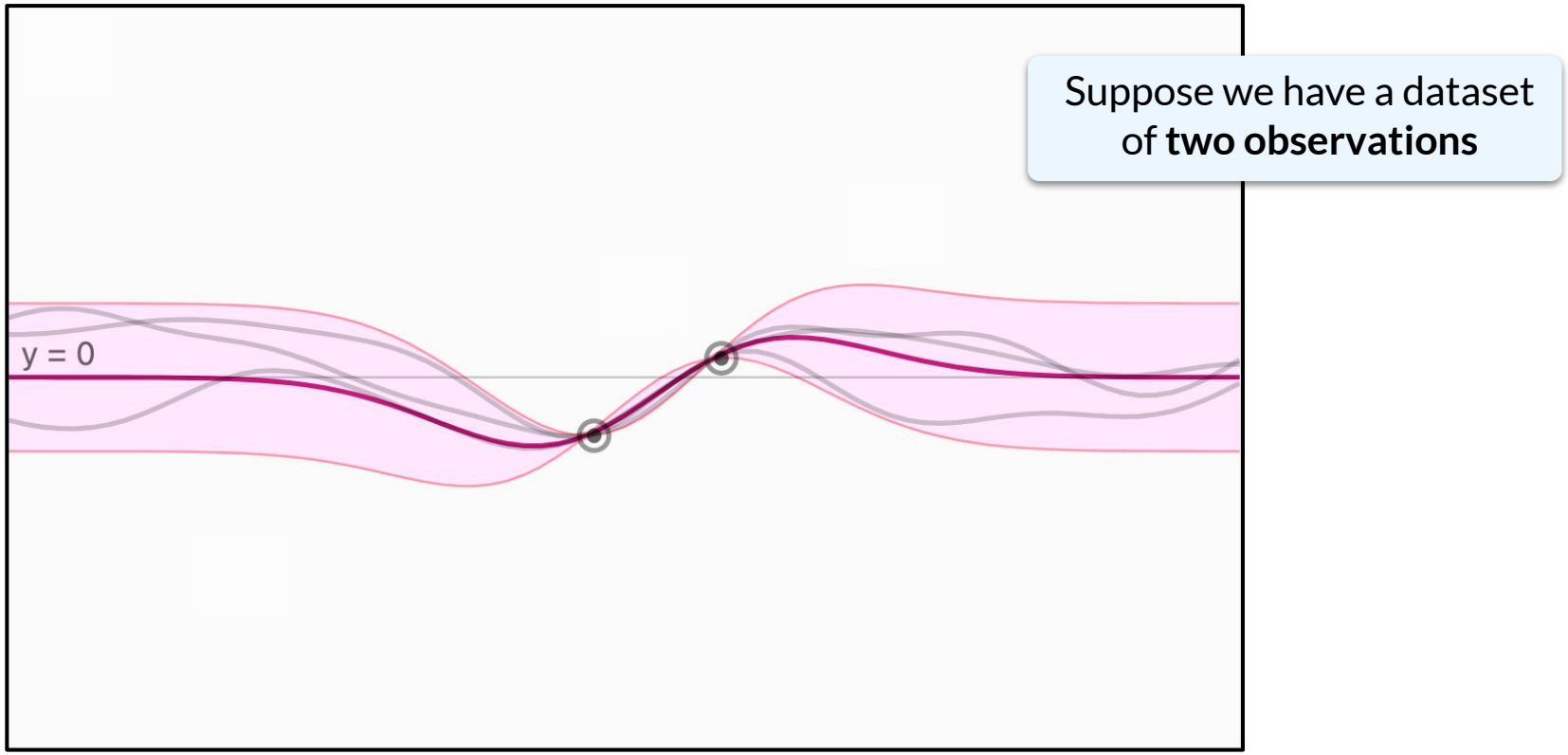

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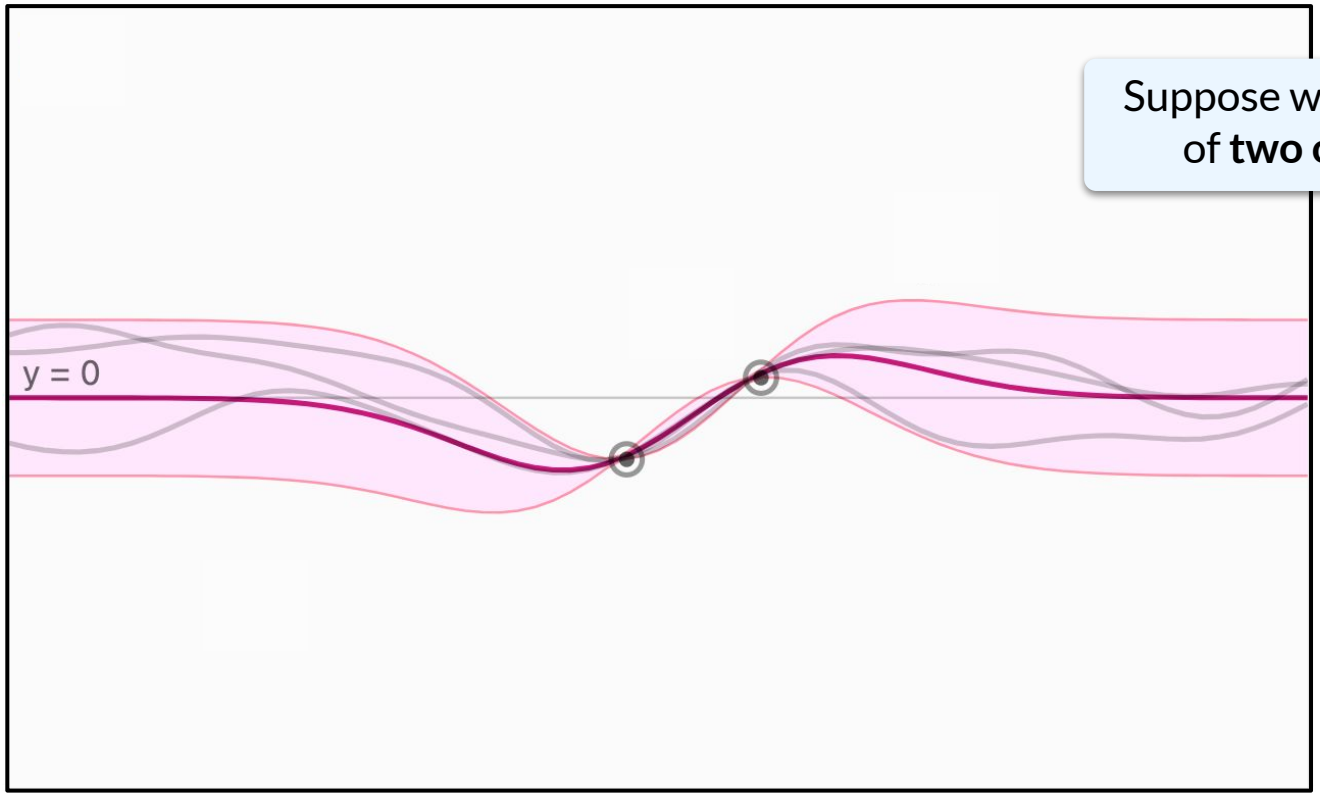
Review — Gaussian Process Posterior

Visualizing this:

Mean function is now **not constant**



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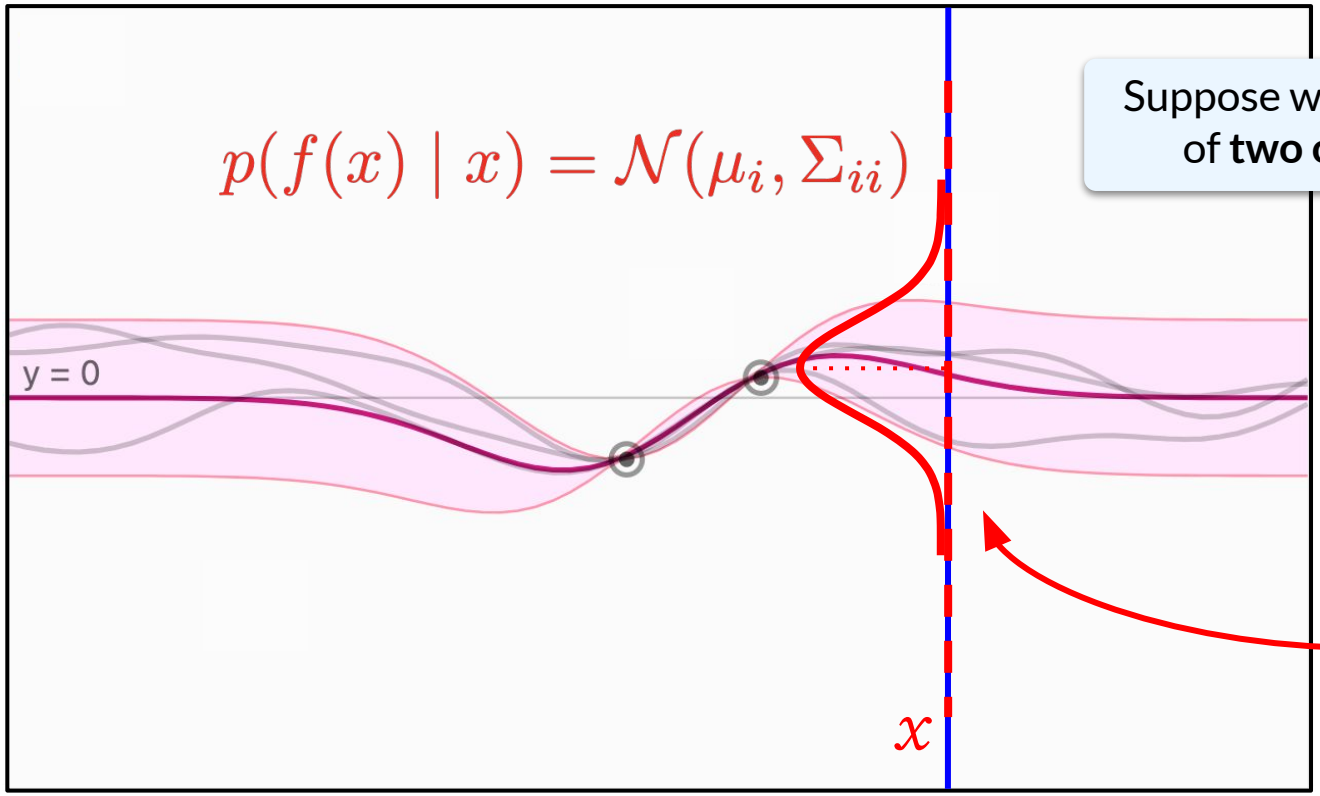

Suppose we have a dataset of **two observations**

Mean function is now **not constant**

To make predictions for a given x, just compute marginal of posterior GP

Source: A Visual Exploration of Gaussian Processes

Review — Gaussian Process Posterior

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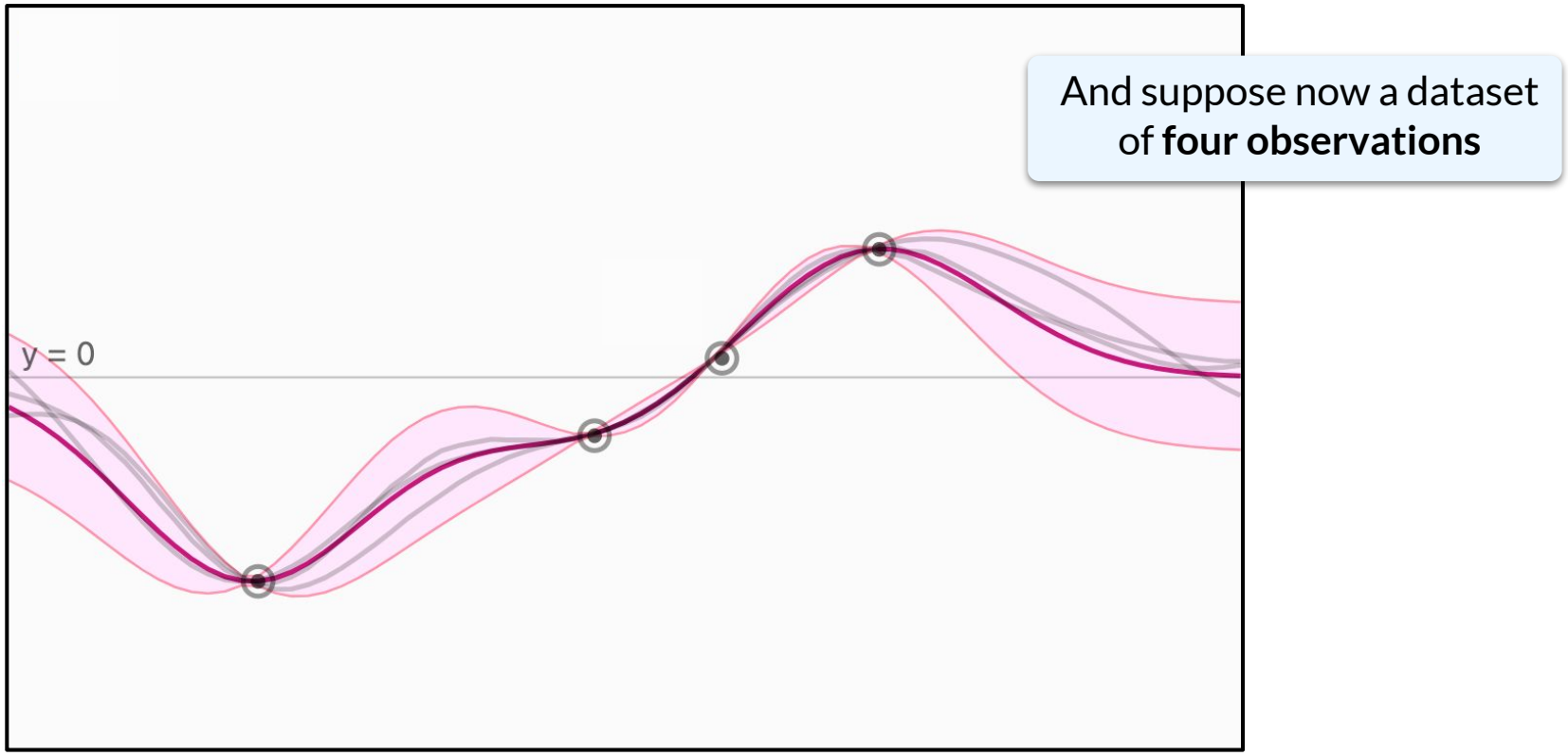

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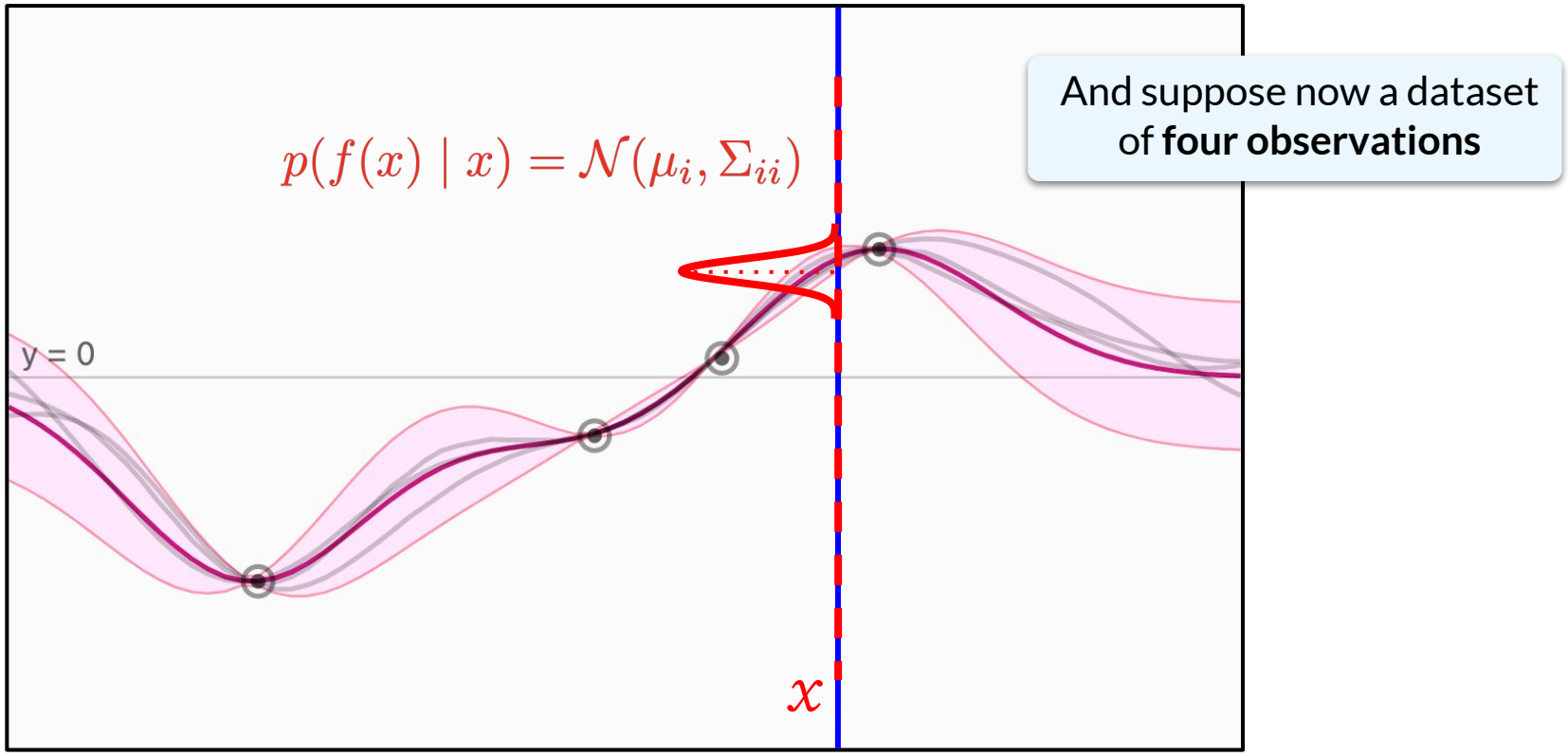

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Gaussian Processes — Summary

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- ⇒ This yields a predictive UQ model!

Deep Uncertainty Models

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We can also define predictive UQ models using neural networks.

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I will go through a few examples of these.

Deep Uncertainty Models

As a running example, we'll look at methods for incorporating predictive uncertainty into the following neural network:

Deep Uncertainty Models —Example: Computational Catalyst Design

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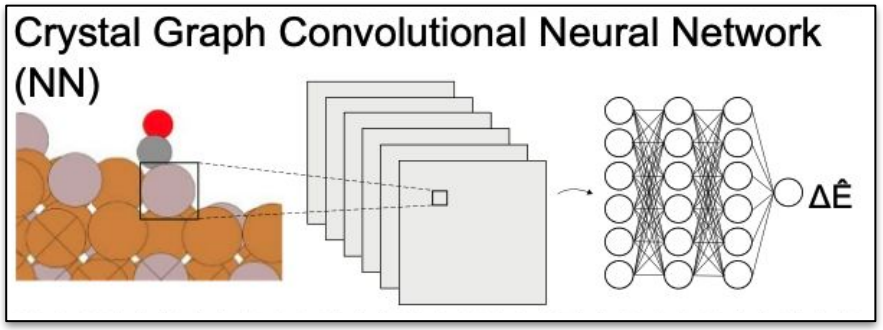

*Xie, Tian, and Jeffrey C. Grossman. "**Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties."** Physical review letters, 2018.*

CGCNN Model *(a graph convolutional neural network model)*

- *Inputs*: three-dimensional atomic structure (a graph).
- *Outputs*: DFT-calculated site adsorption energies ΔE.

  (⇒ *Regression*).

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Deep Uncertainty Models —Example: Computational Catalyst Design

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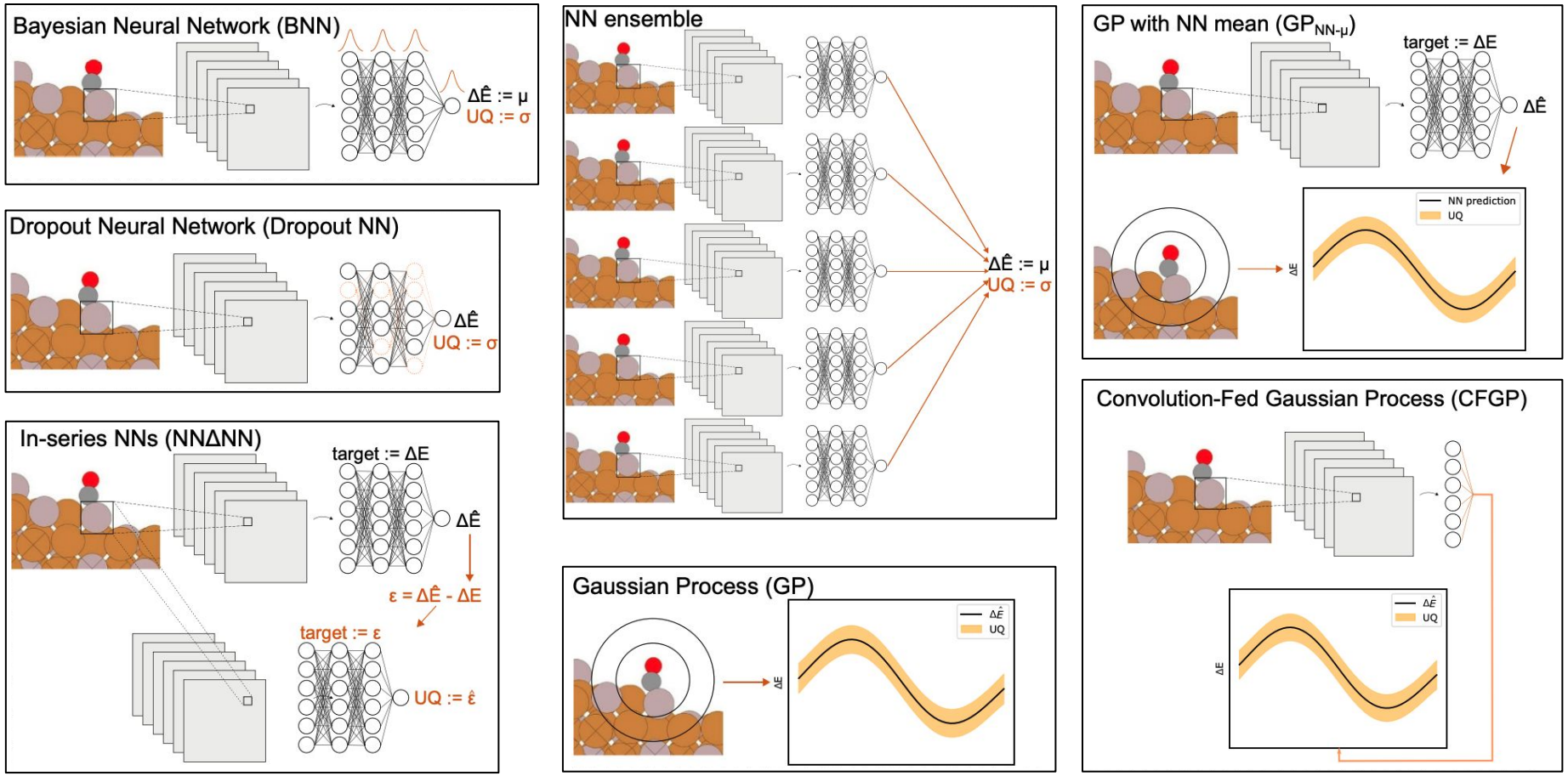
⇒ there are many ways this can be done, and it's an active area of research!

Deep Uncertainty Models —Example: Computational Catalyst Design



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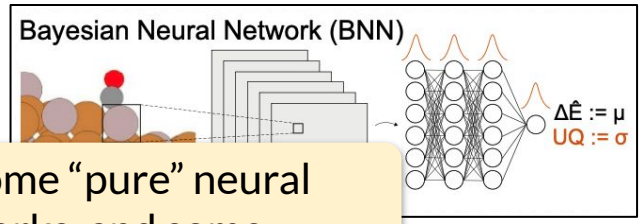
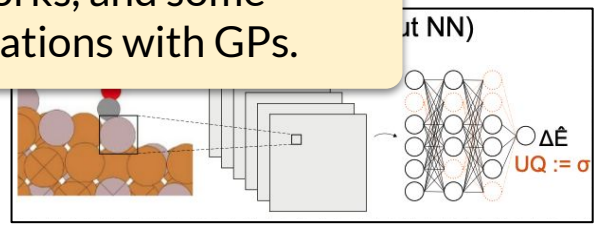
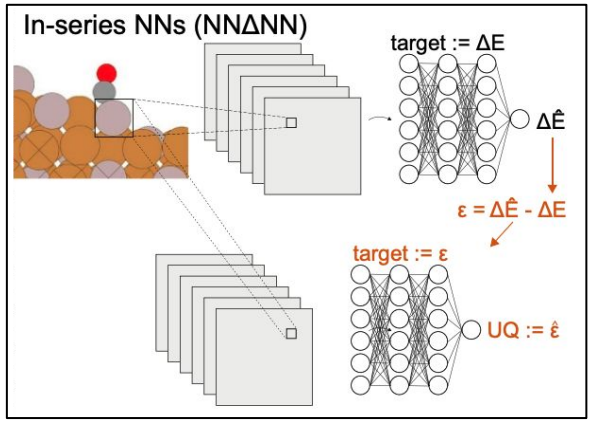
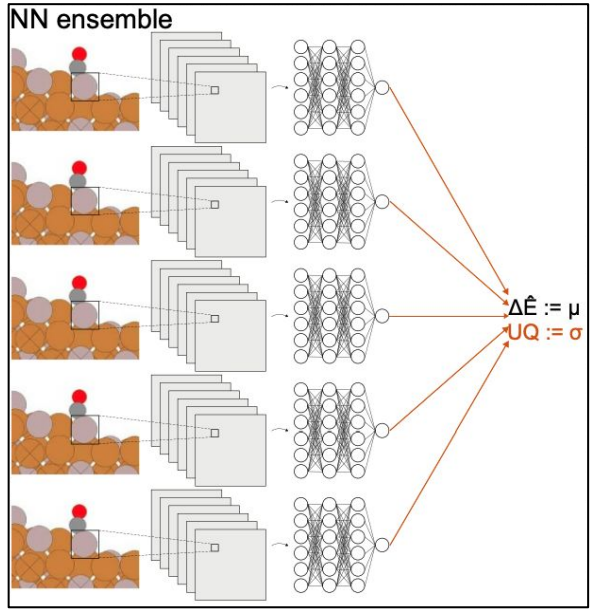
Deep Uncertainty Models —Example: Computational Catalyst Design

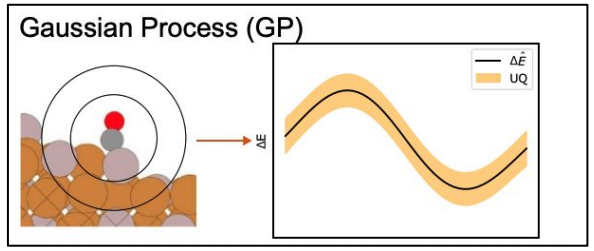
Note: some “pure” neural networks, and some combinations with GPs.

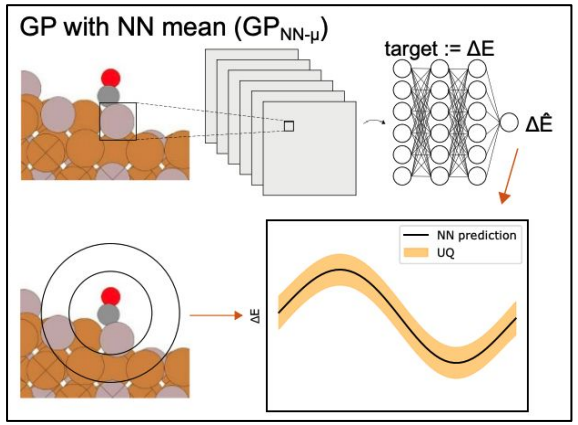


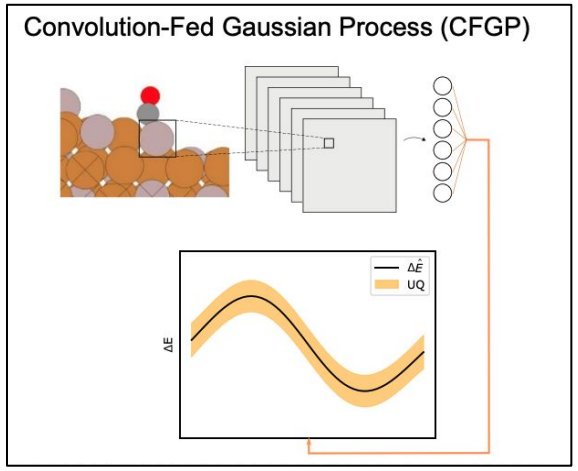












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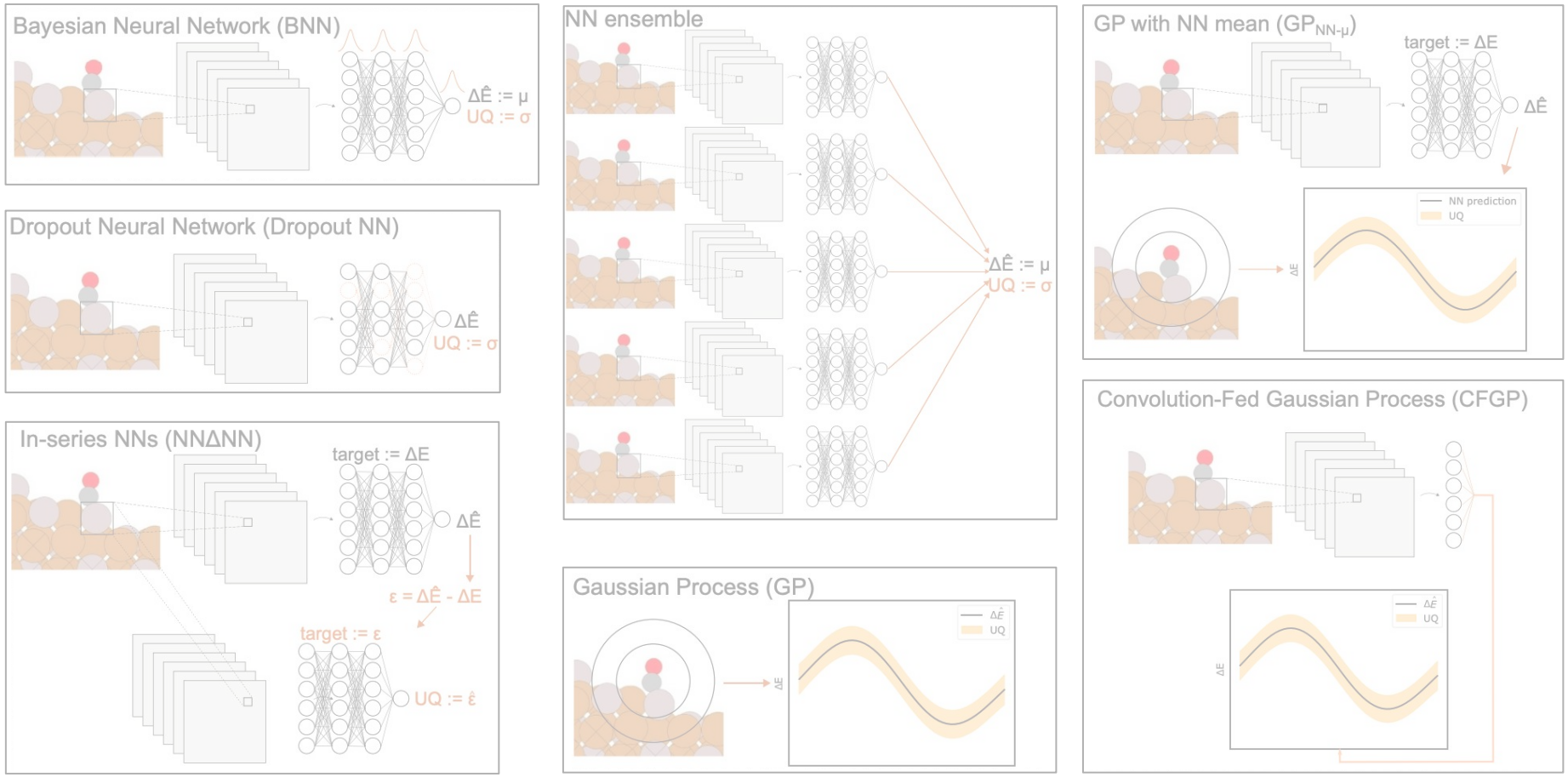

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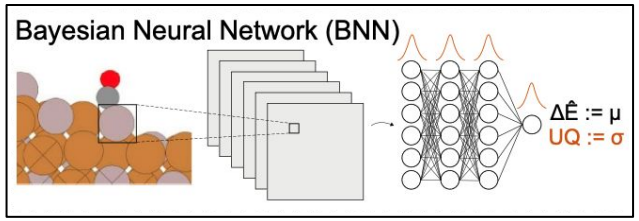

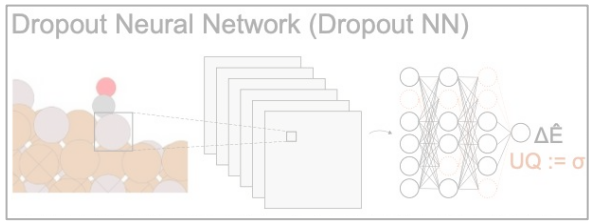

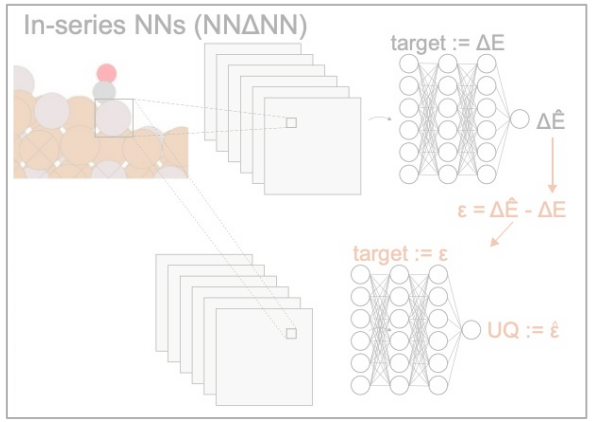

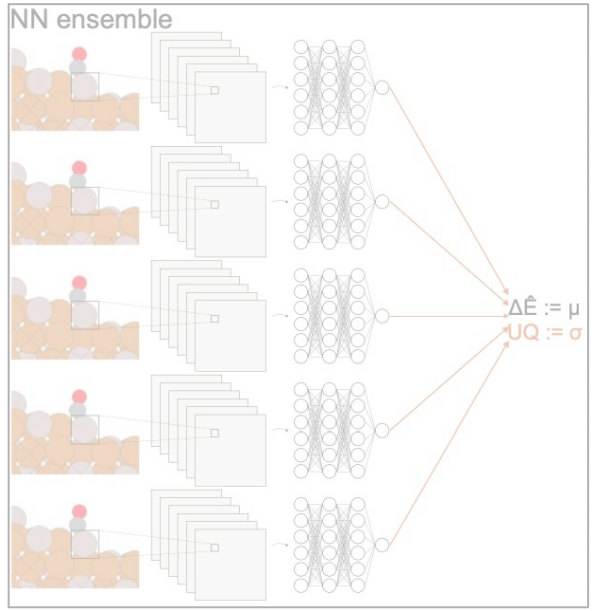

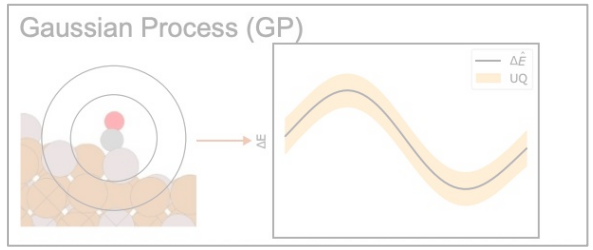

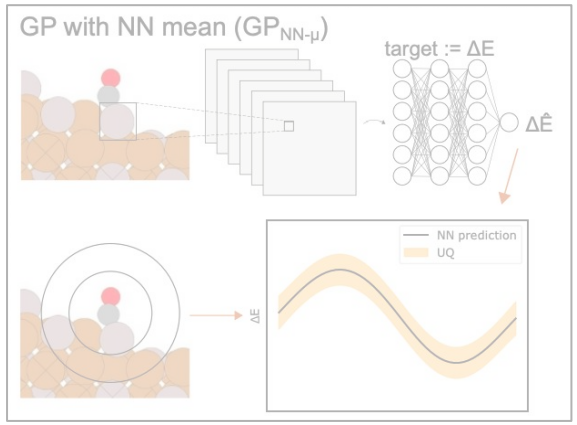

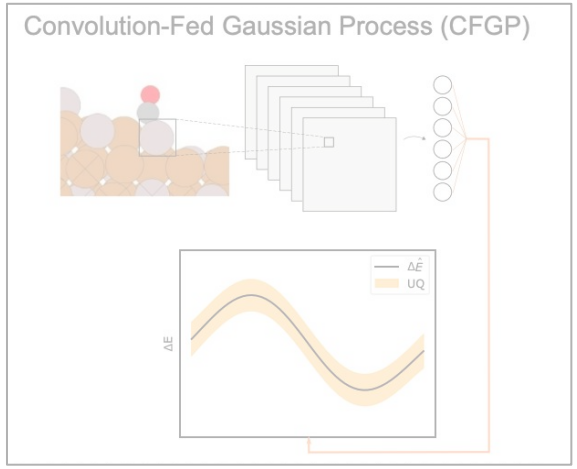

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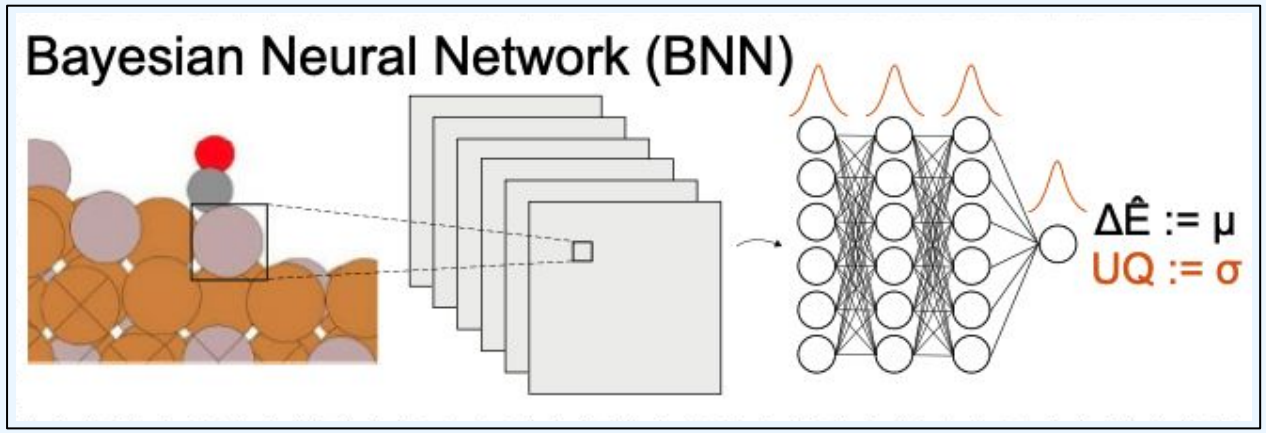

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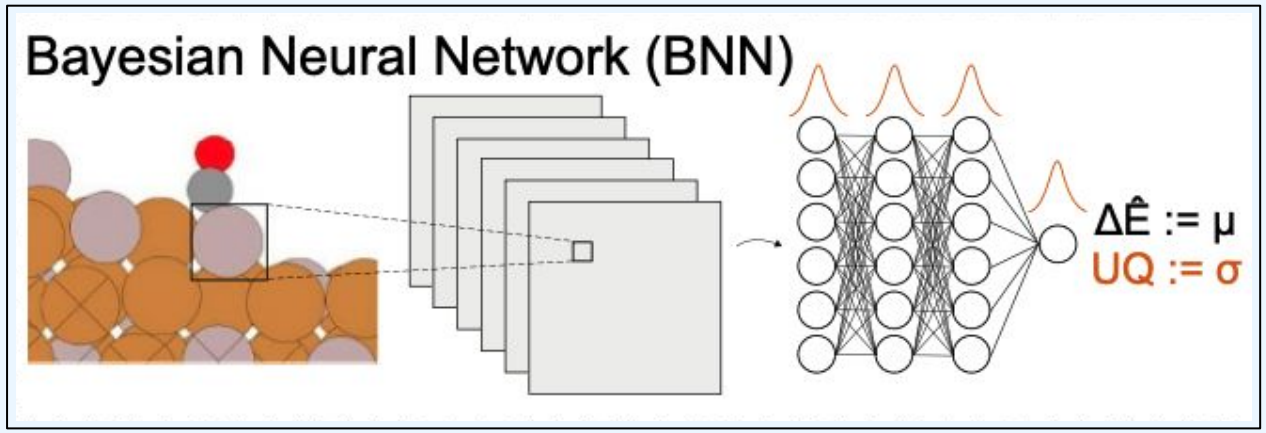

- Define a prior on neural network weights.
- In training, compute posterior over neural network weights (rather than a point estimate).
- Often using some type of MCMC (*e.g.*, LMC) or variational inference.

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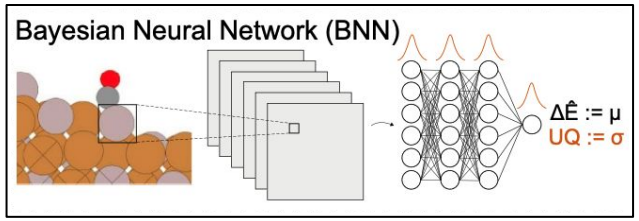

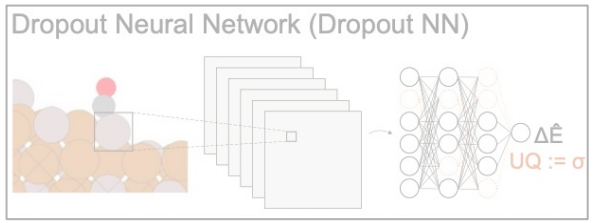

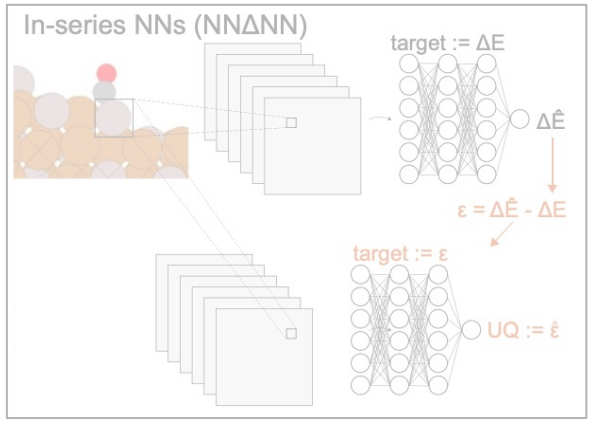

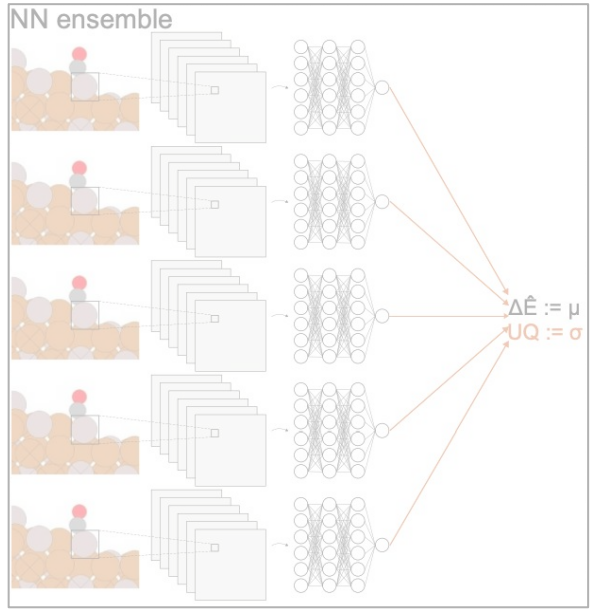

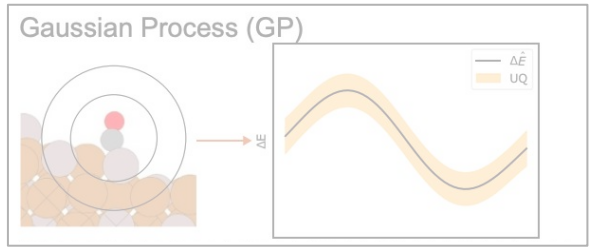

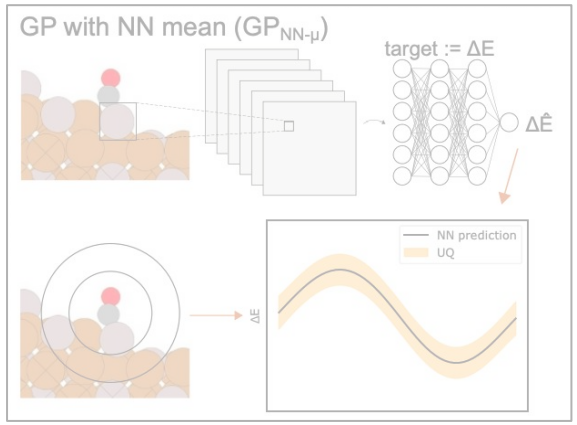

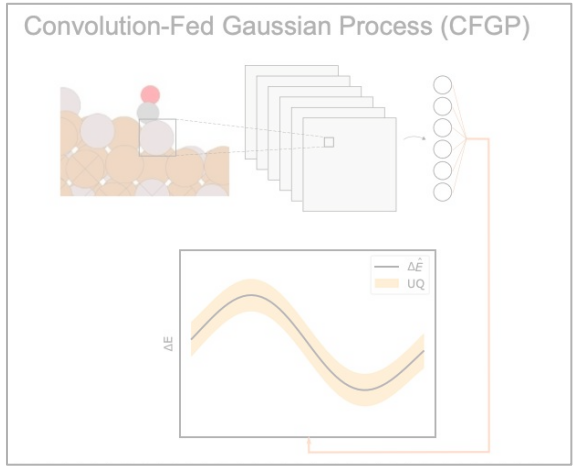

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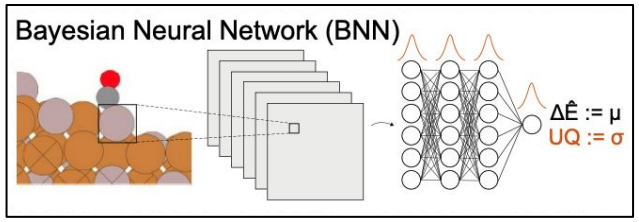

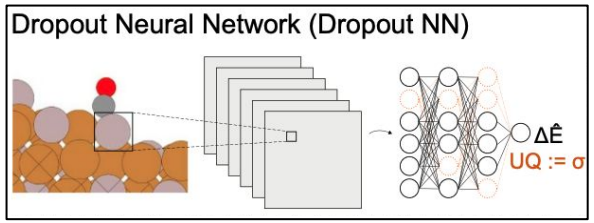

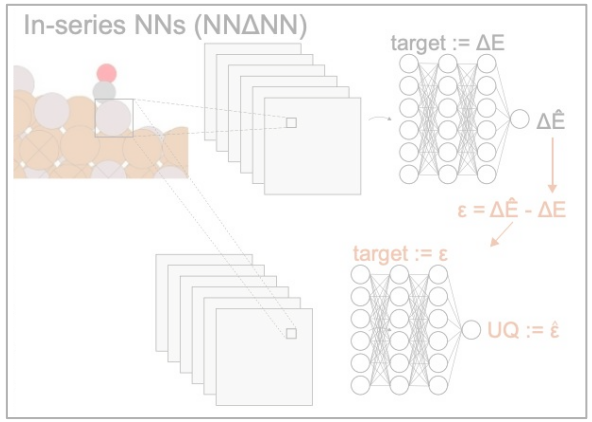

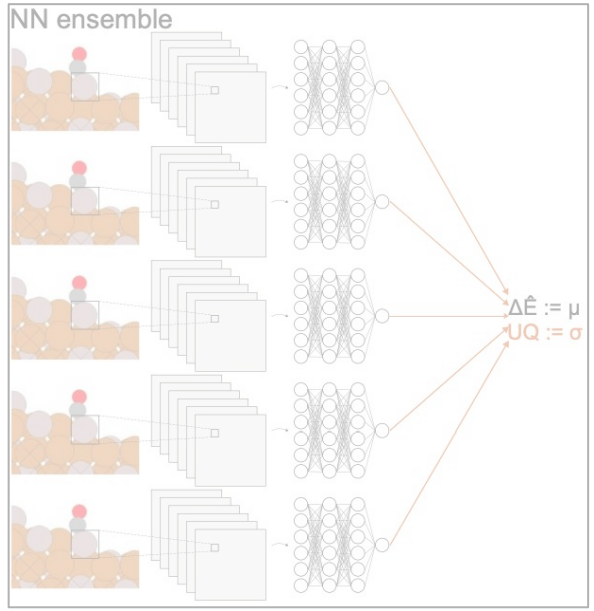

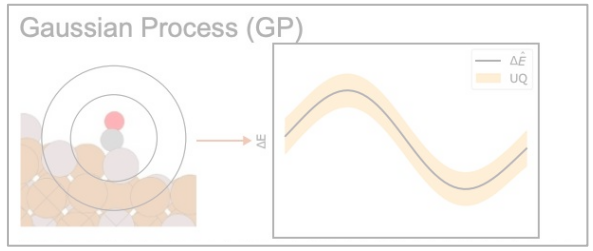

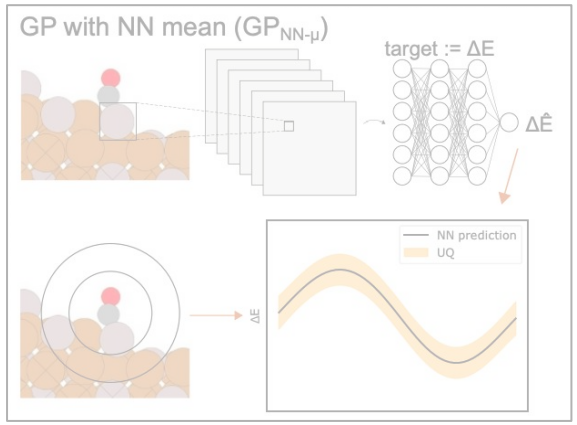

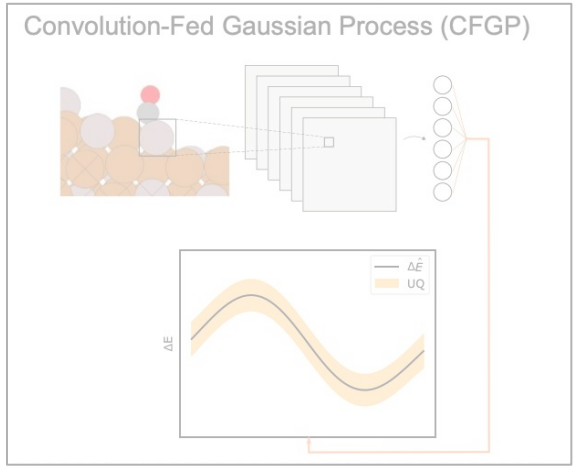

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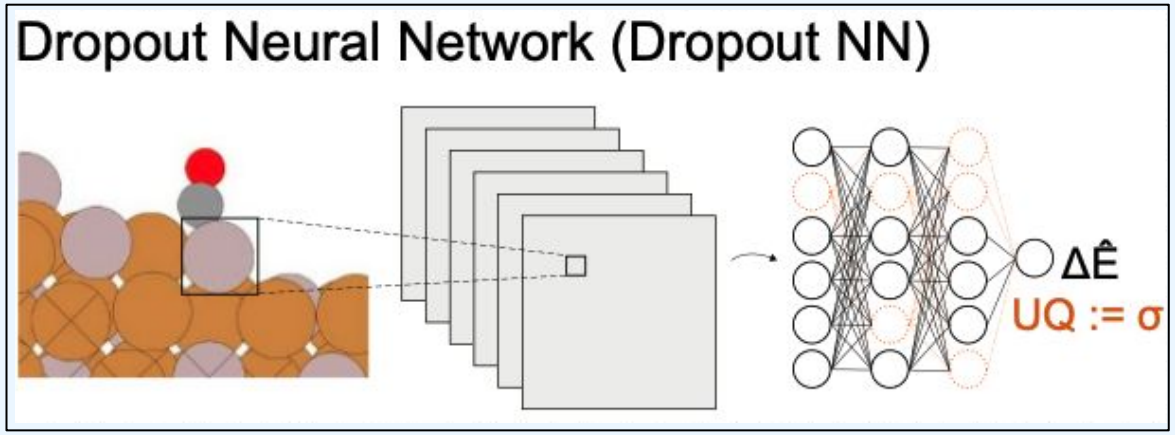

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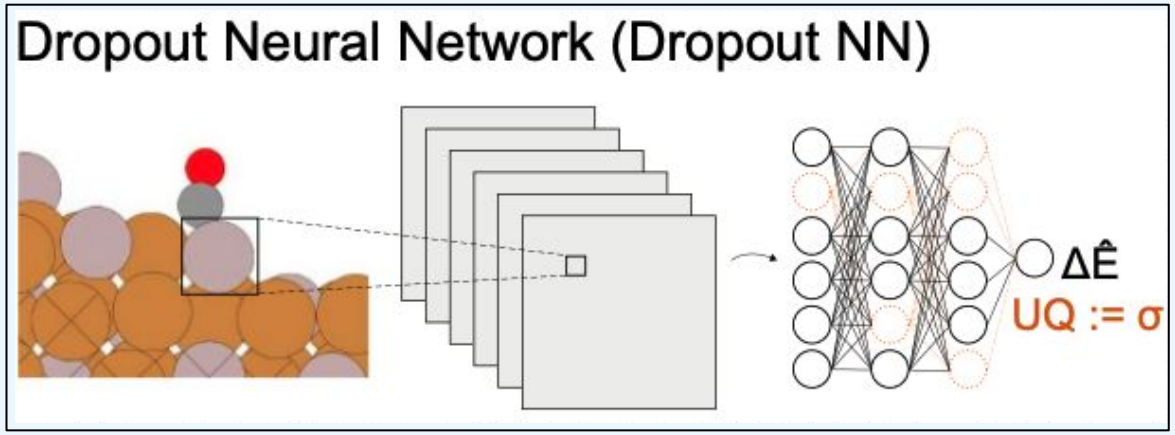

- During train/inference-time, perform *Monte Carlo Dropout*.
- (*I.e.*, set a random fraction of the neuron's outputs to zero during forward pass of the model).
- ⇒ A set of forward passes yields a set of samples from an output distribution.

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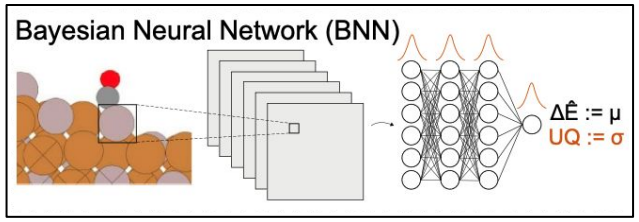

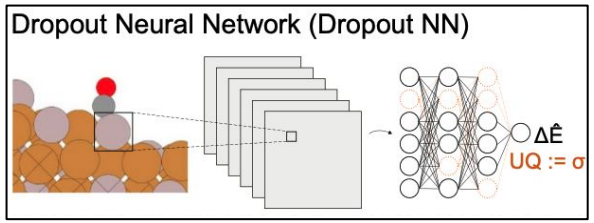

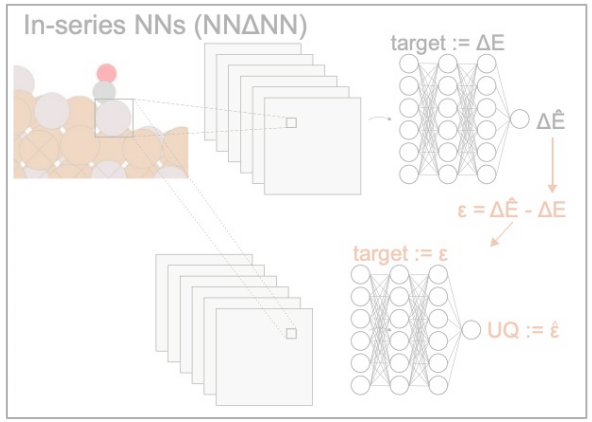

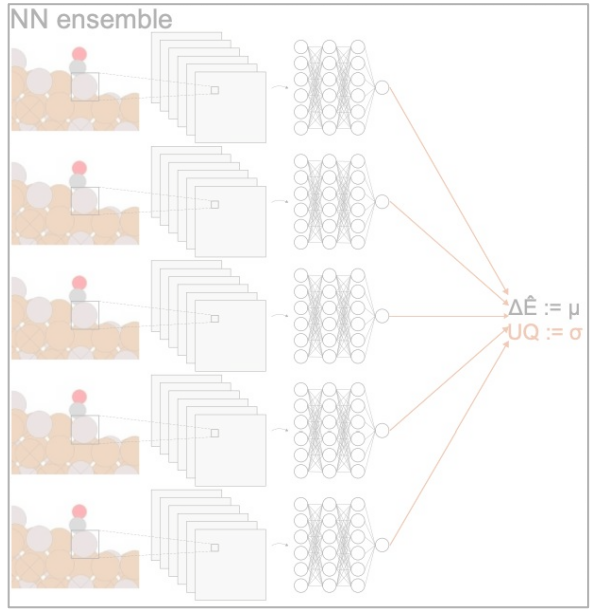

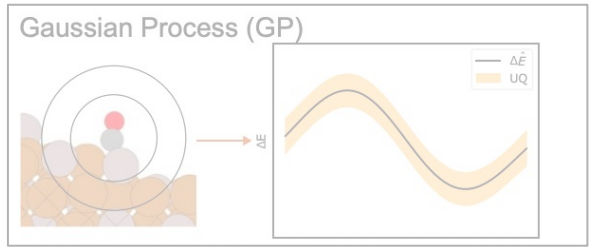

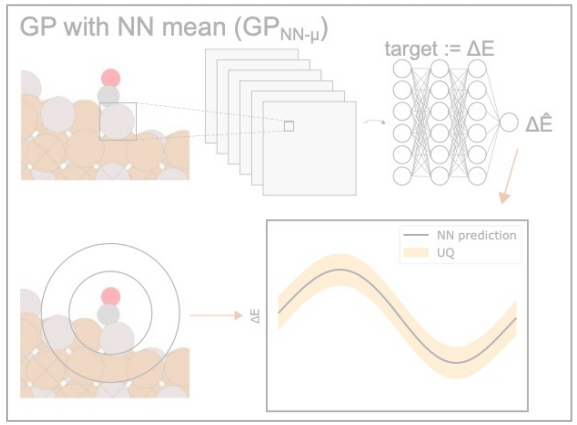

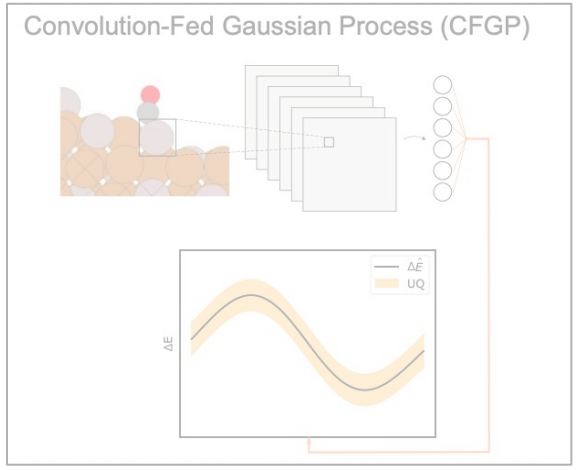

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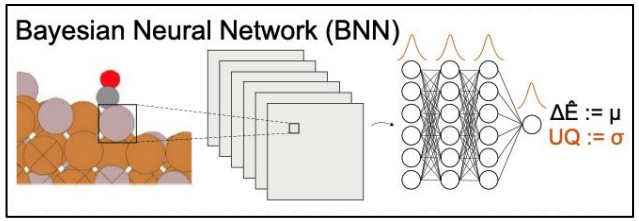

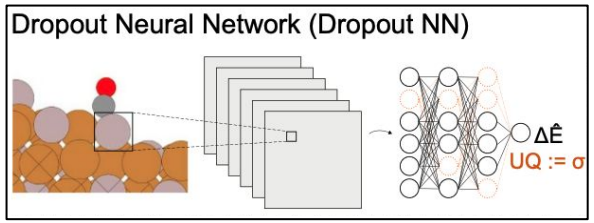

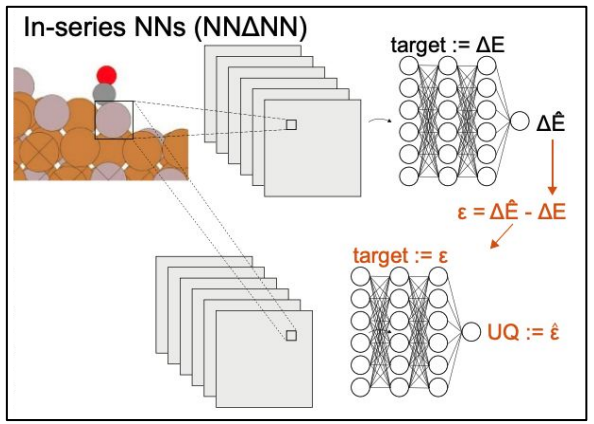

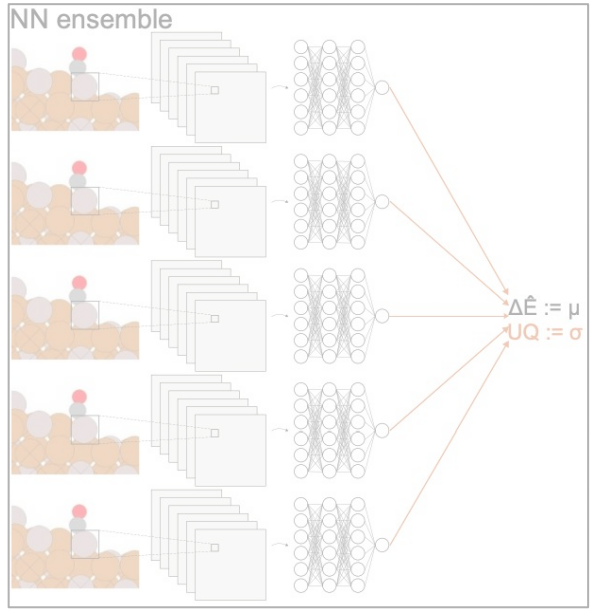

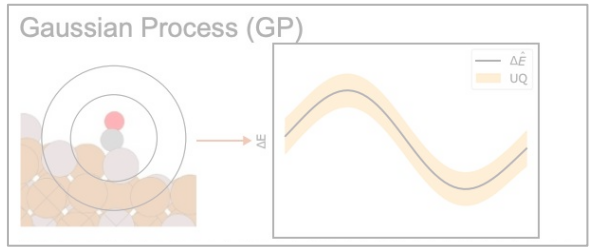

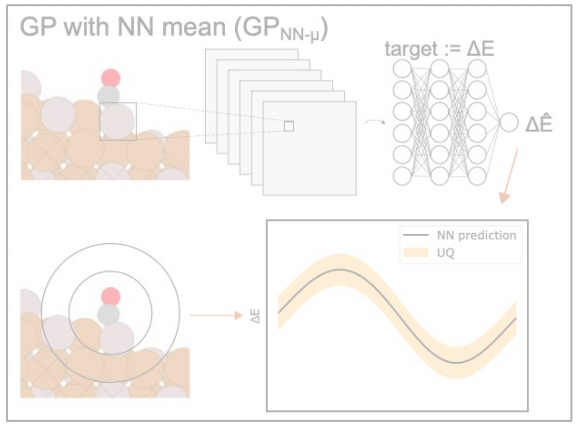

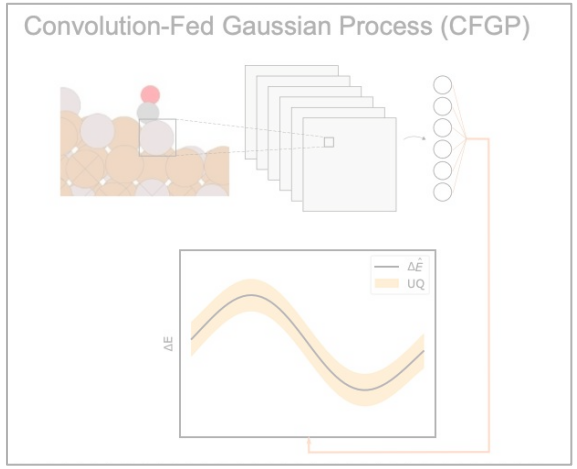

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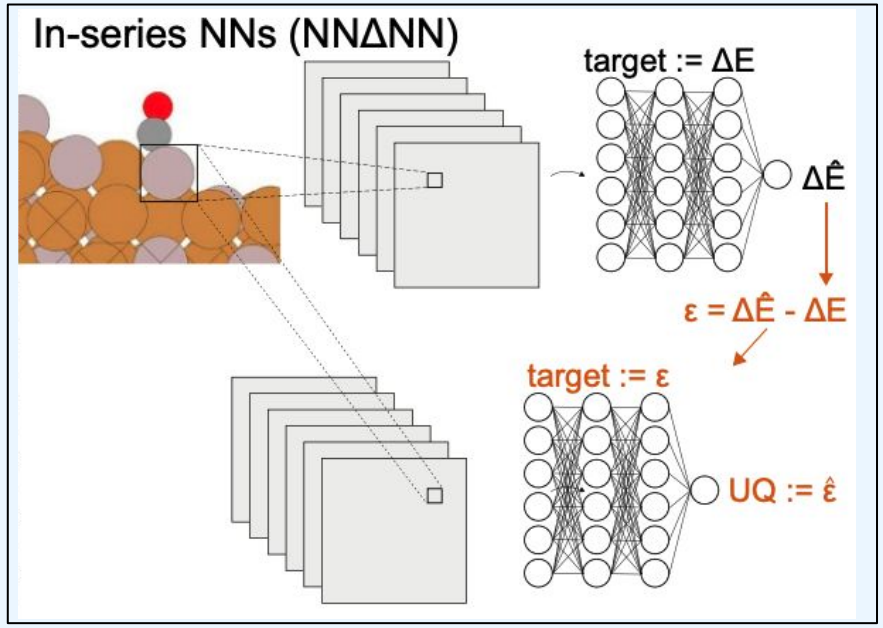

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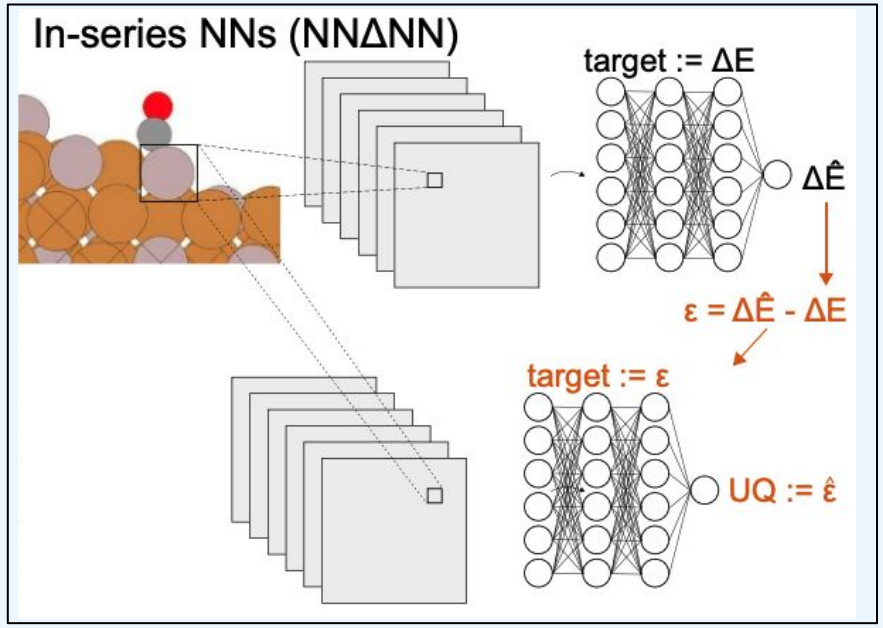

- First train a neural network for point prediction.
- Then compute residuals on a held-out set.
- Then use another neural network to try and predict residuals.

- ⇒ Second network predicts error, which can be used as UQ model.

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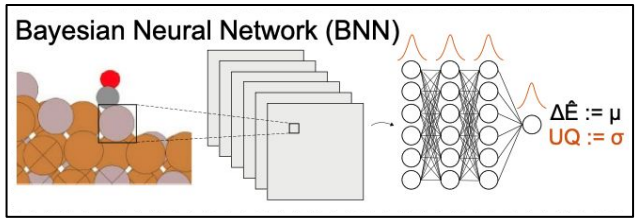

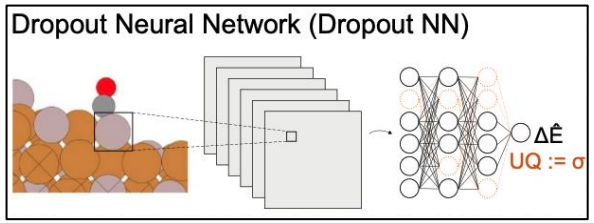

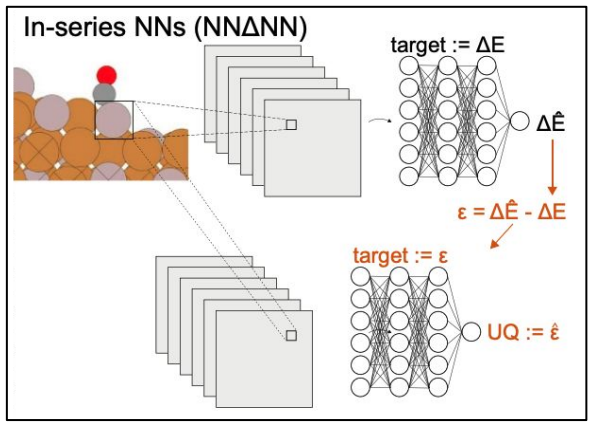

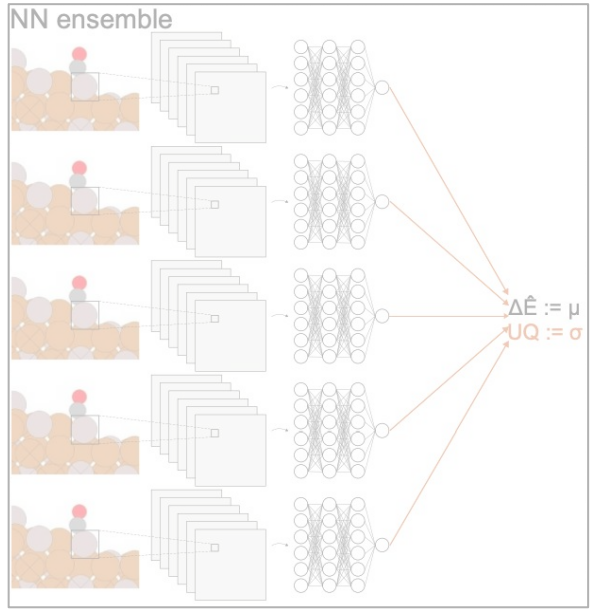

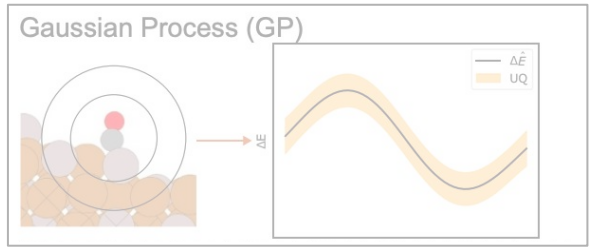

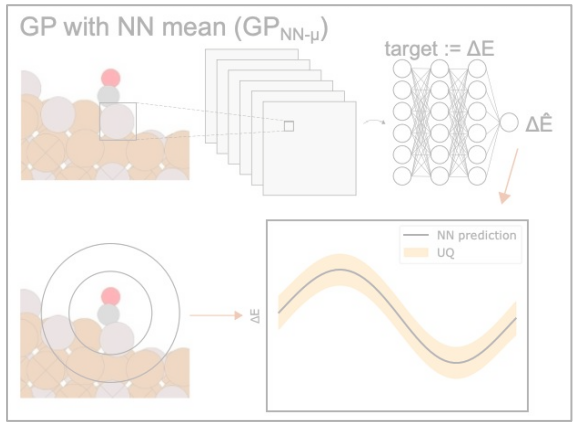

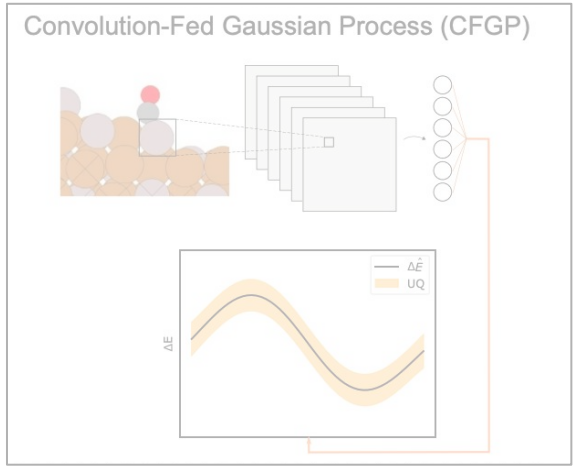

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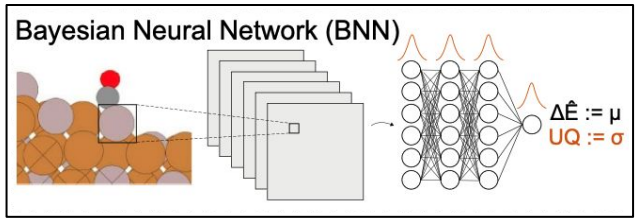

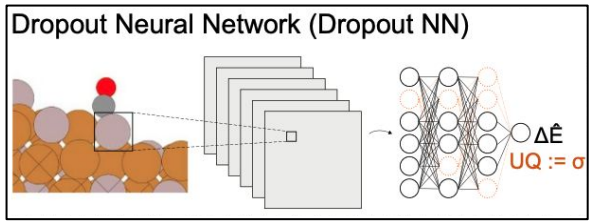

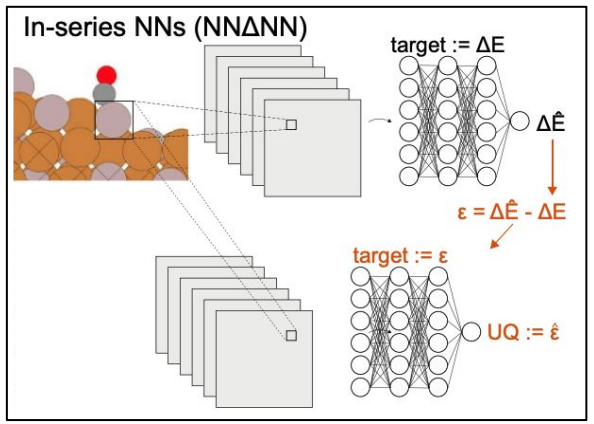

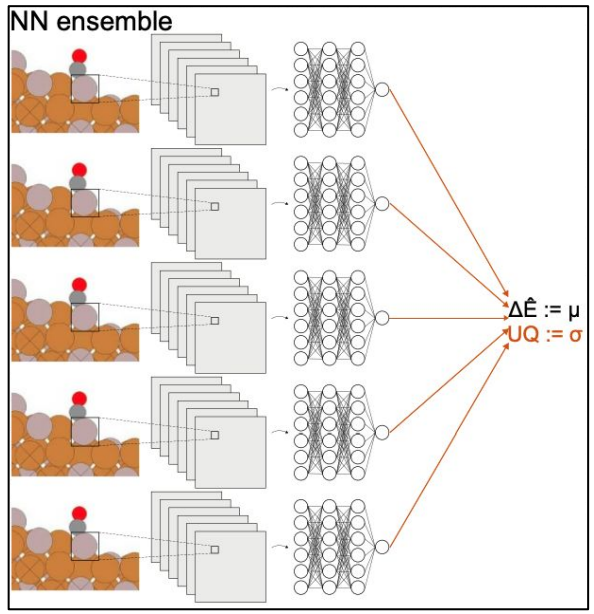

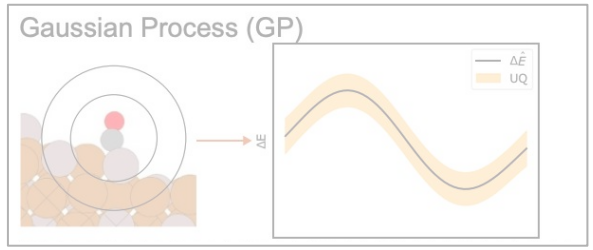

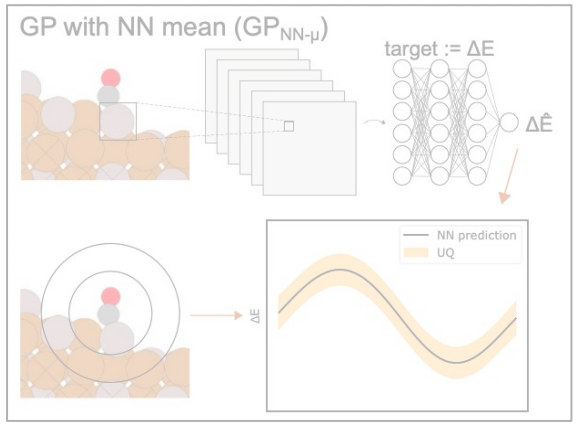

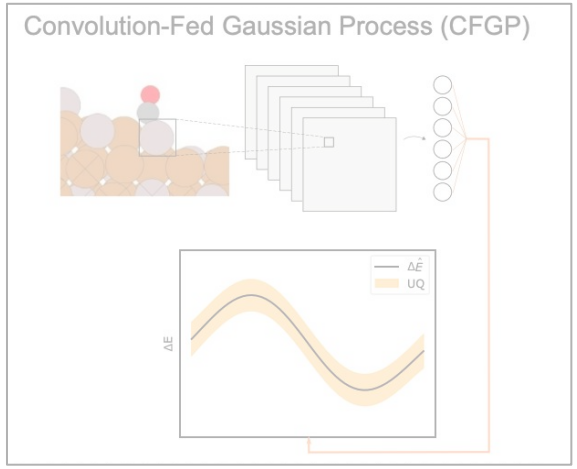

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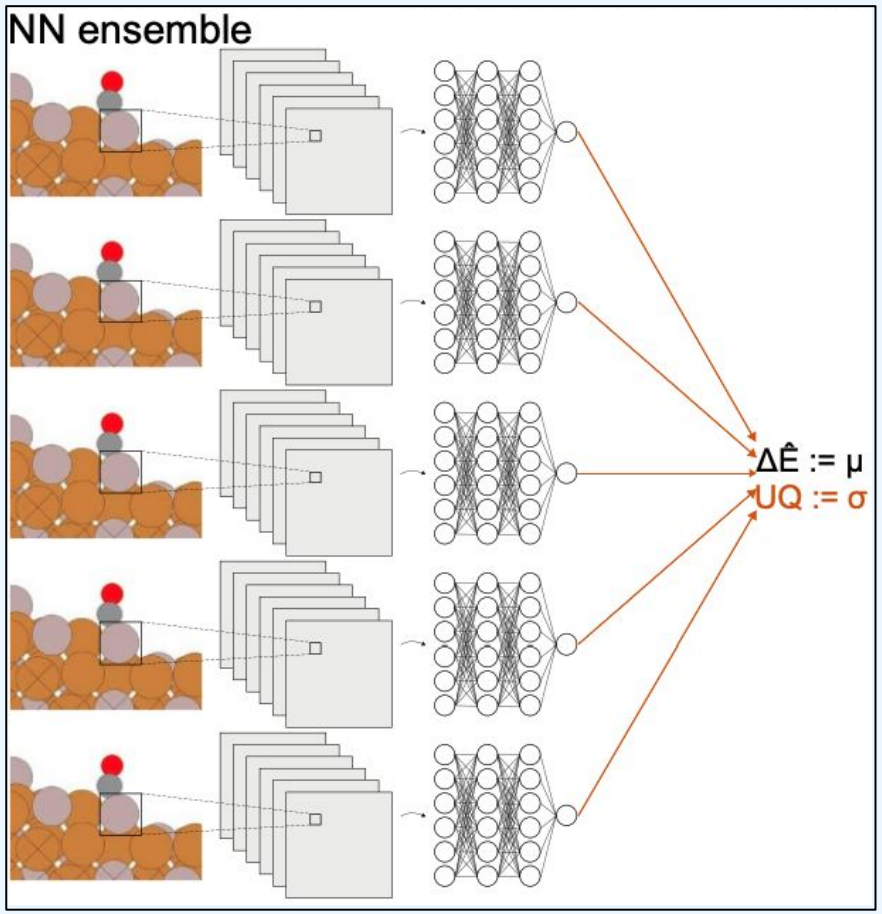

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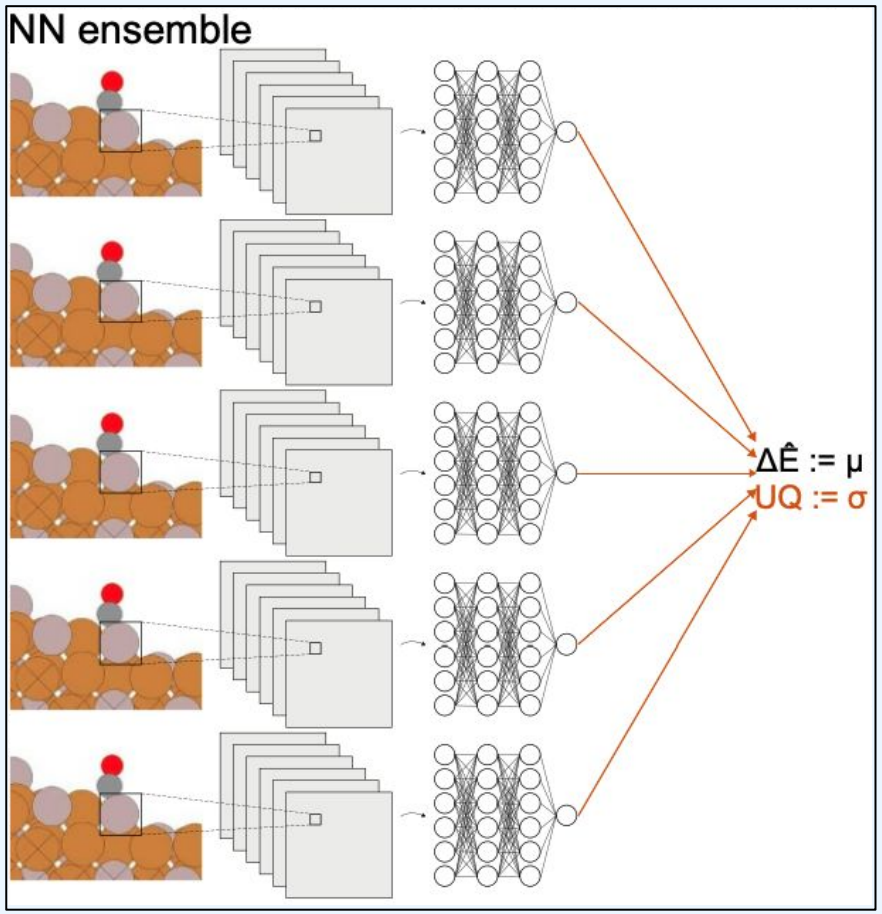

- Train a set of neural networks.
- Often each neural network has a different initialization, subset of data, or hyperparameter setting.
- Use diversity of predictions (agreement) as a measure of uncertainty in predictions.

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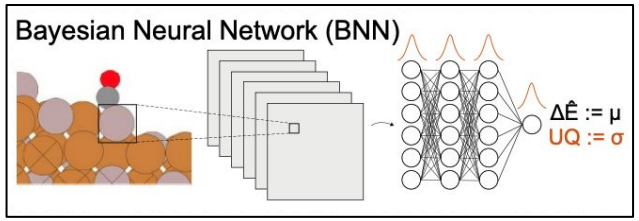

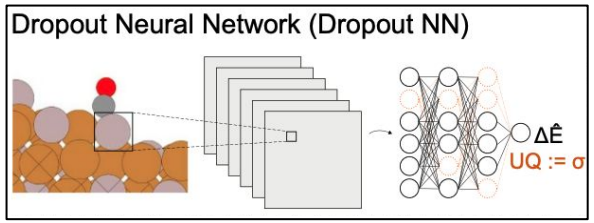

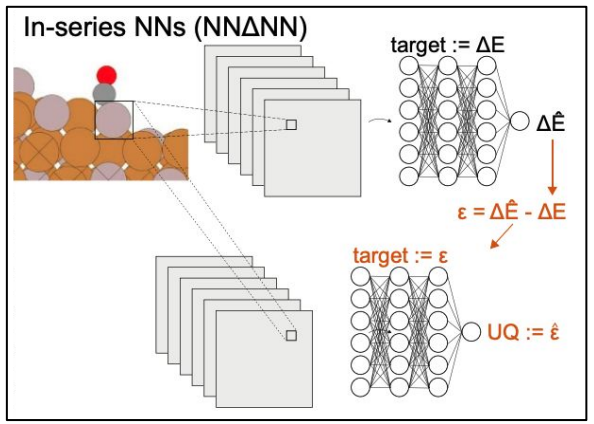

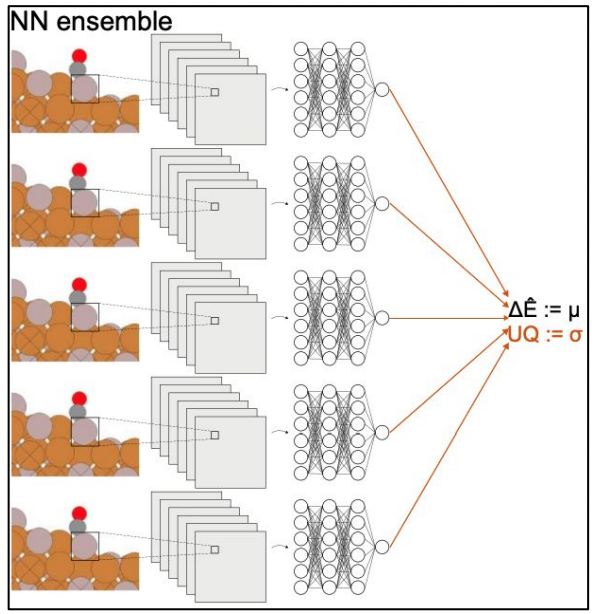

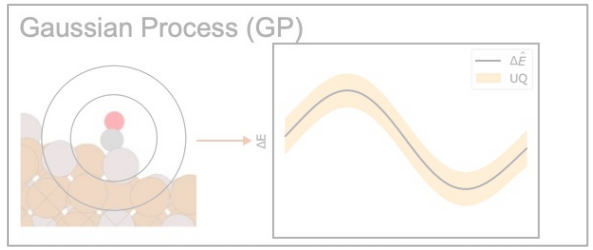

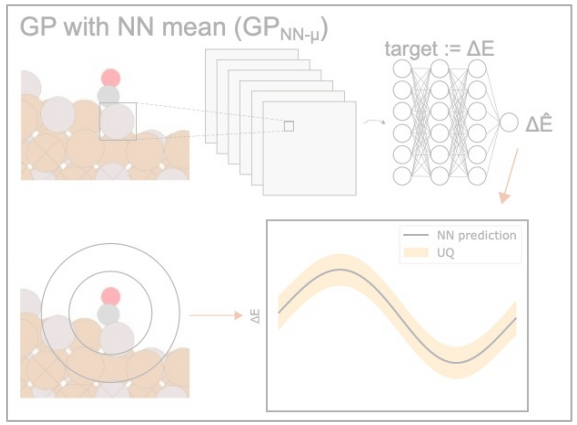

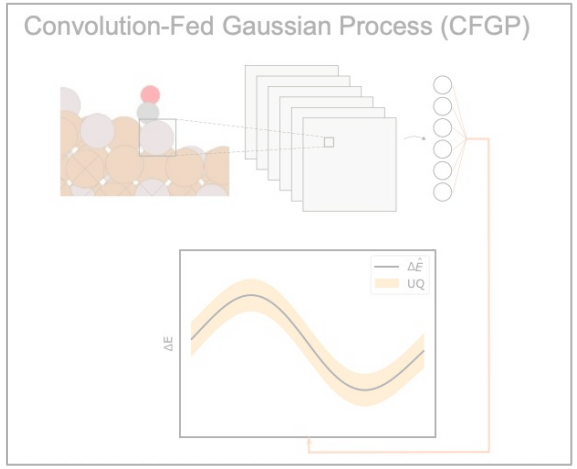

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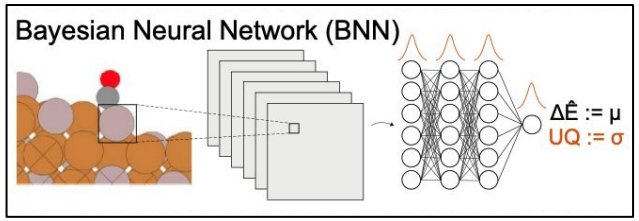

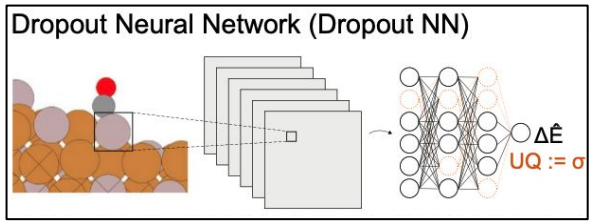

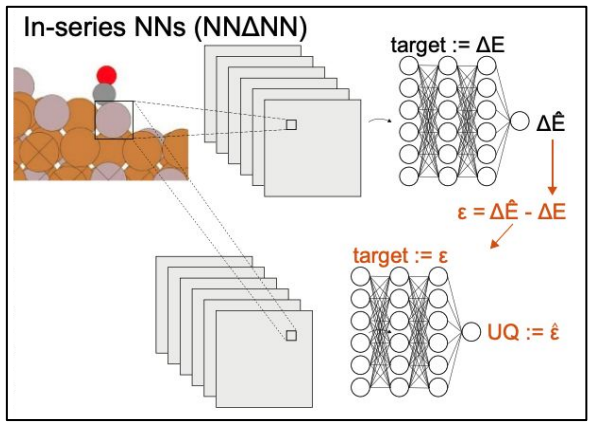

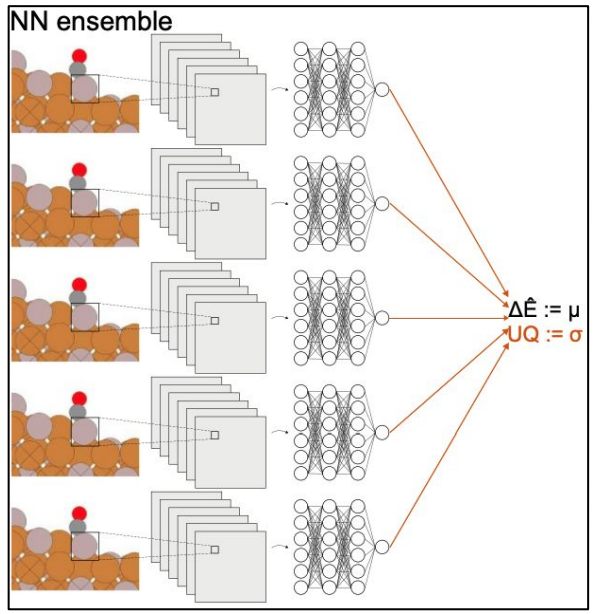

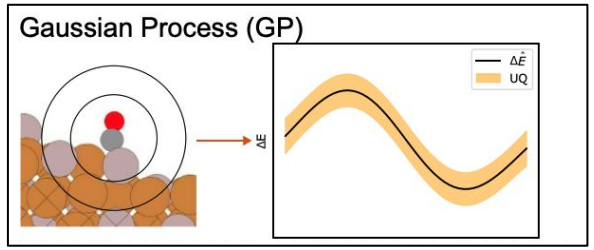

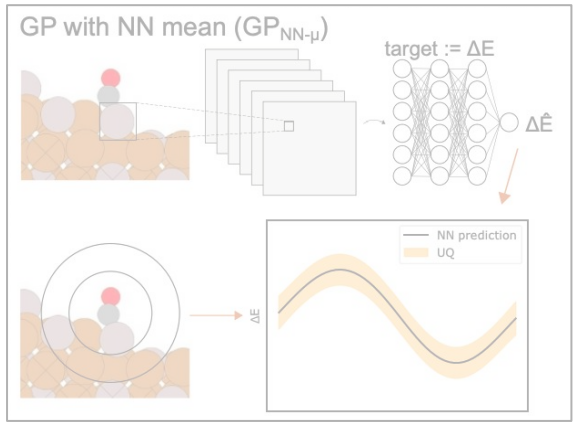

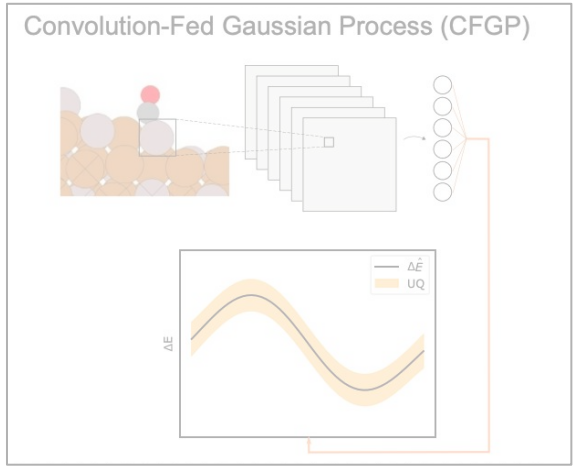

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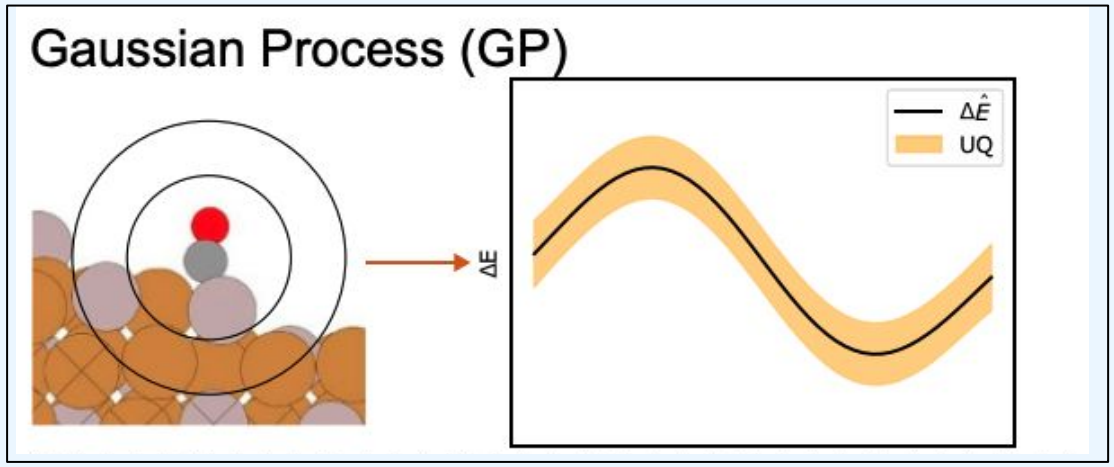

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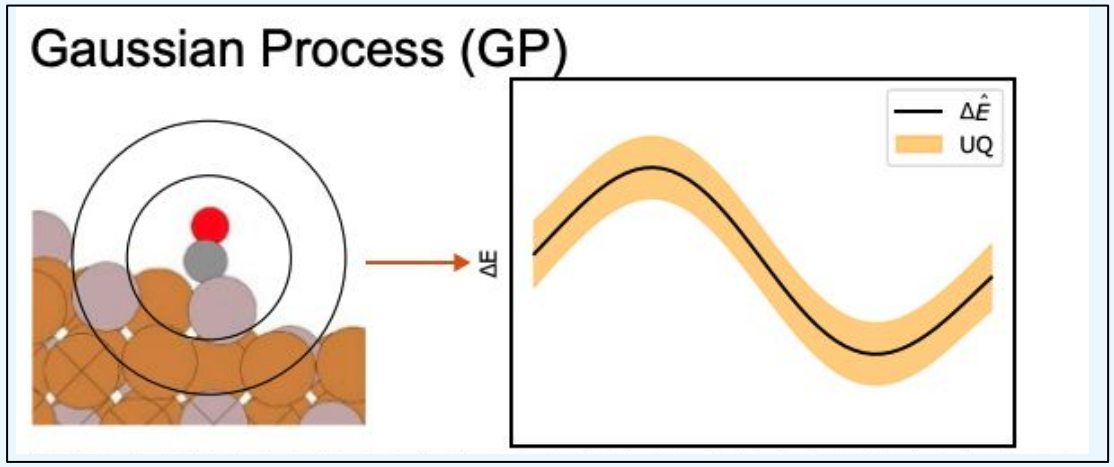

- Define some appropriate mean and kernel function on graph inputs.
- This yields a valid GP, which can make predictions on new inputs (new graphs)
- *Difficulty*: hard to hand-design good kernel function, & doesn't use NN.

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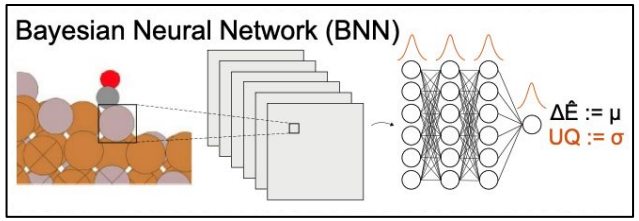

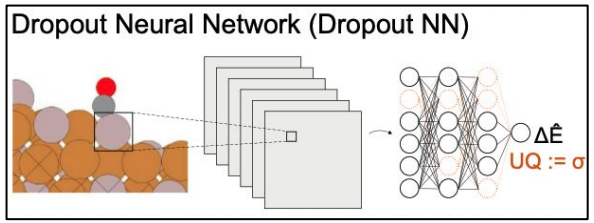

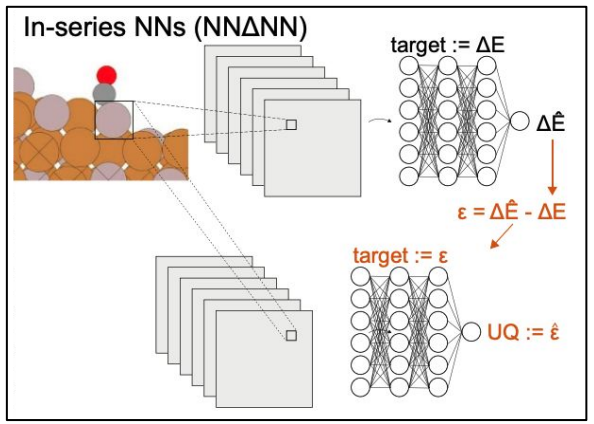

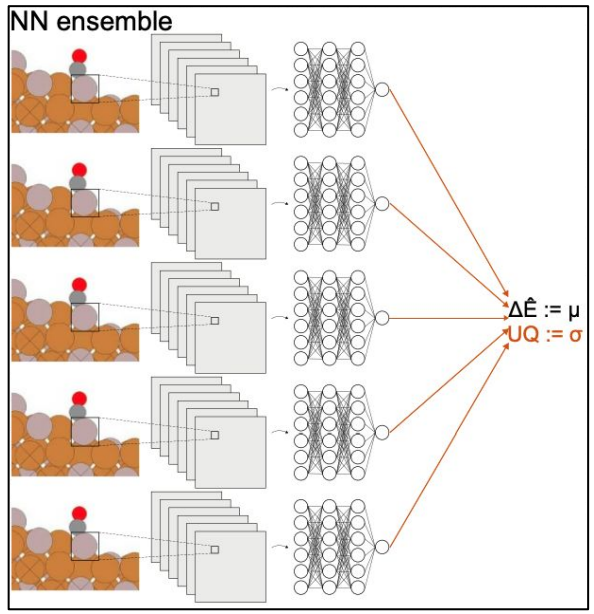

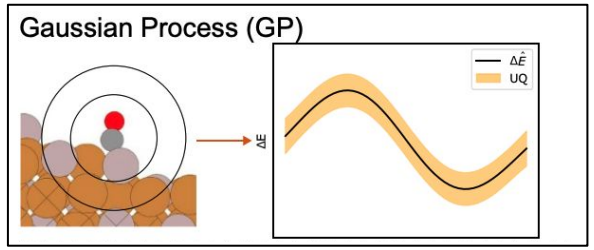

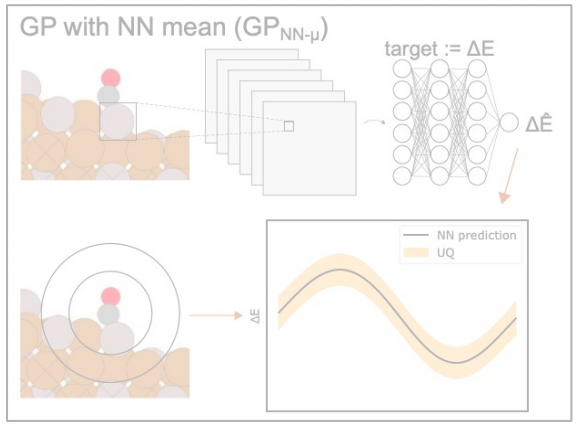

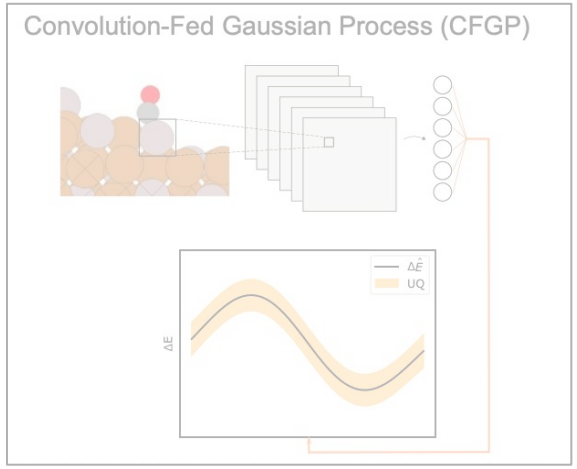

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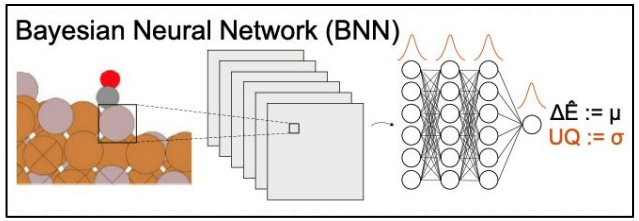

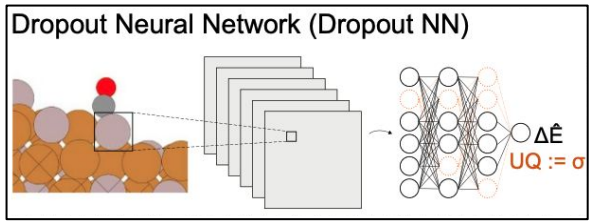

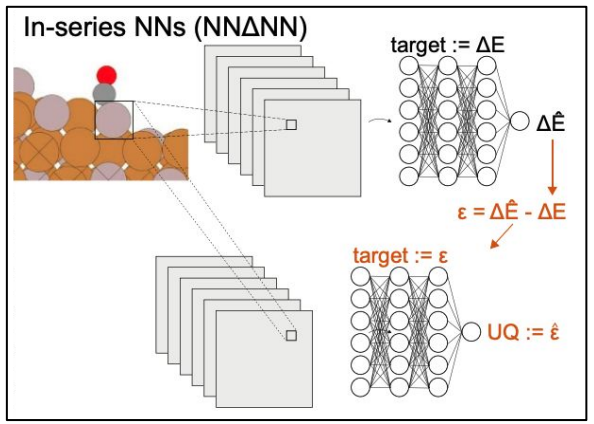

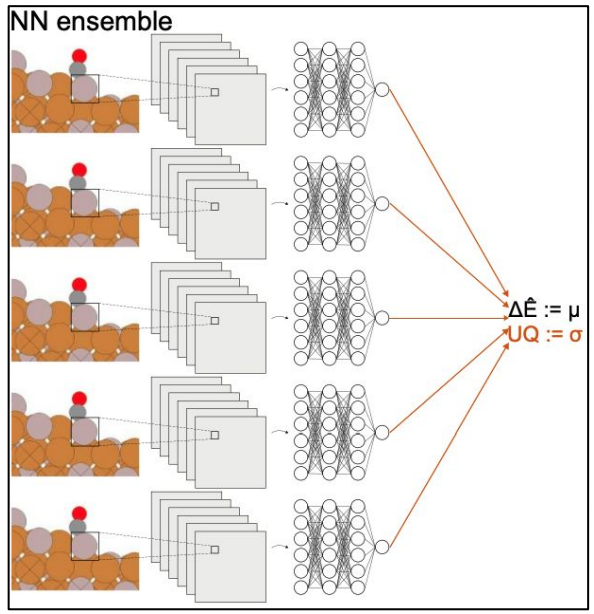

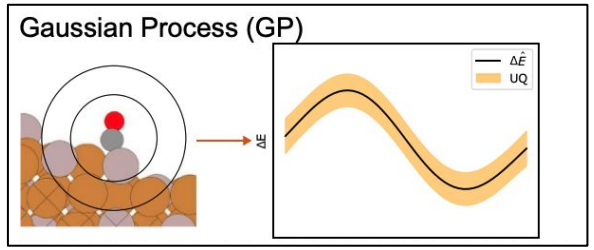

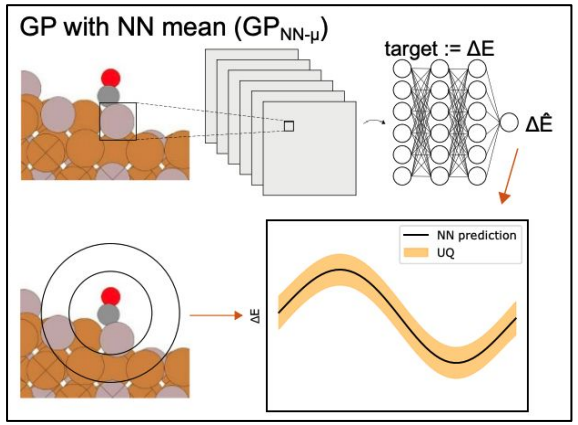

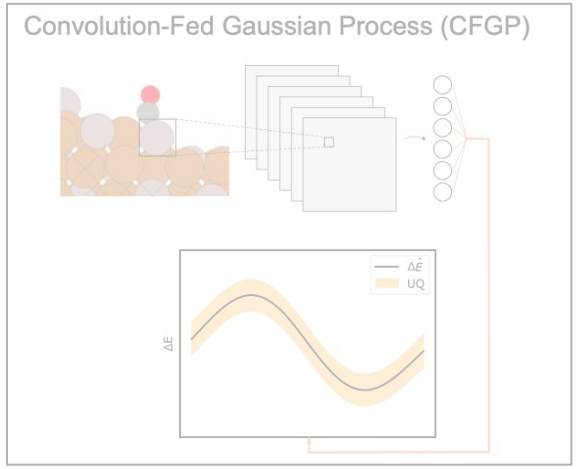

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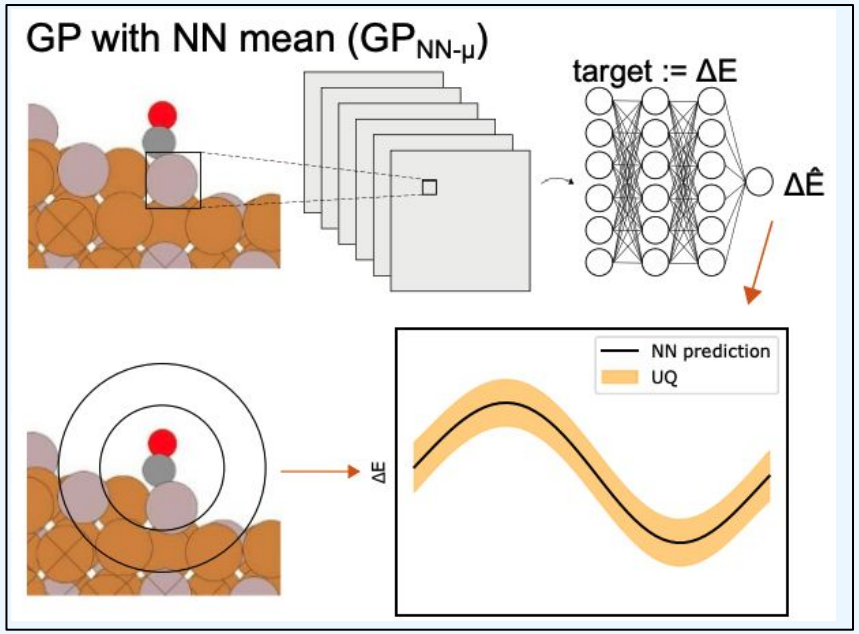

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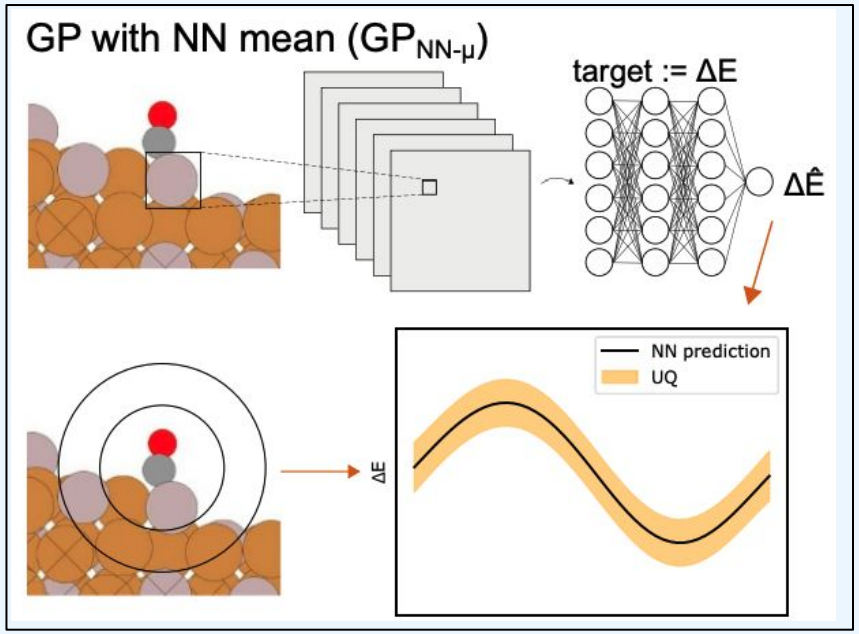

- In GPs, the prior mean fn is usually set to be **0.**
- But it could be anything…
- Here, we can set the prior mean function to be the output of a neural network model!

- Downside: still need to define a kernel function on graph inputs.

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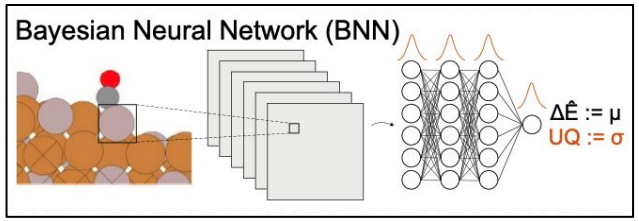

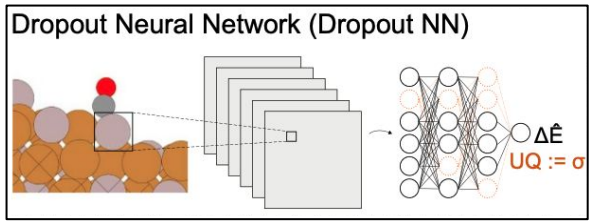

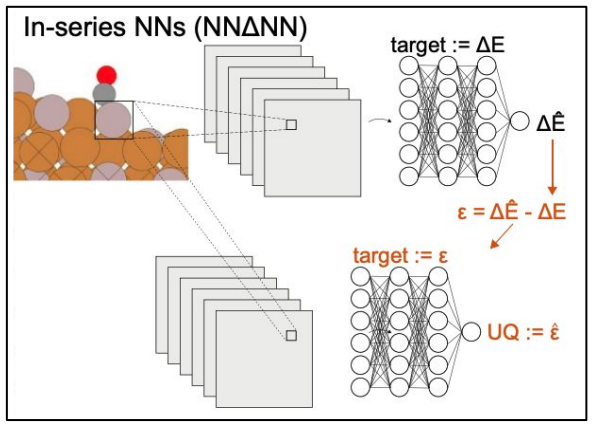

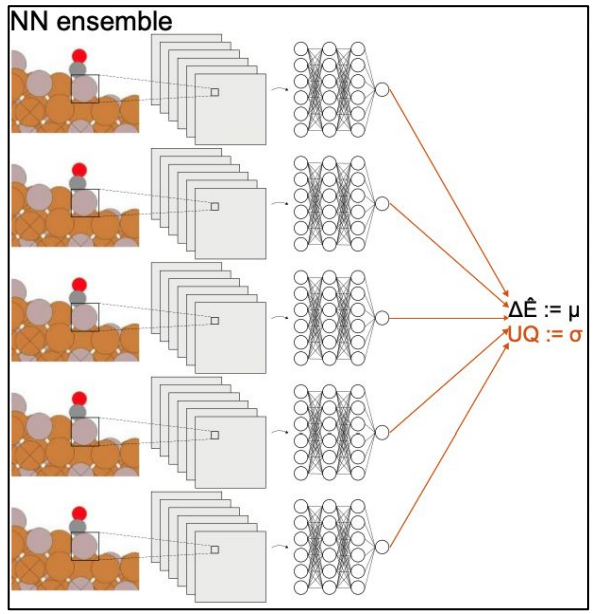

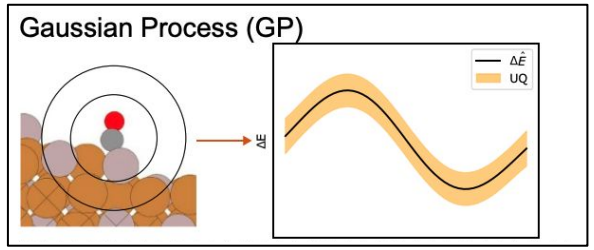

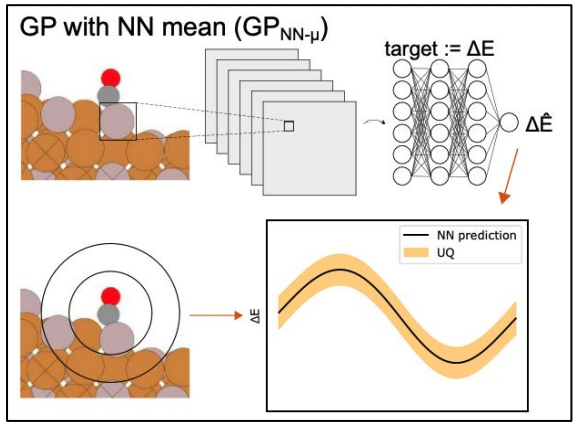

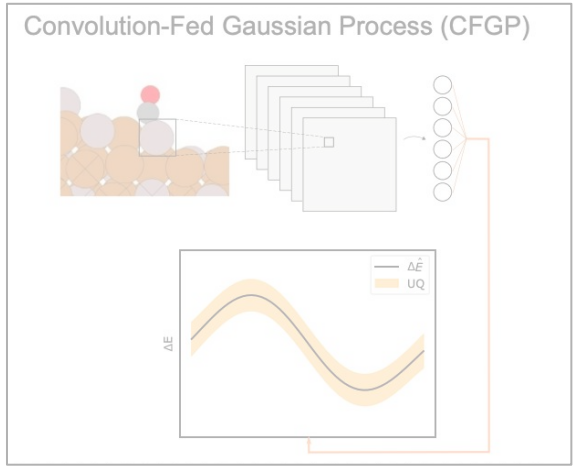

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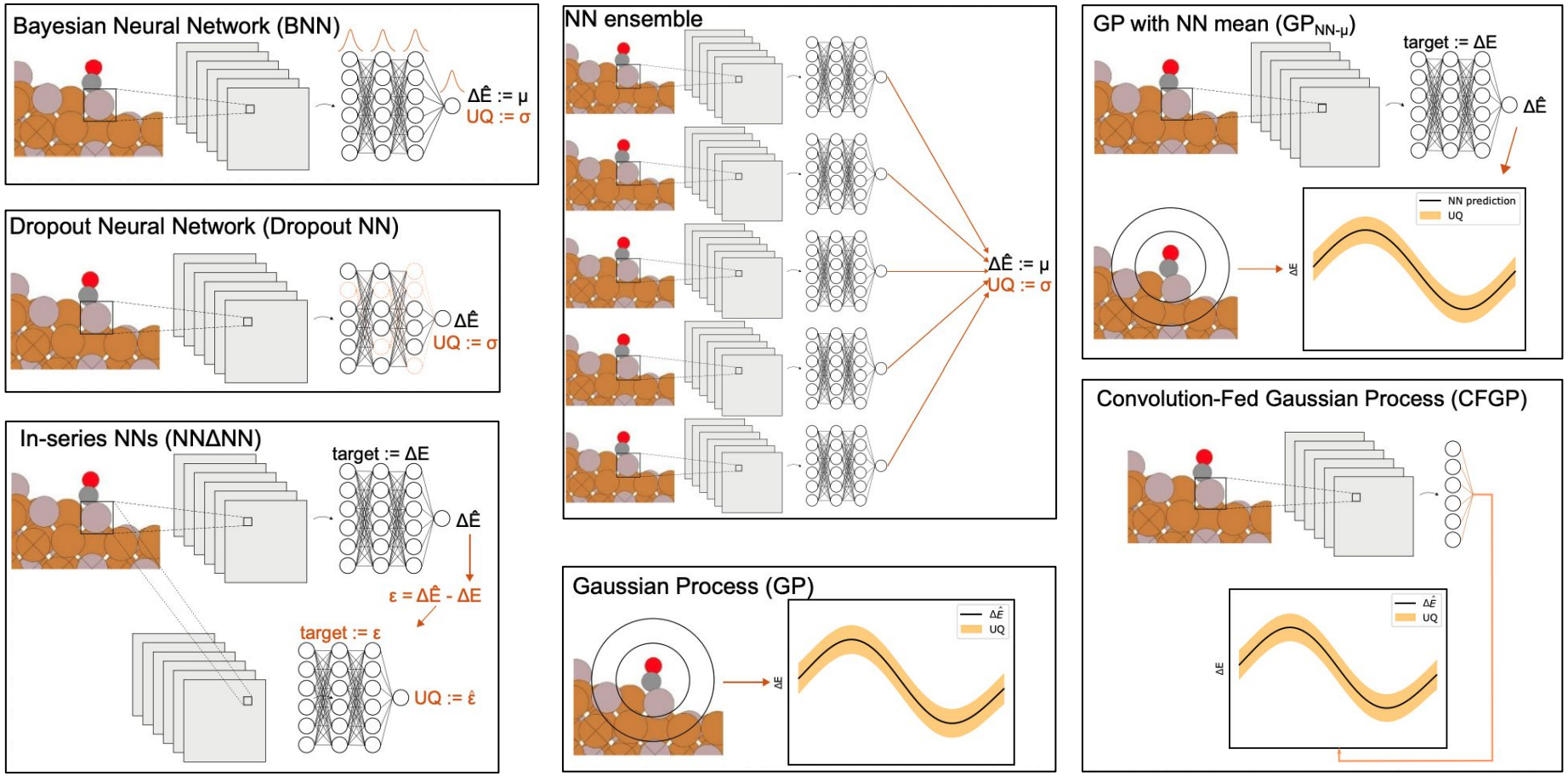

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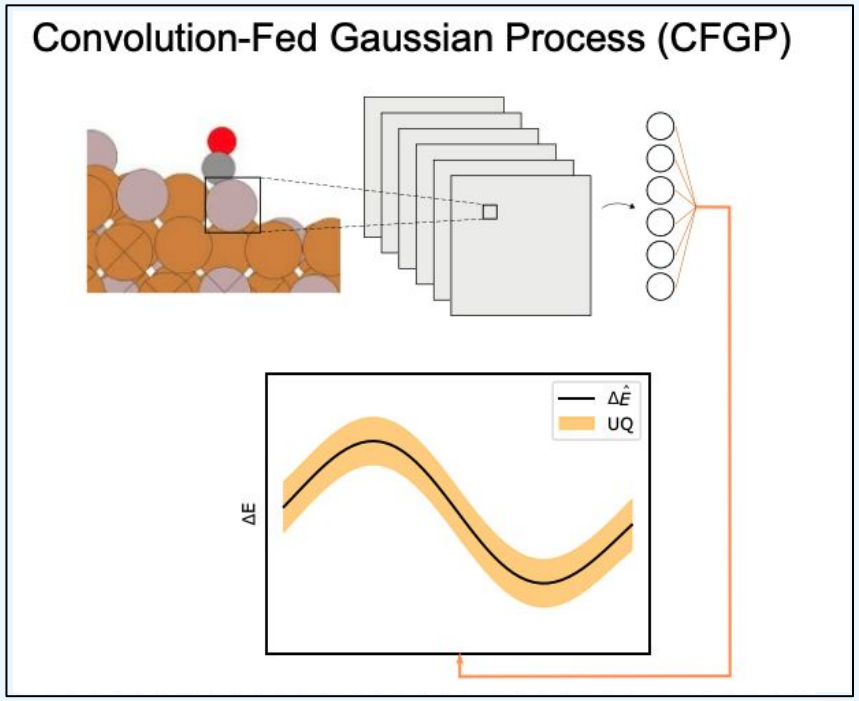

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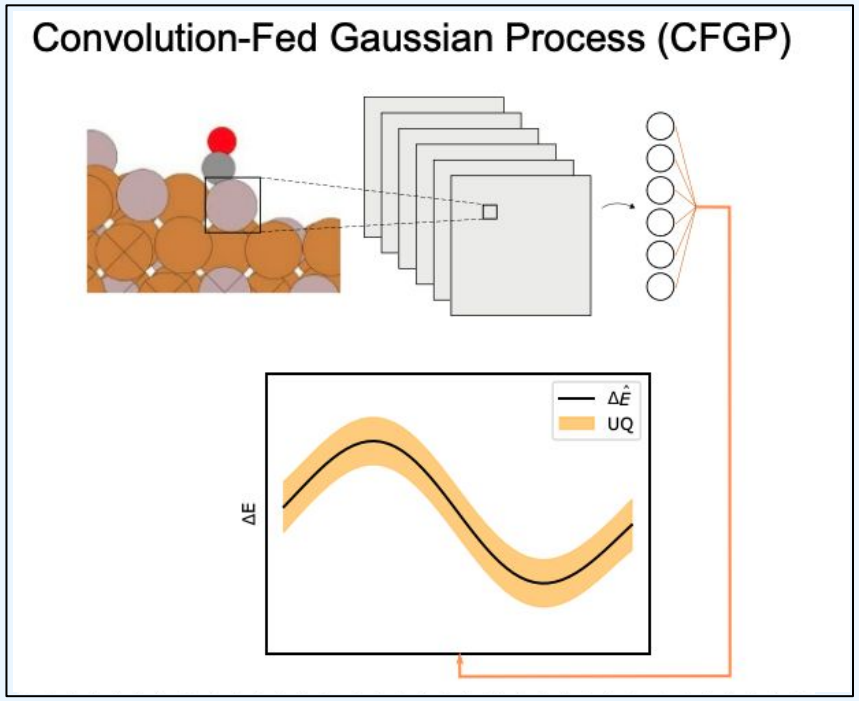

- Here, we use the neural network to learn good representations *(e.g., for a GP)*.
- For any input, first make a prediction w/ neural network.
- Use output at an intermediate layer as new transformed input (into a continuous space).
- Then define a Gaussian process on this new representation of inputs.

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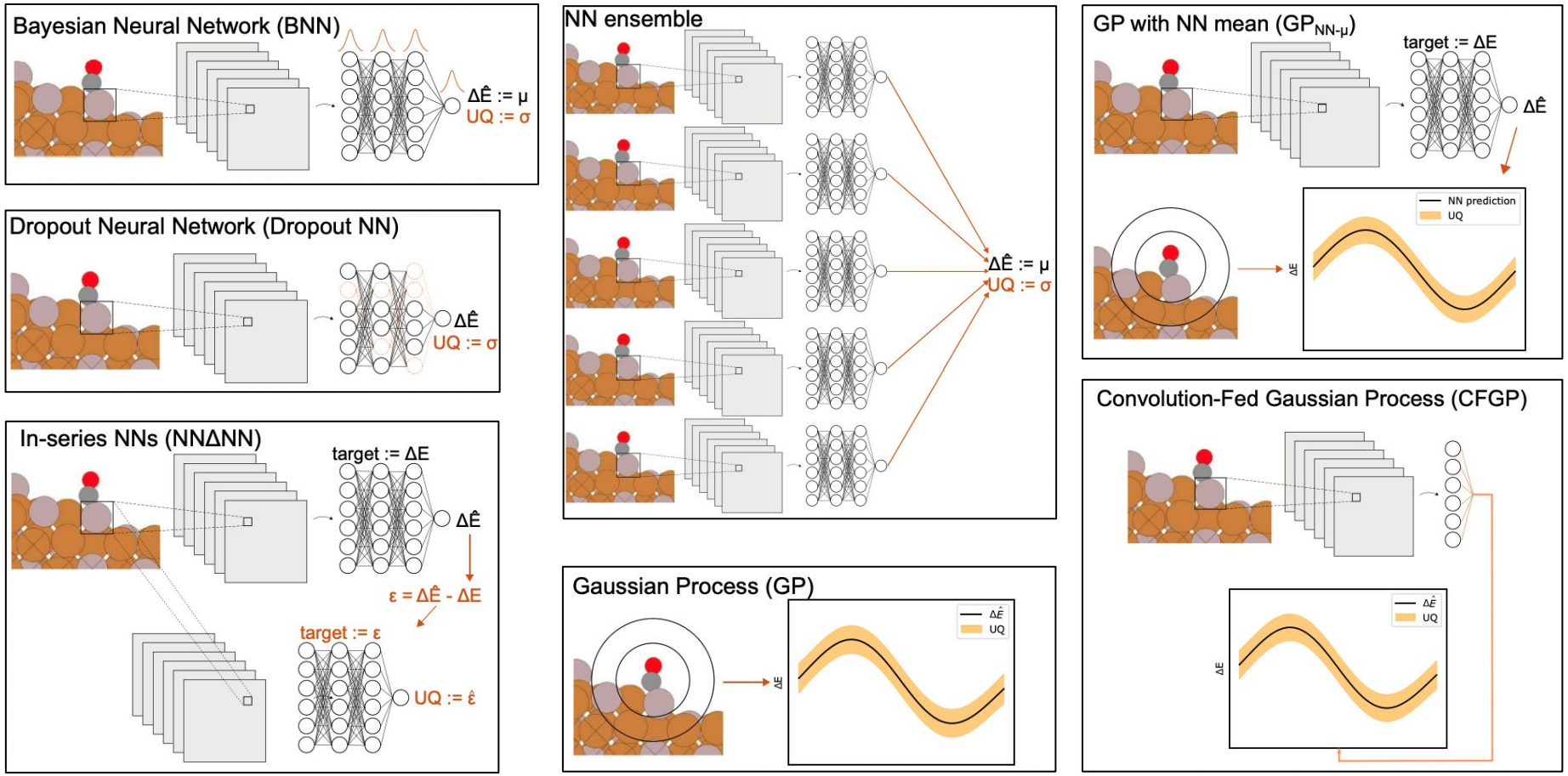

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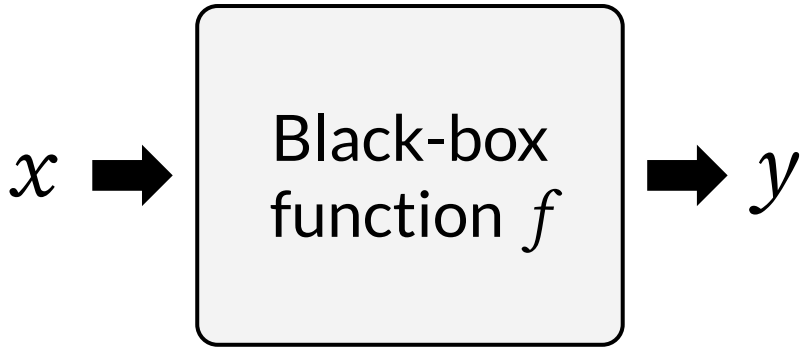
Bayesian Optimization

Expensive Black-box Functions

Expensive Black-box Functions

Unknown

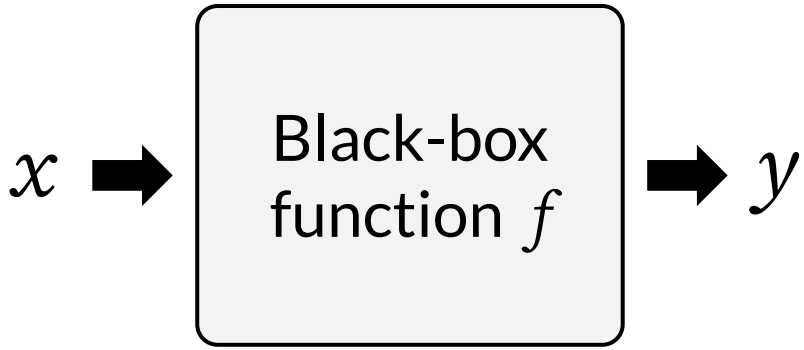
Many real-world systems can be modeled as an **expensive black-box function** f.



Expensive Black-box Functions

Many real-world systems can be modeled as an **expensive black-box function** f.

MATERIALS SCIENCE



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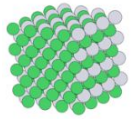
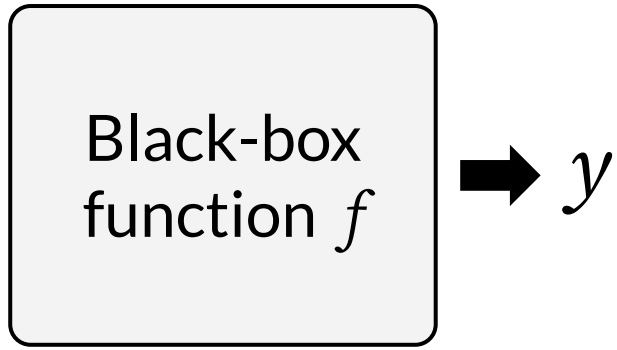
MATERIALS SCIENCE

Material Composition



[0.2, 0.5, 0.3]
Pt Sn Au



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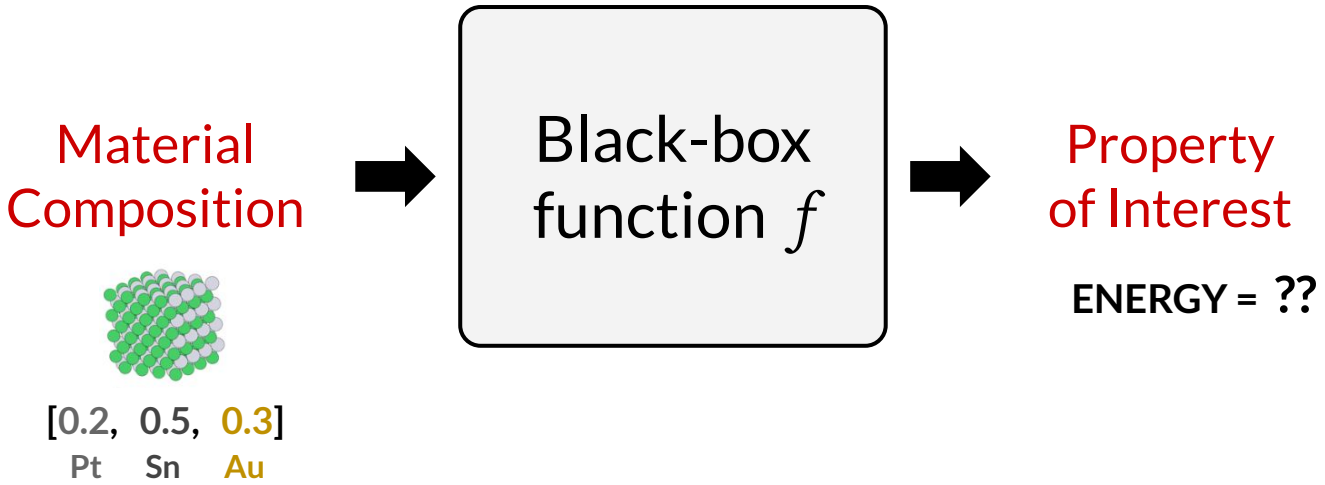

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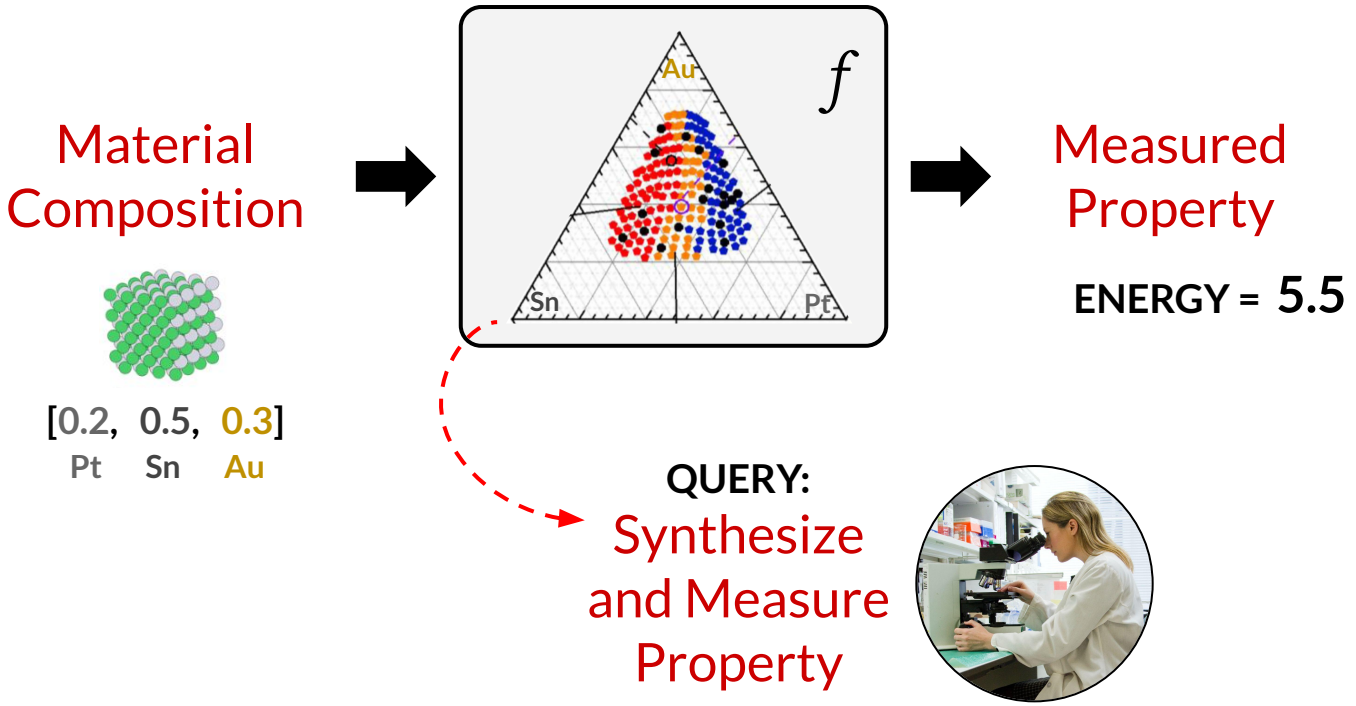

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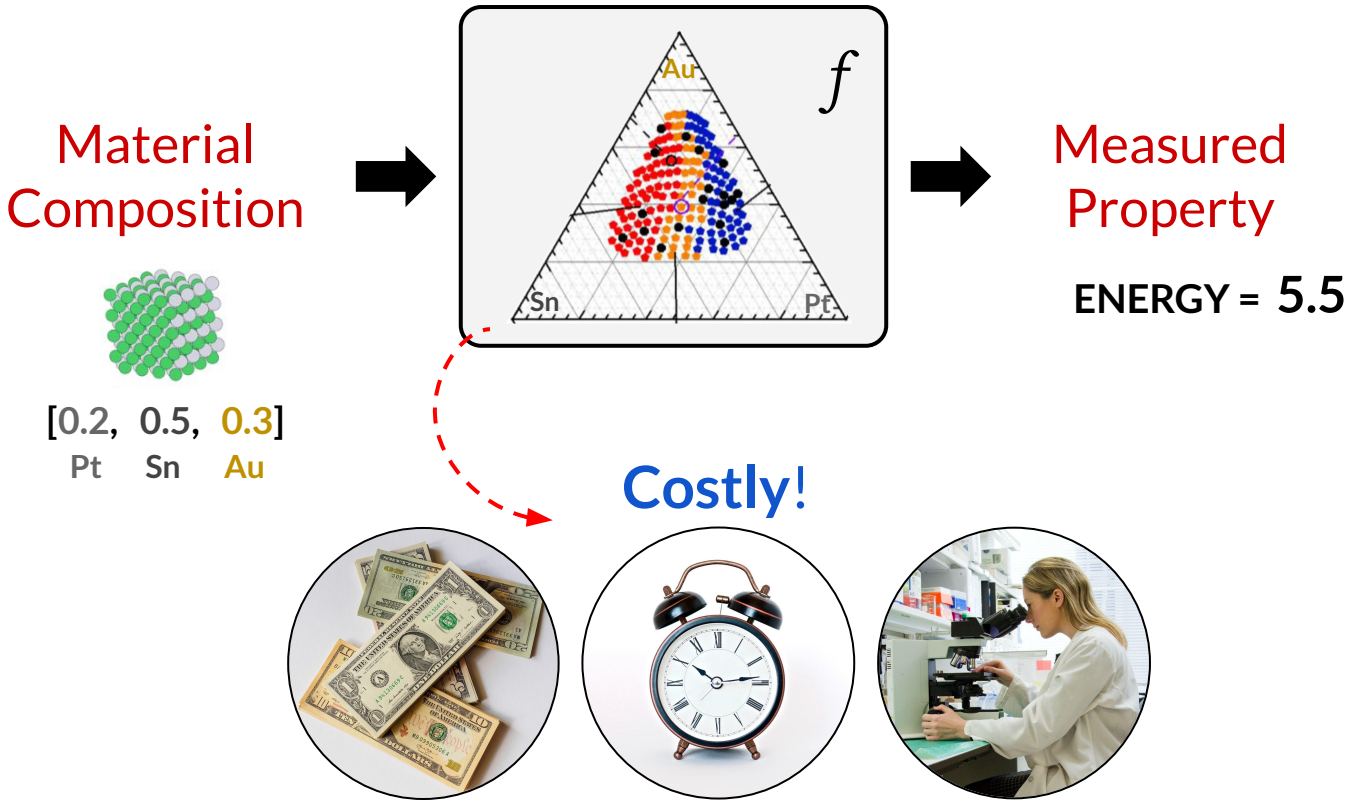

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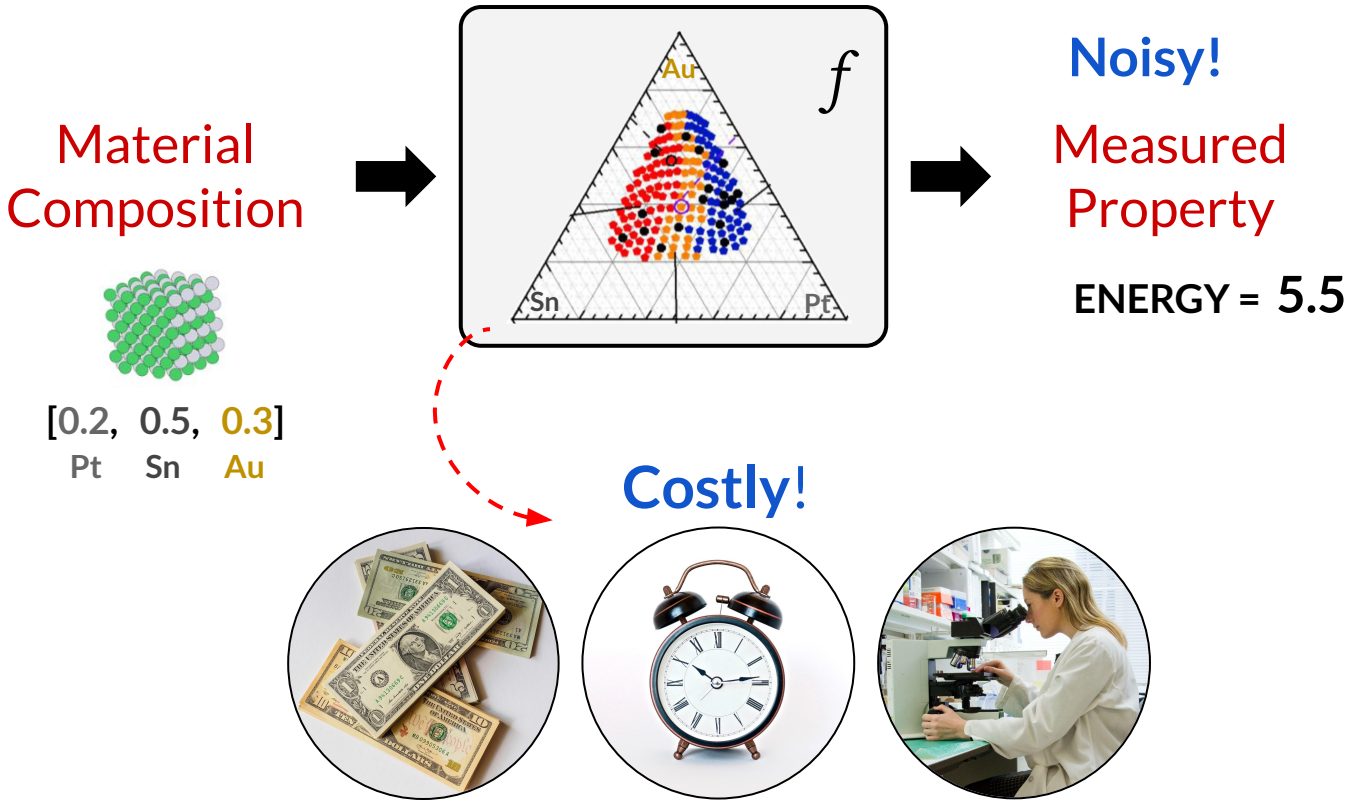

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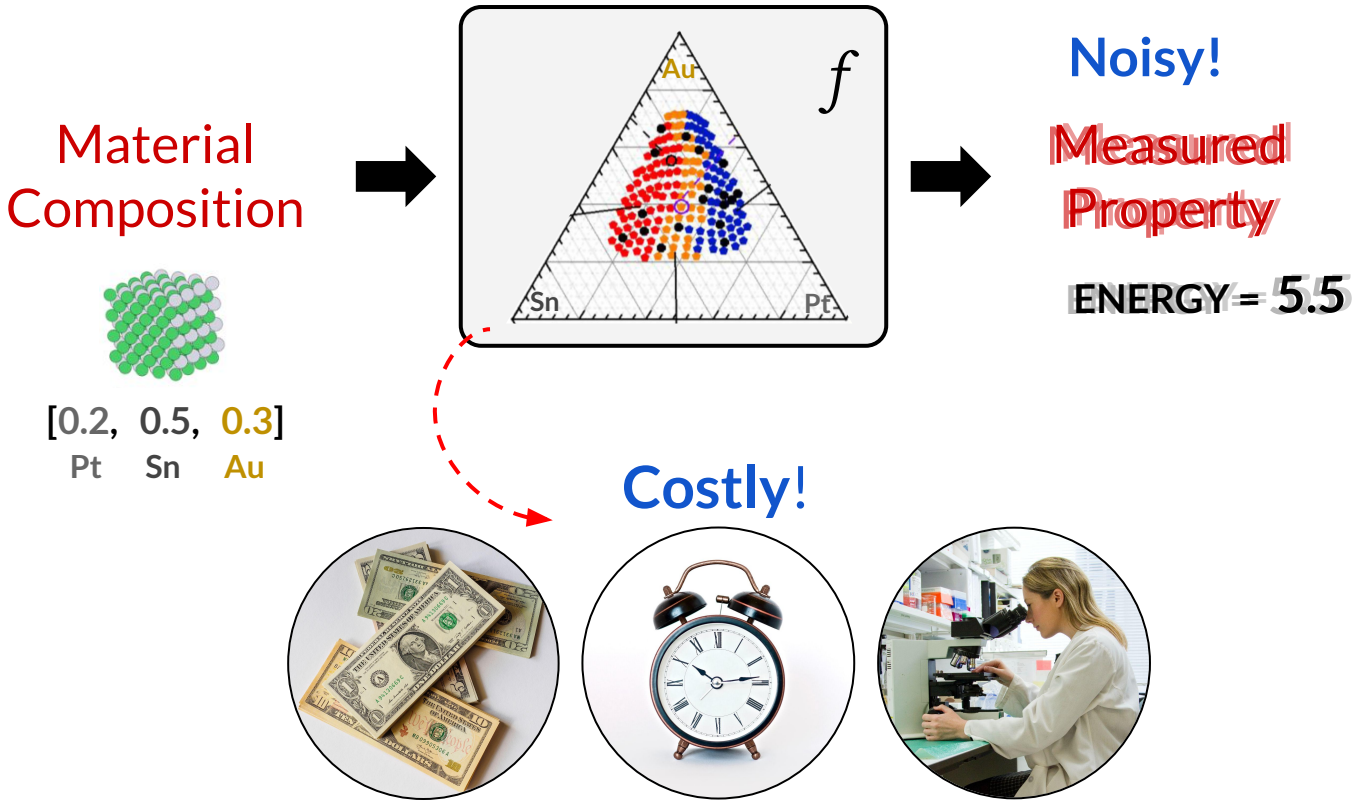

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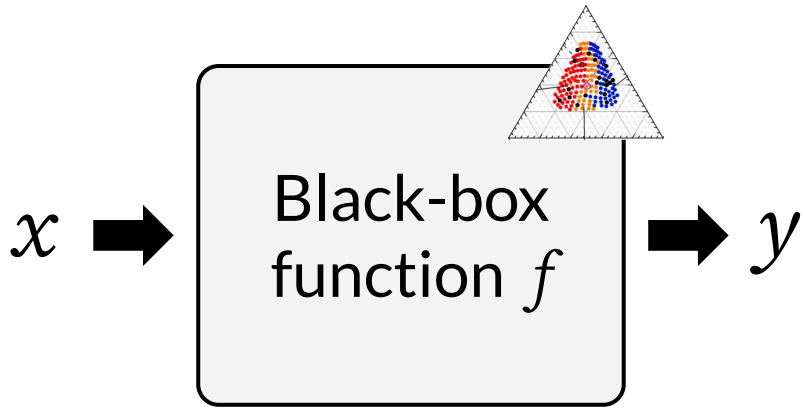

Use this symbol

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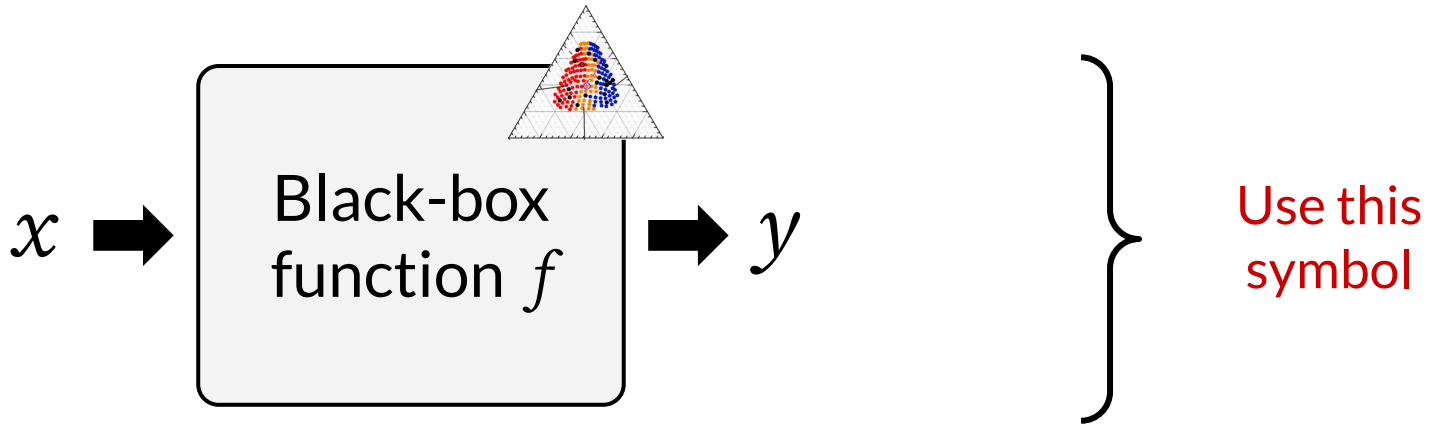


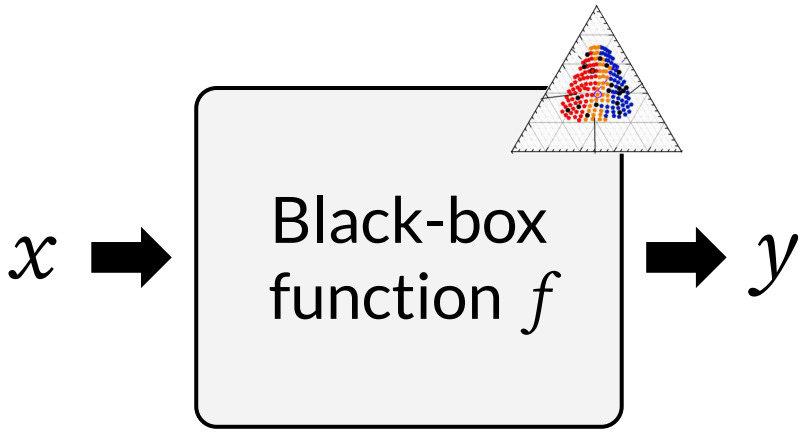
Leads to task of **black-box global optimization**.

Black-Box Global Optimization

Black-Box Global Optimization

Suppose we have an **expensive black-box function** $f : \mathcal{X} \to \mathbb{R}$.

Can ***query*** f

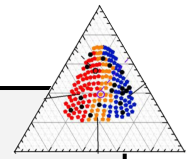


Observe $y \sim f(x) + \varepsilon$

Black-Box Global Optimization

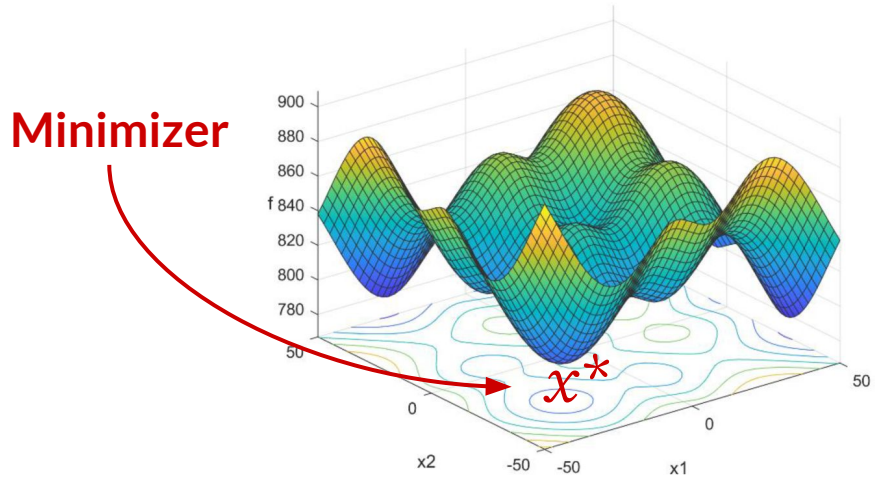
Suppose we have an **expensive black-box function** $f : \mathcal{X} \to \mathbb{R}$.

Can ***query*** f x → Black-box function f → y **Observe** $y \sim f(x) + \varepsilon$



Goal: estimate the location of a global optima.

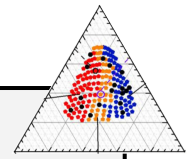
$$x^* = \arg\min_{x \in \mathcal{X}} f(x)$$



Black-Box Global Optimization

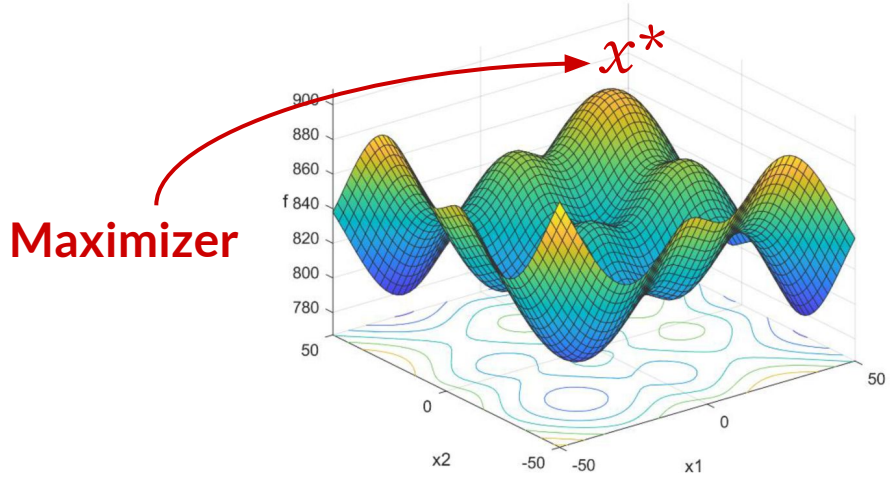
Suppose we have an **expensive black-box function** $f : \mathcal{X} \to \mathbb{R}$.

Can ***query*** f x → Black-box function f → y **Observe** $y \sim f(x) + \varepsilon$



Goal: estimate the location of a global optima.

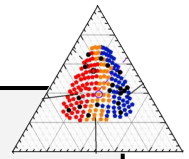
$$x^* = \arg\max_{x \in \mathcal{X}} f(x)$$



Black-Box Global Optimization

Suppose we have an **expensive black-box function** $f : \mathcal{X} \to \mathbb{R}$.

Can ***query*** f x ➡ Black-box function f ➡ y **Observe** $y \sim f(x) + \varepsilon$

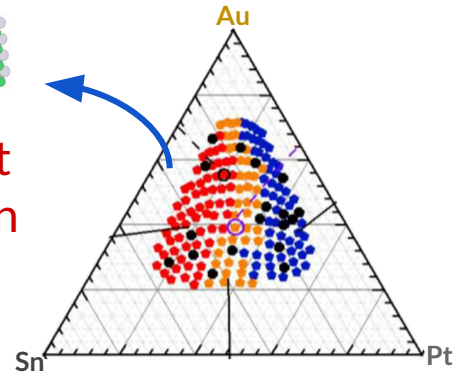


Goal: estimate the location of a global optima.

$$x^* = \arg\max_{x \in \mathcal{X}} f(x)$$

$x^* =$ 

"Greatest activation energy"



Black-Box Global Optimization

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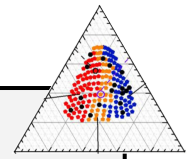
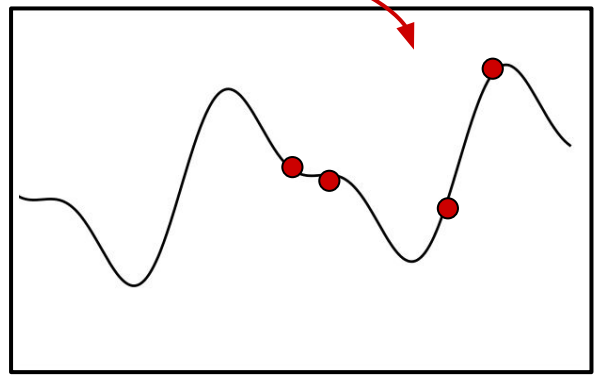


Goal: estimate the location of a global optima.

In a **limited budget** of T queries.

Few queries

No gradient information



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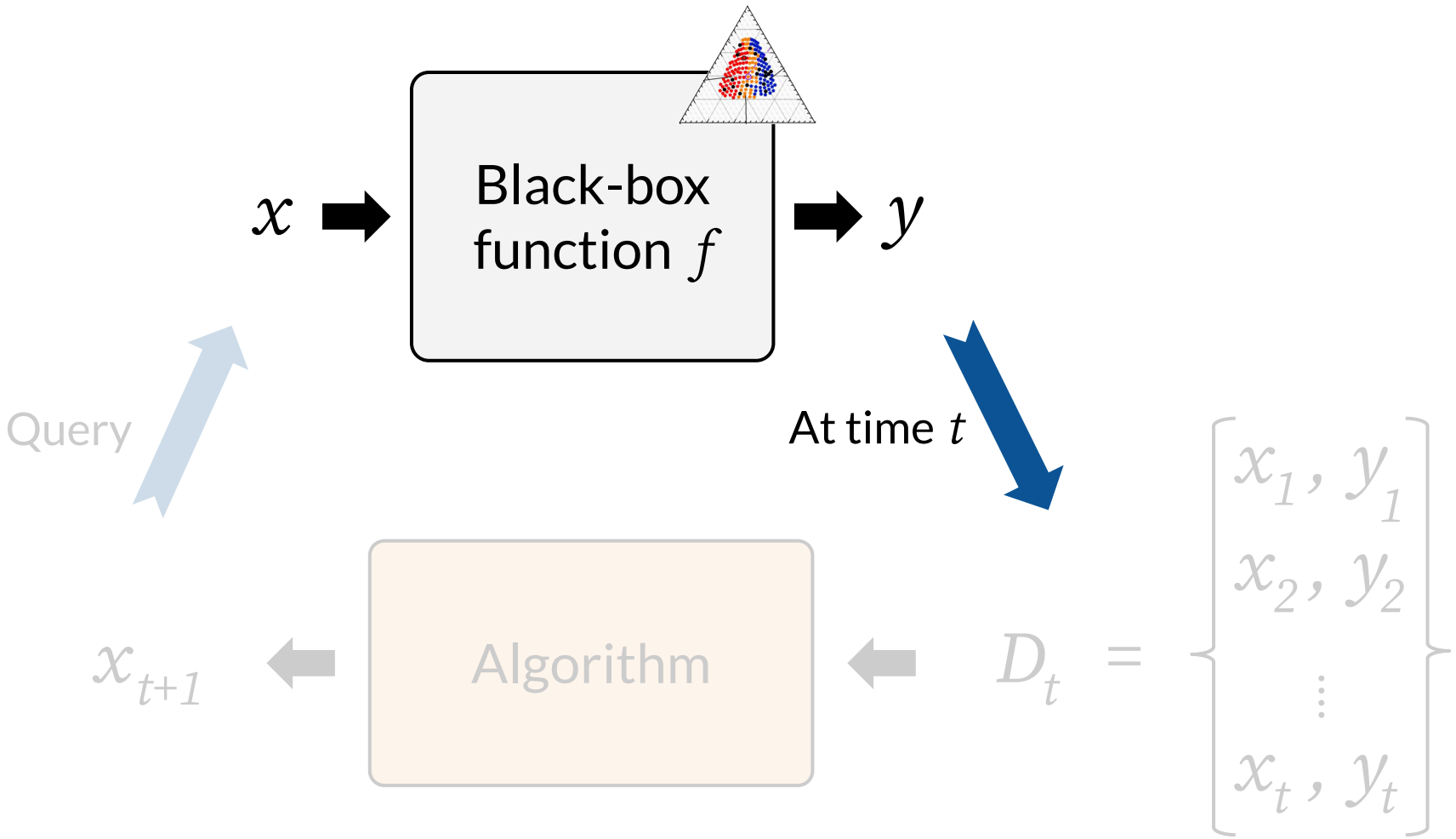

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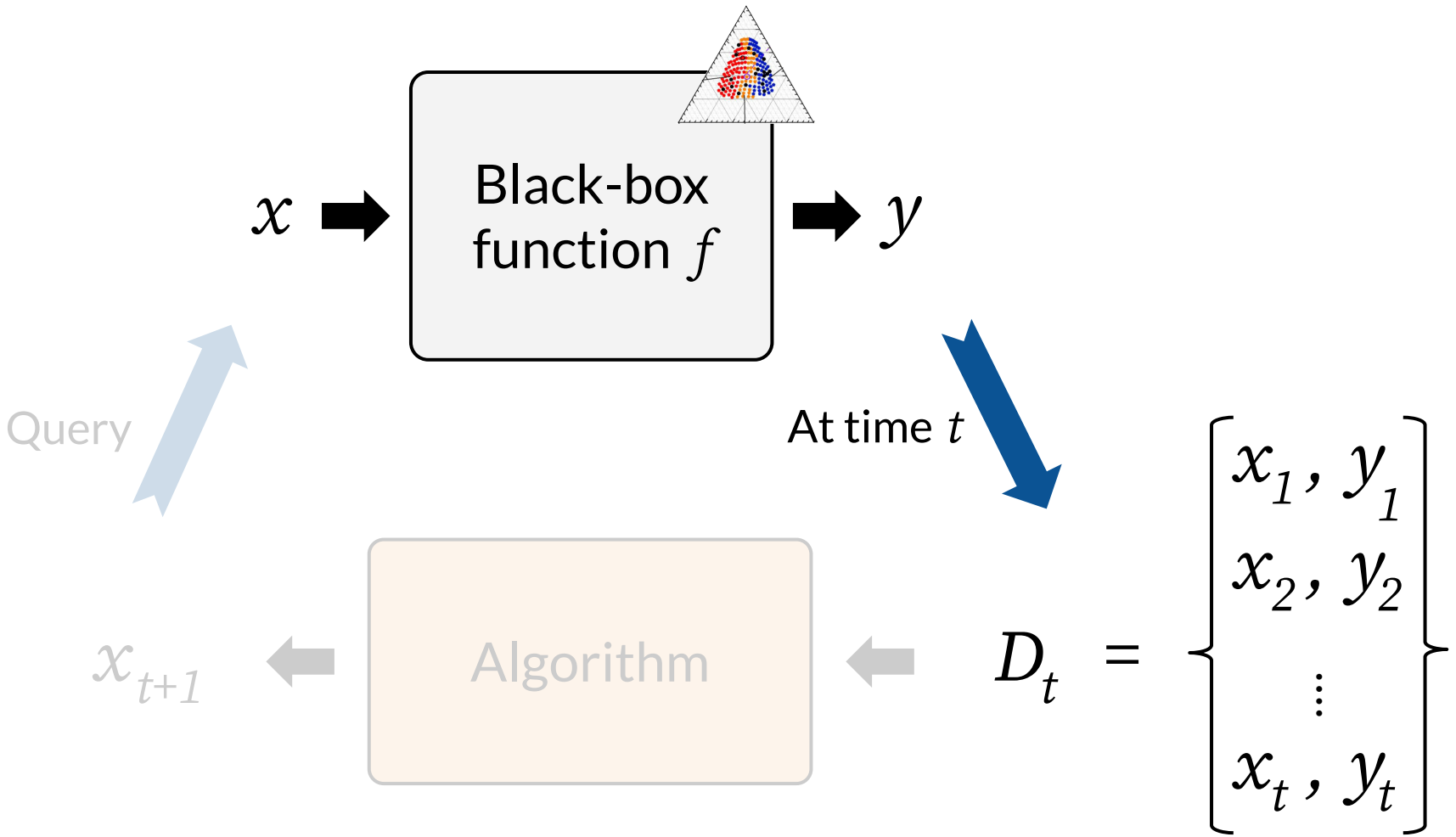

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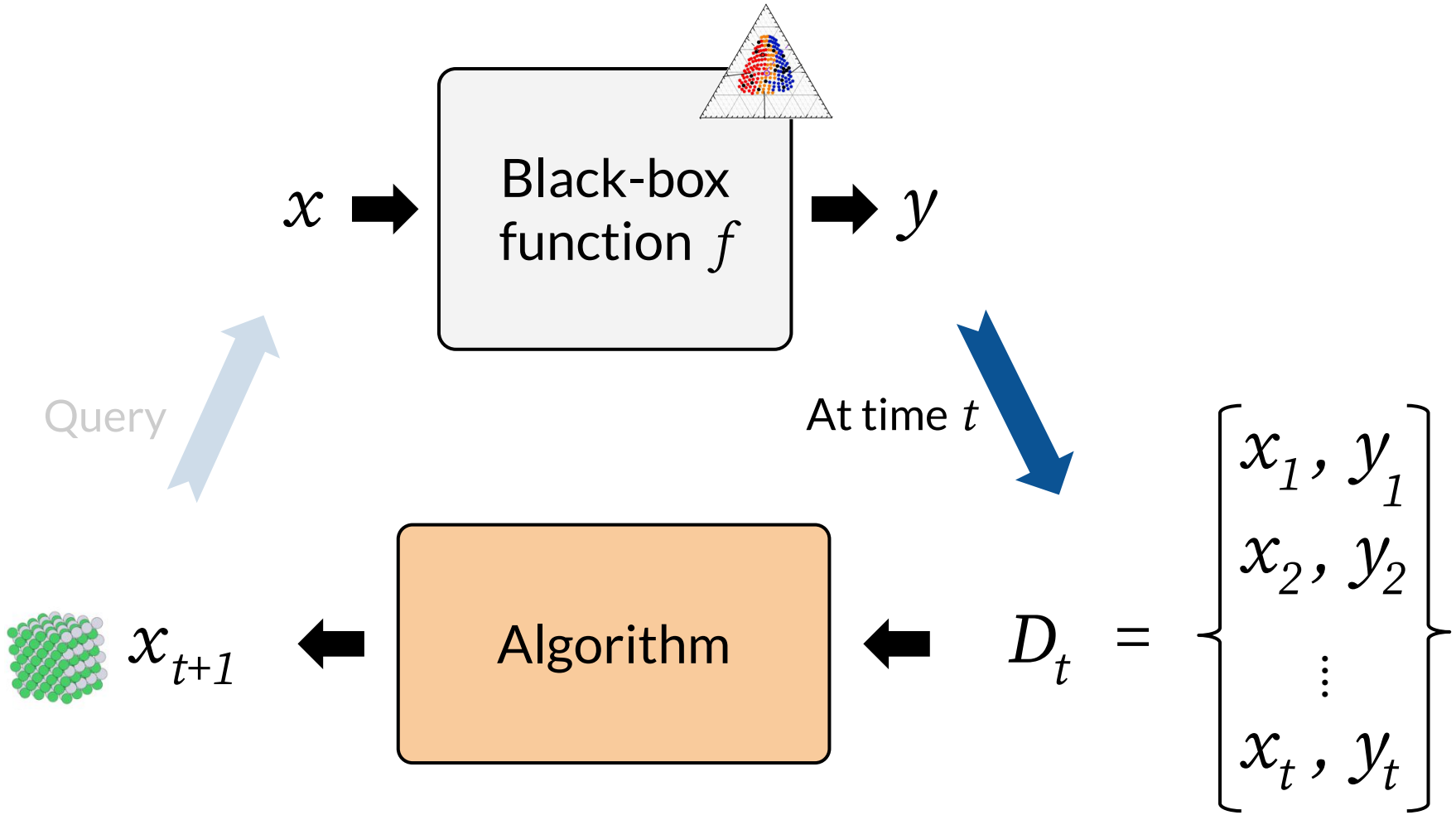

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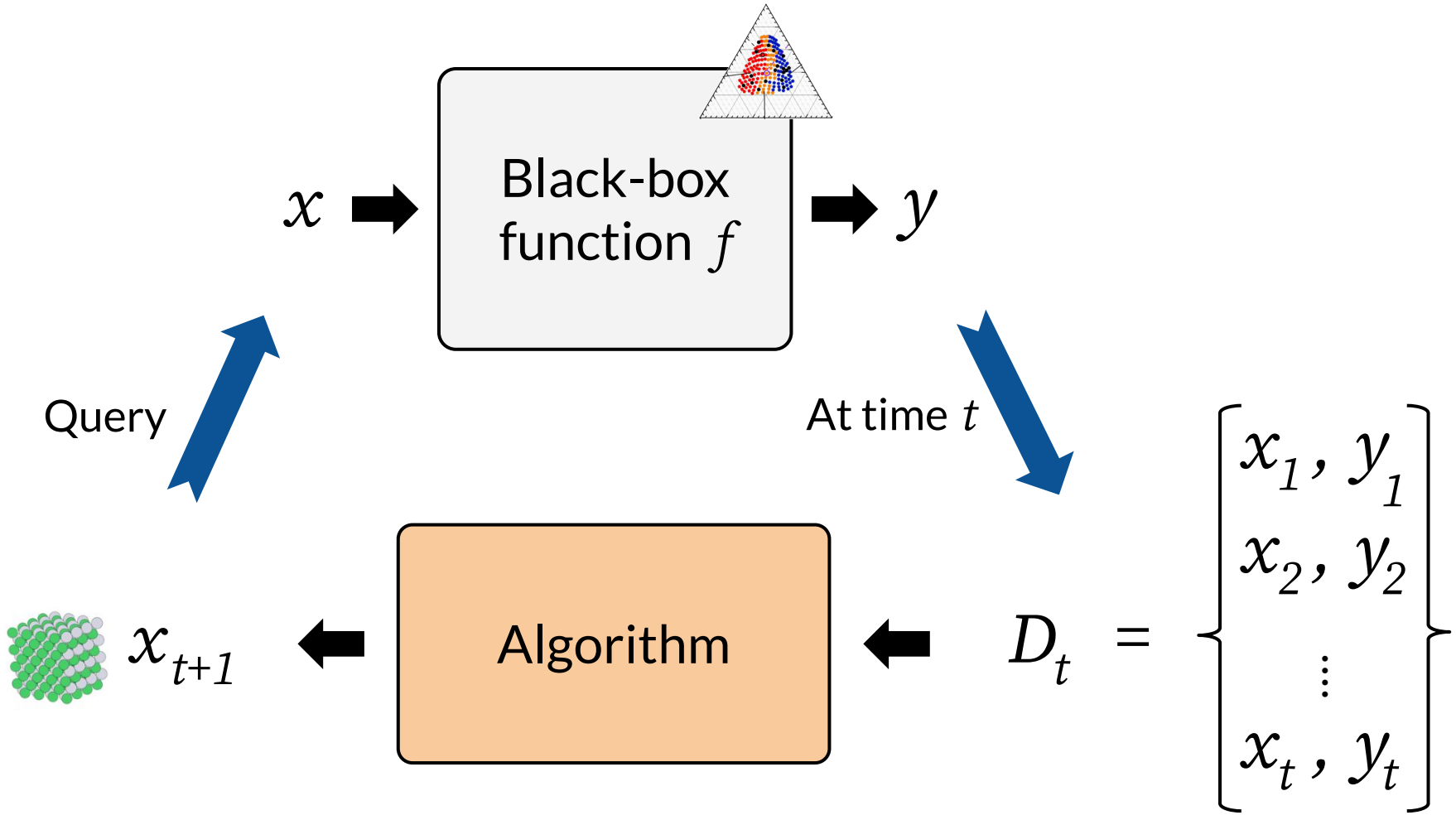

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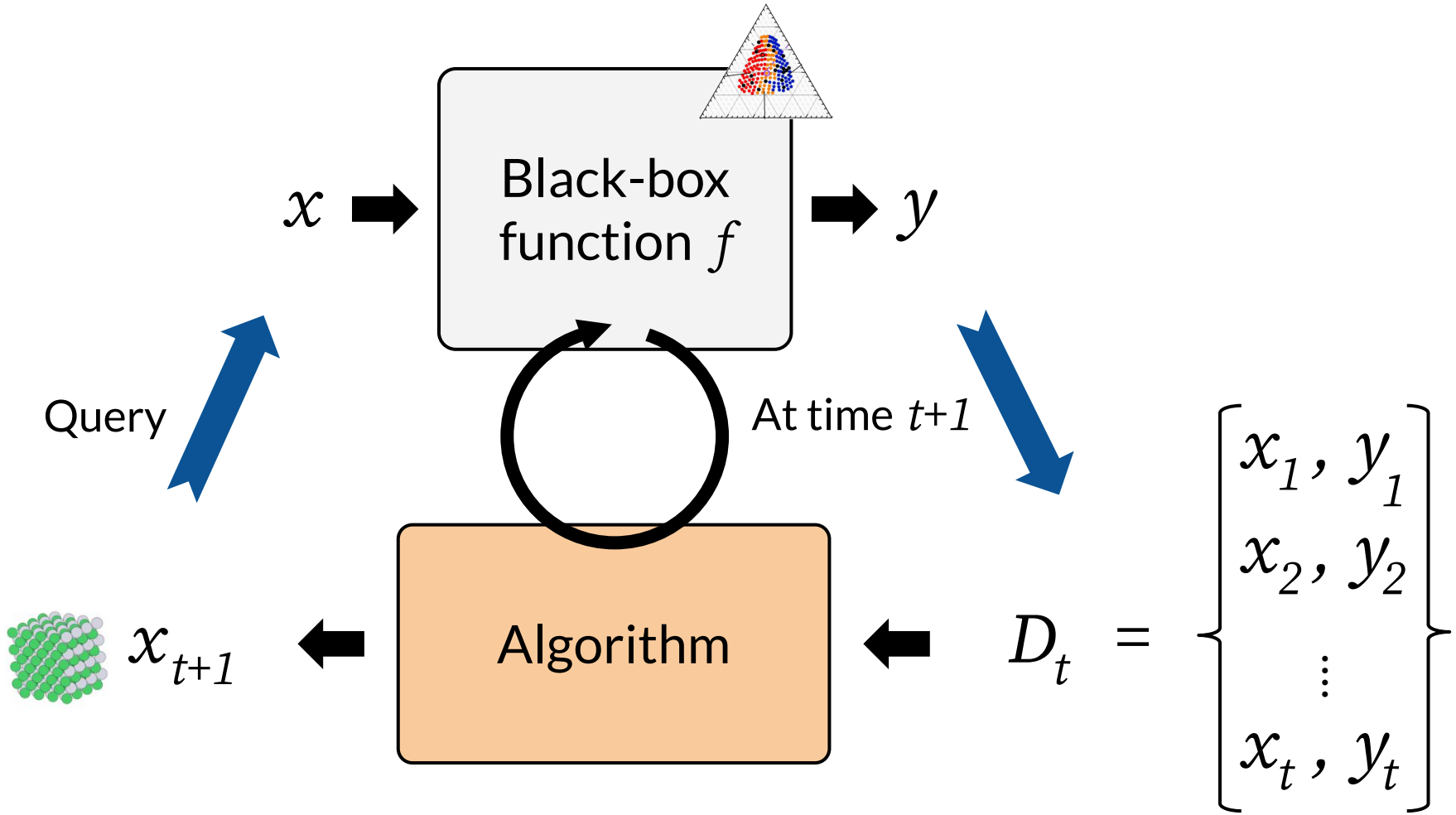

Bayesian Optimization — Motivation

Derivative-free optimization:

- Evolutionary or genetic algorithms [FOW, 1966]
- Trust region methods [LM, 1944-1963]
- Nelder-Mead / simplex methods [NM, 1965]
- Simulated annealing [P, 1970; KGV, 1983]

Bayesian Optimization — Motivation

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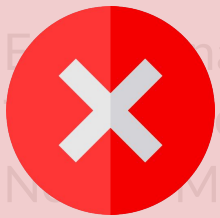

Can require 1000s of queries!

Need:

- Better sample-efficiency.
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What is Bayesian Opt? Uses a (probabilistic) predictive model to aid in optimization.

Bayesian Optimization — Motivation

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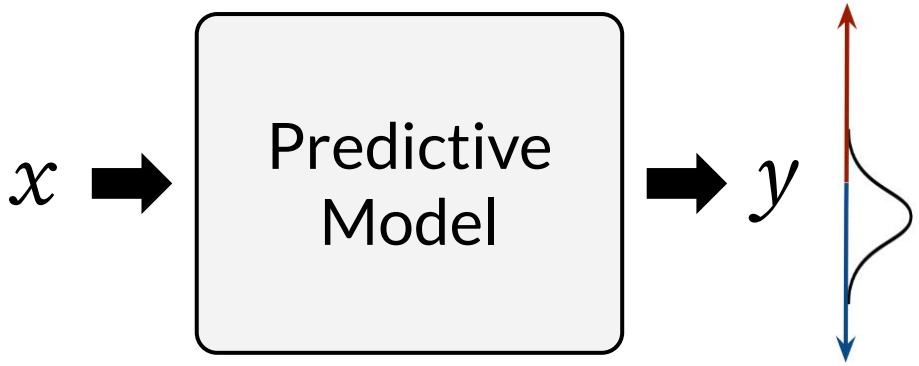

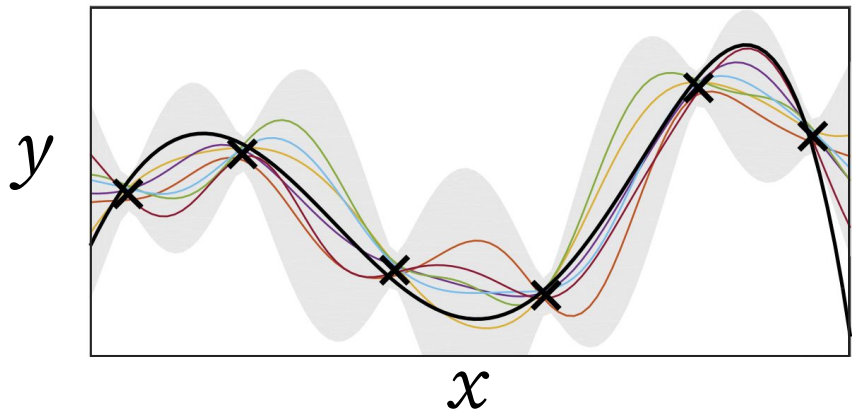

Bayesian Optimization — Motivation

Derivative-free optimization:

- Random search, Grid search, Factorial designs [FOW, 1966]
- Response surface methods [L, M, 1944-1963]
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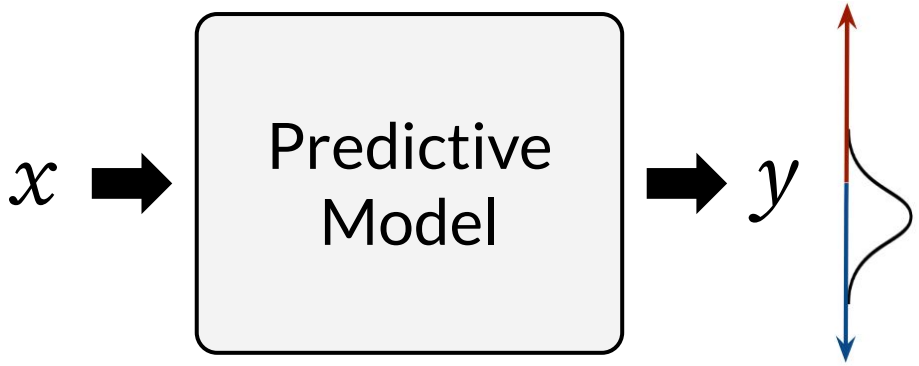

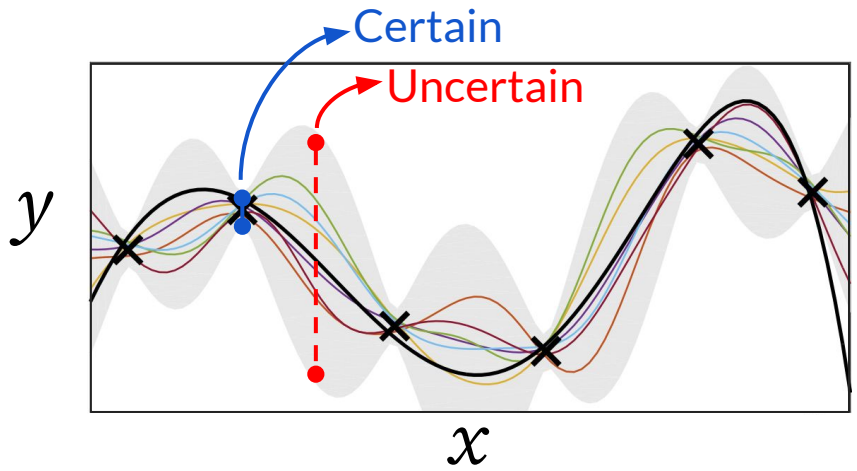

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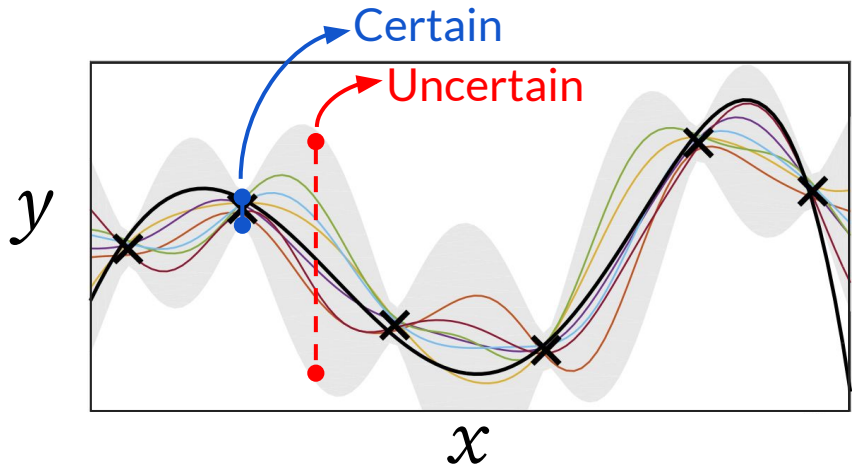
Model used for *intelligent* decision making ⇒ sample-efficient opt



Bayesian Optimization — Algorithm Overview

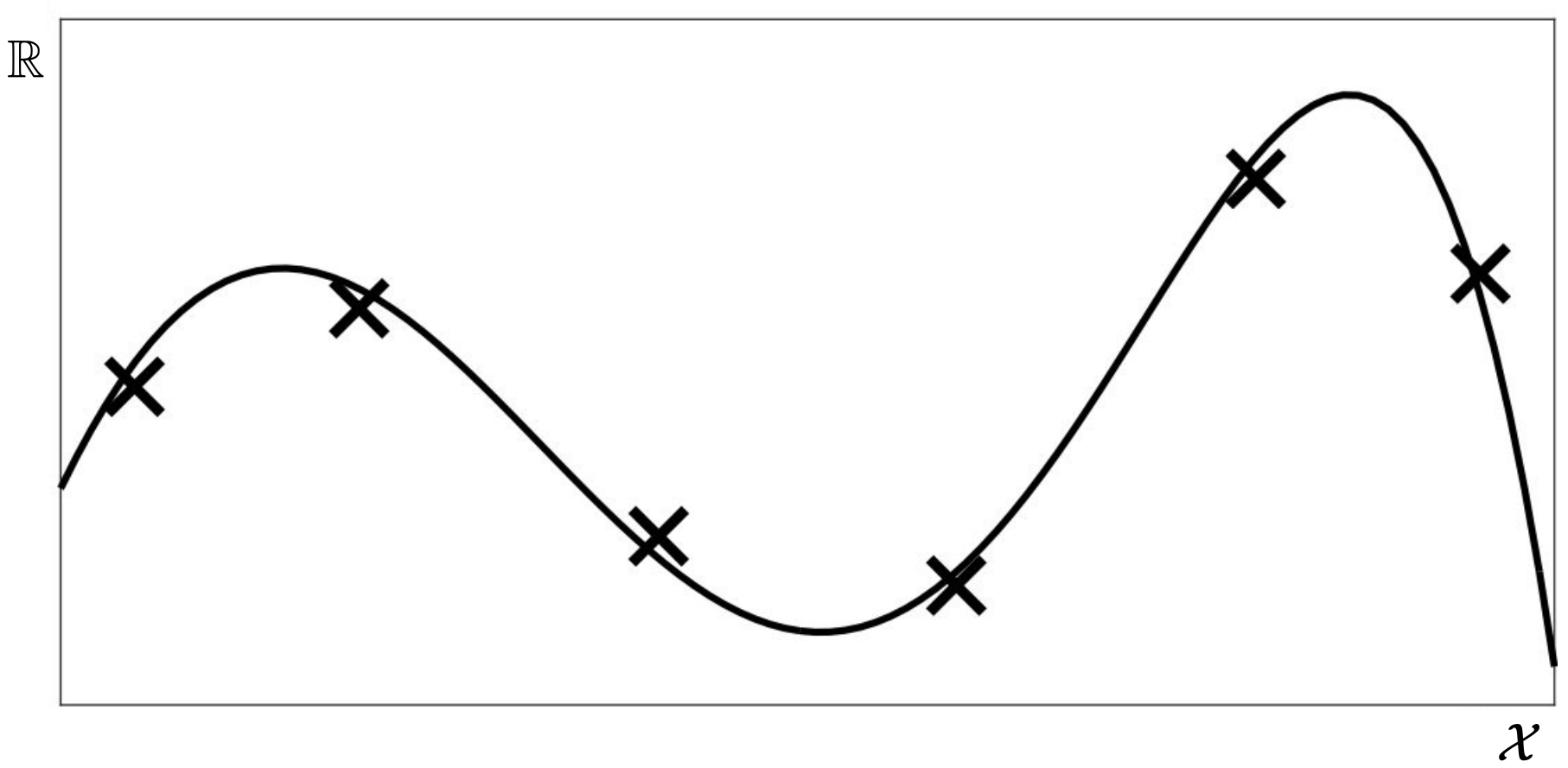
At each iteration of BO, three steps:

Bayesian Optimization — Algorithm Overview

At each iteration of BO, three steps:

1. Fit model to dataset.
2. Optimize an *acquisition function* to select next point to query.
3. Query black-box function.

Bayesian Optimization — Visualization



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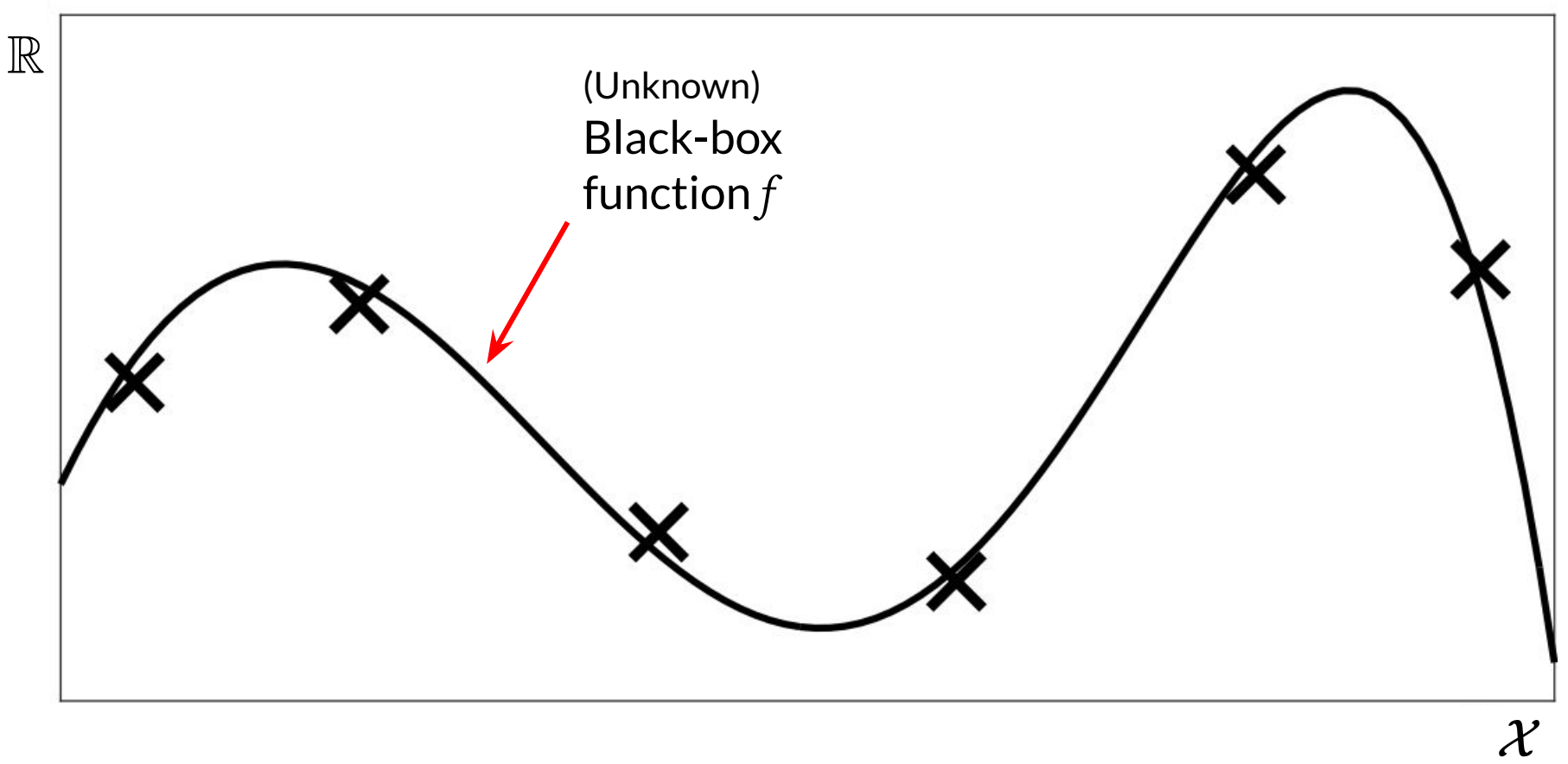
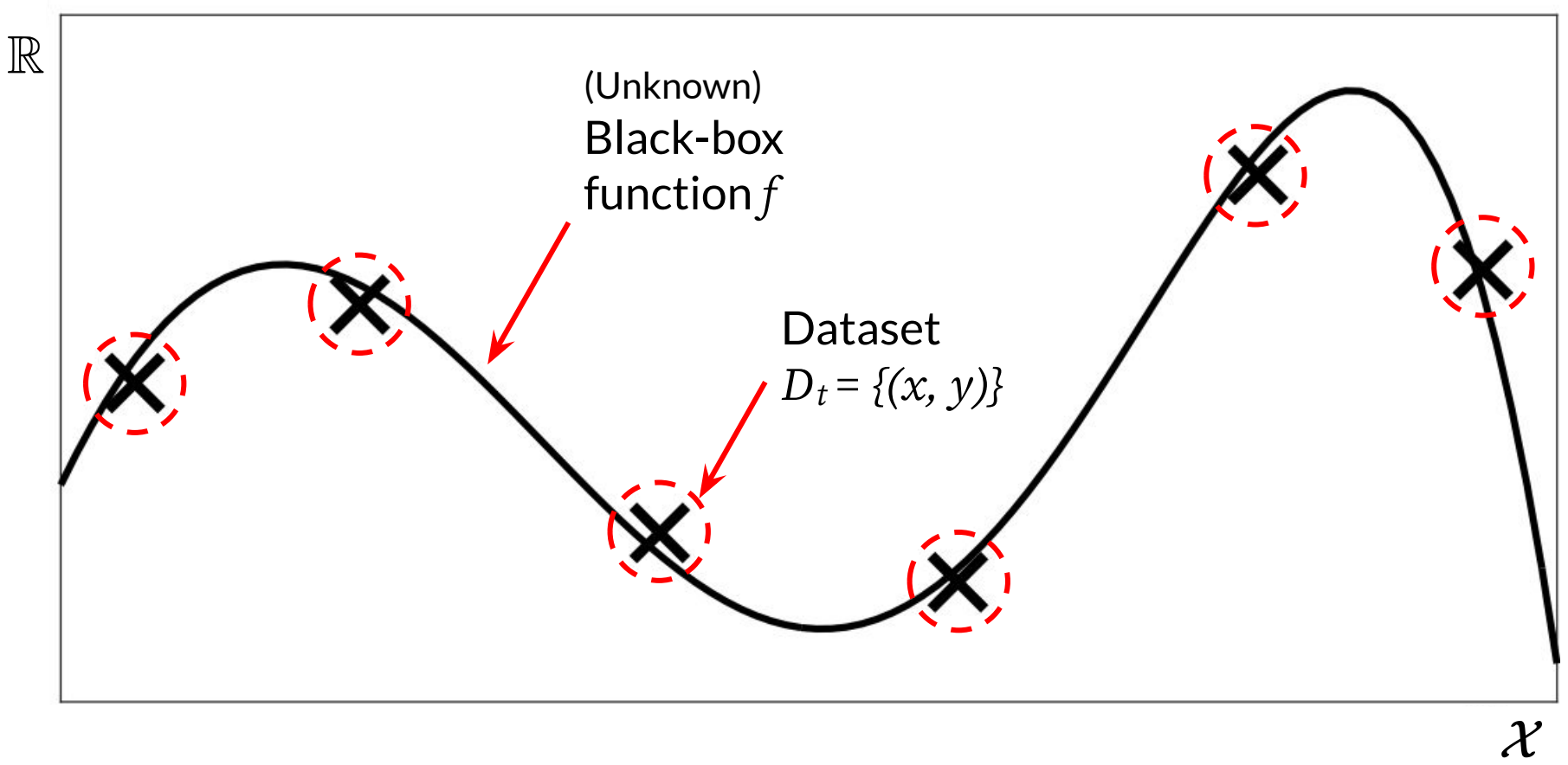


Unknown black-box f

Bayesian Optimization — Visualization



Unknown black-box f, and dataset of (x, y) pairs.

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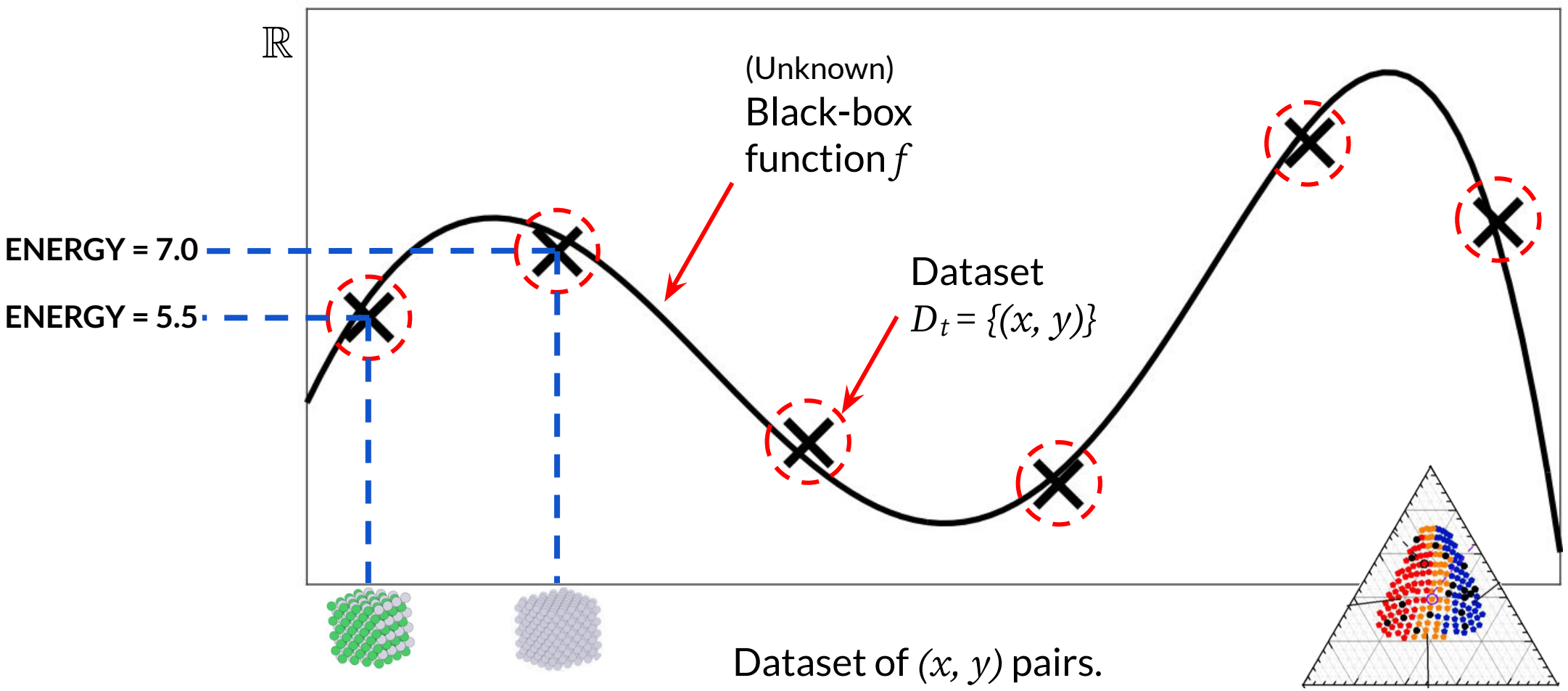

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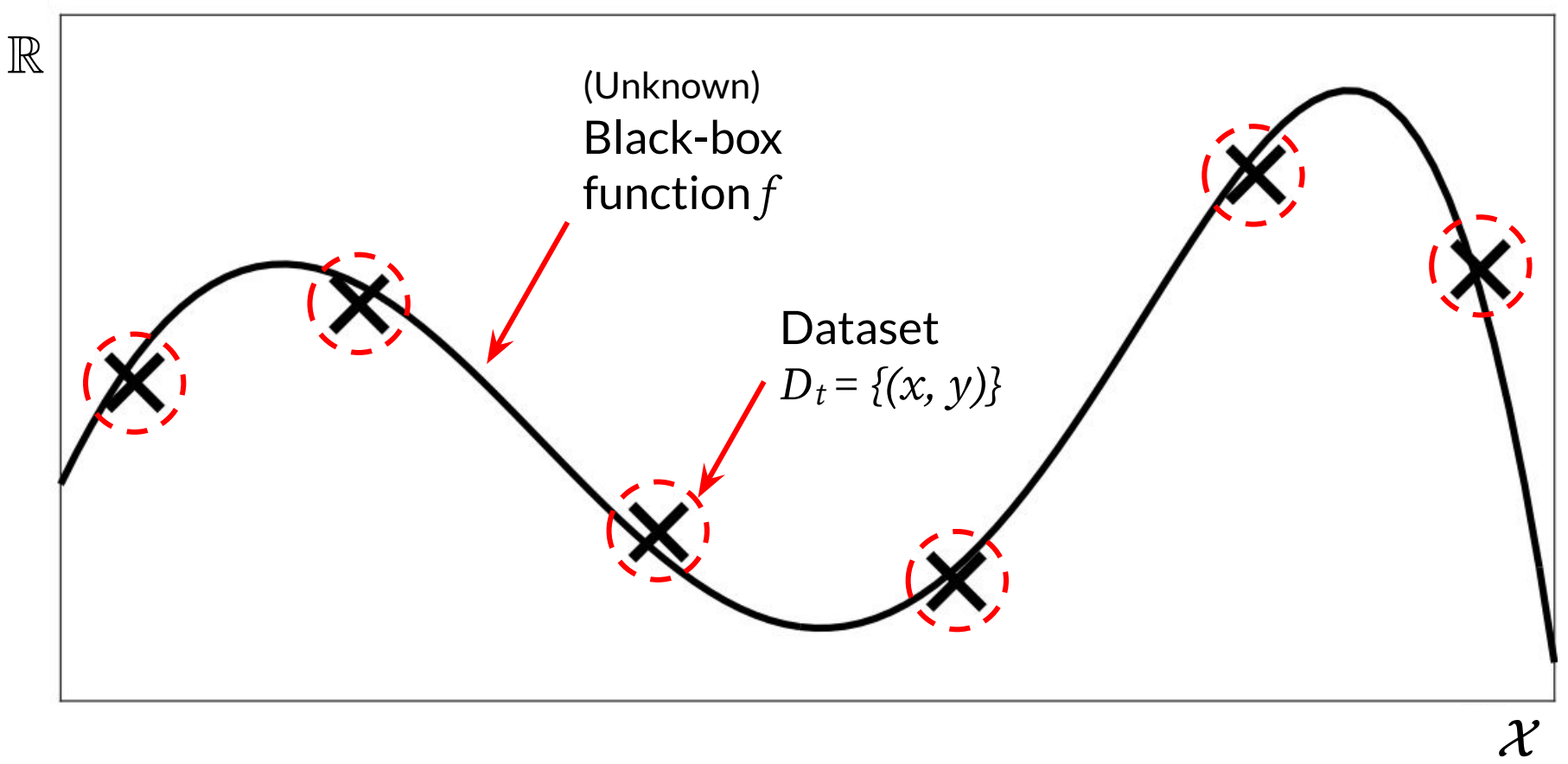

Dataset of (x, y) pairs.

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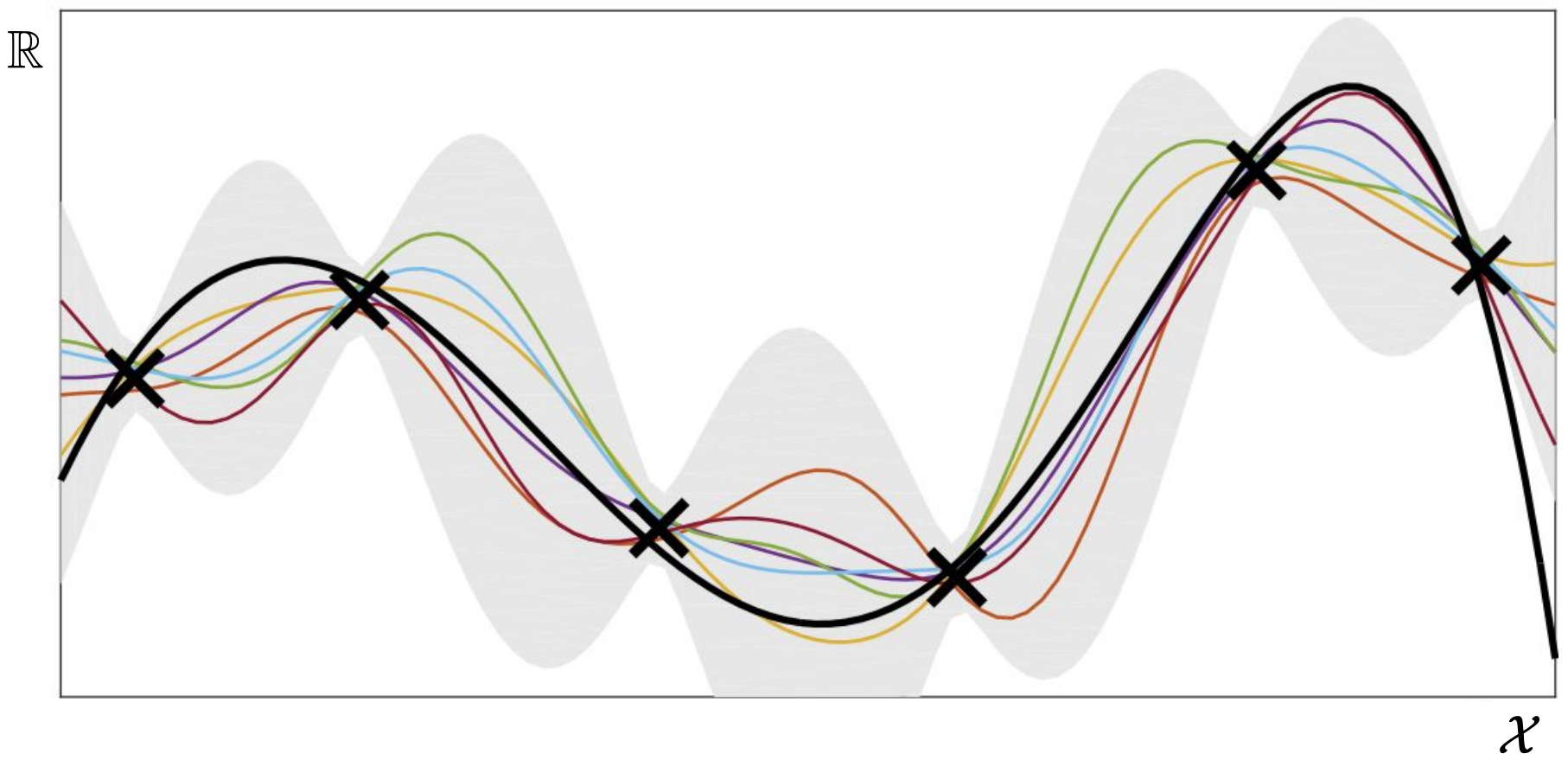

Given this dataset, can fit probabilistic model.

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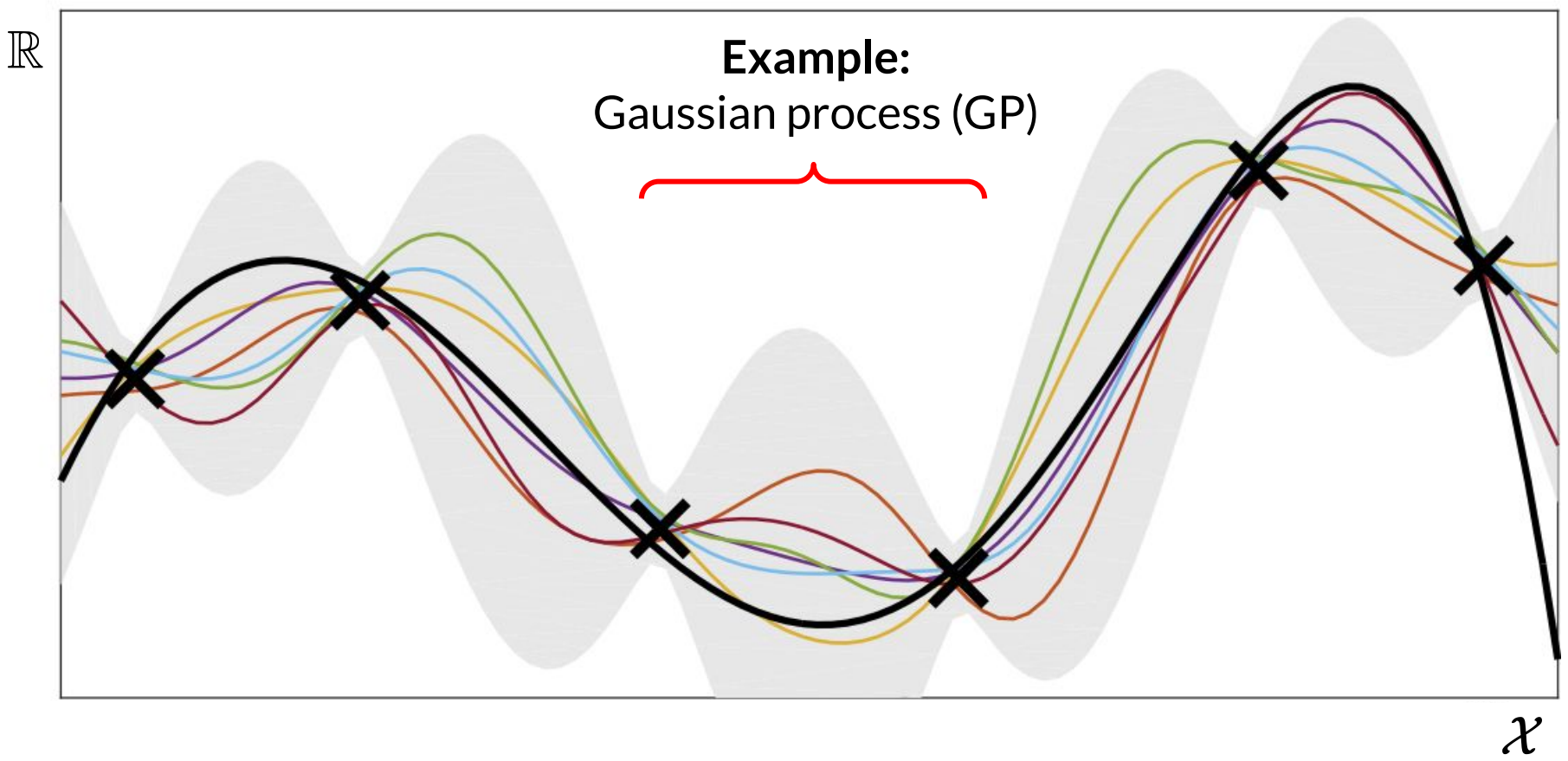

A popular choice for this model is a **Gaussian Process**.

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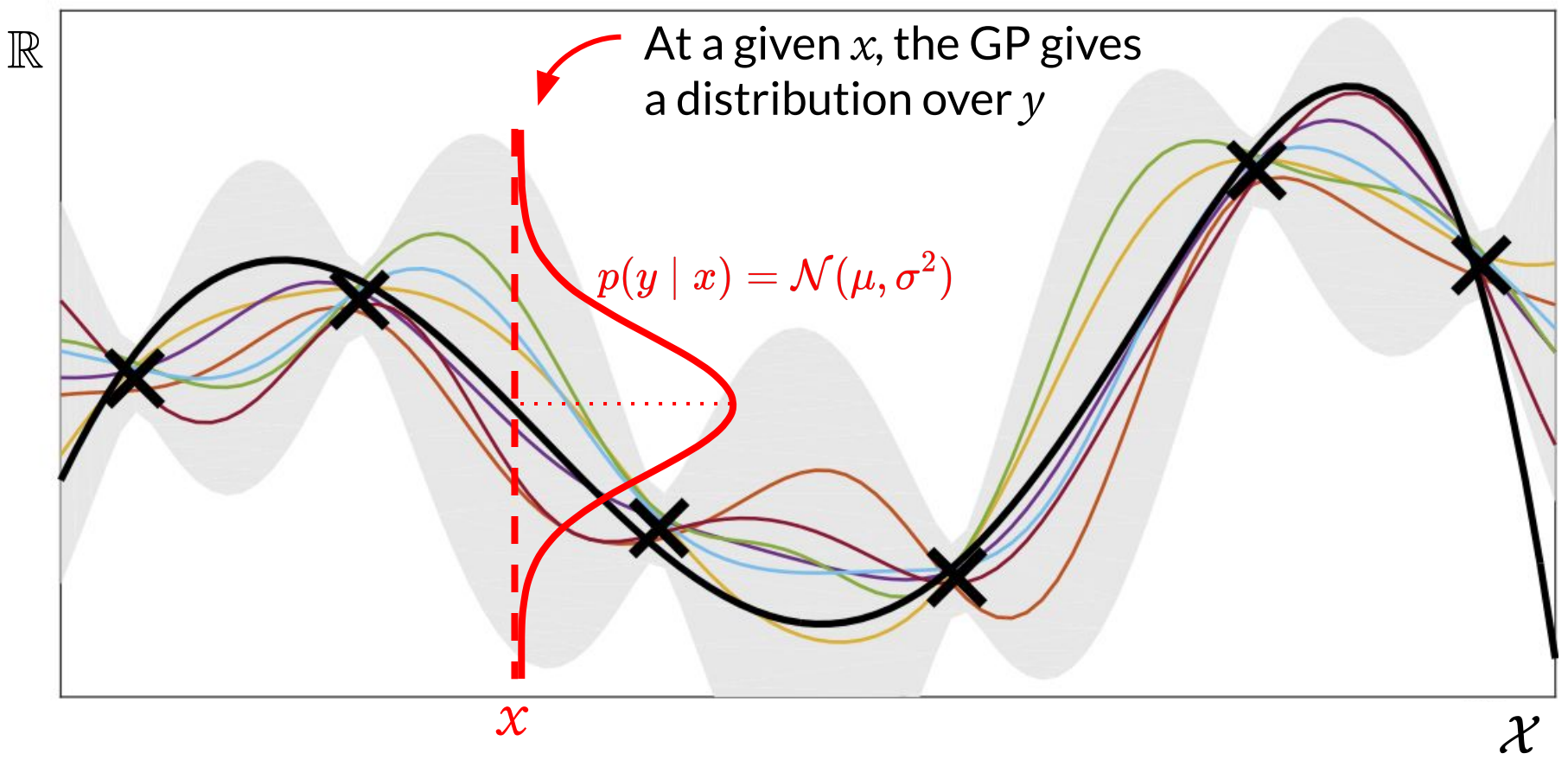

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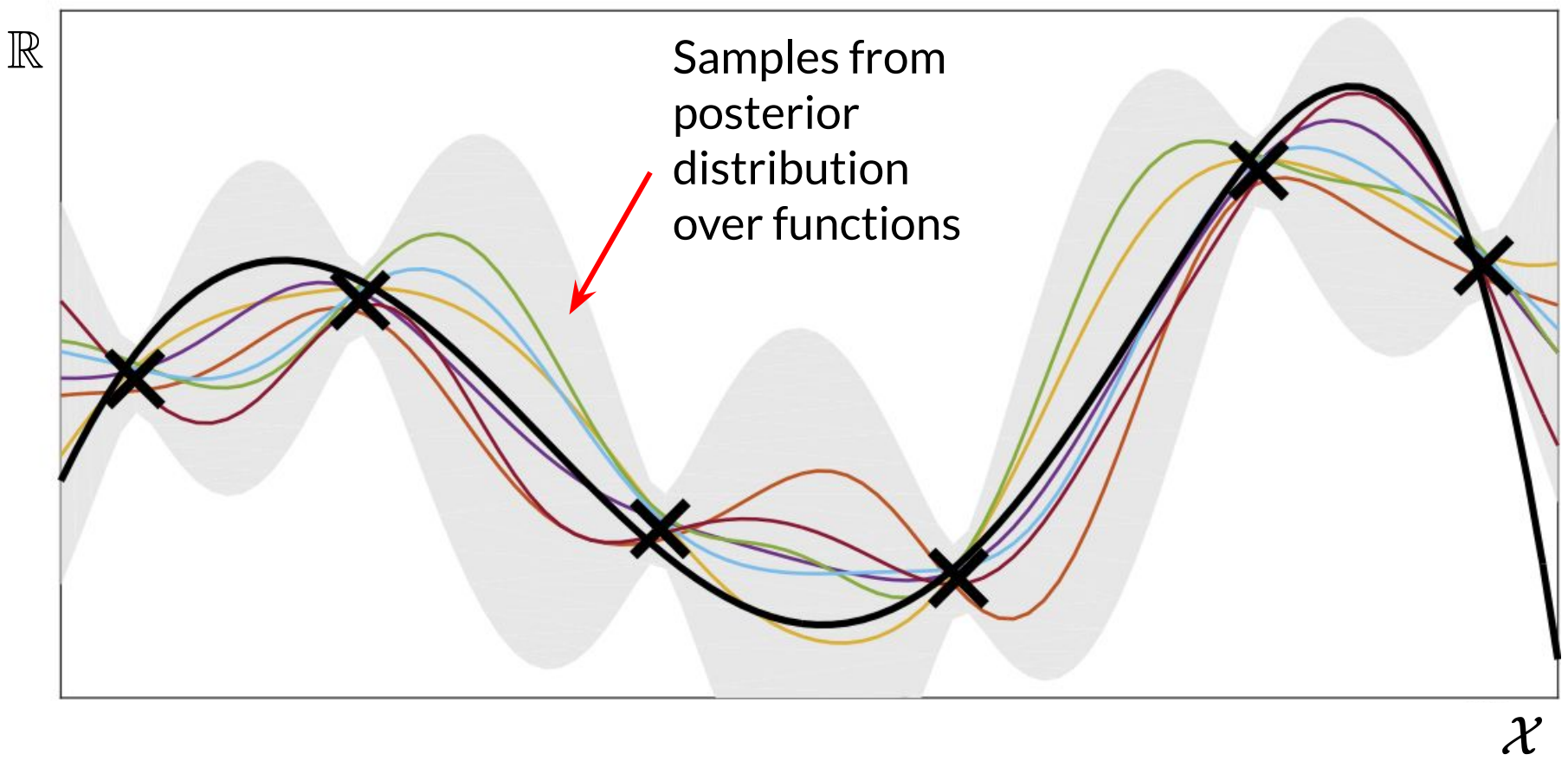

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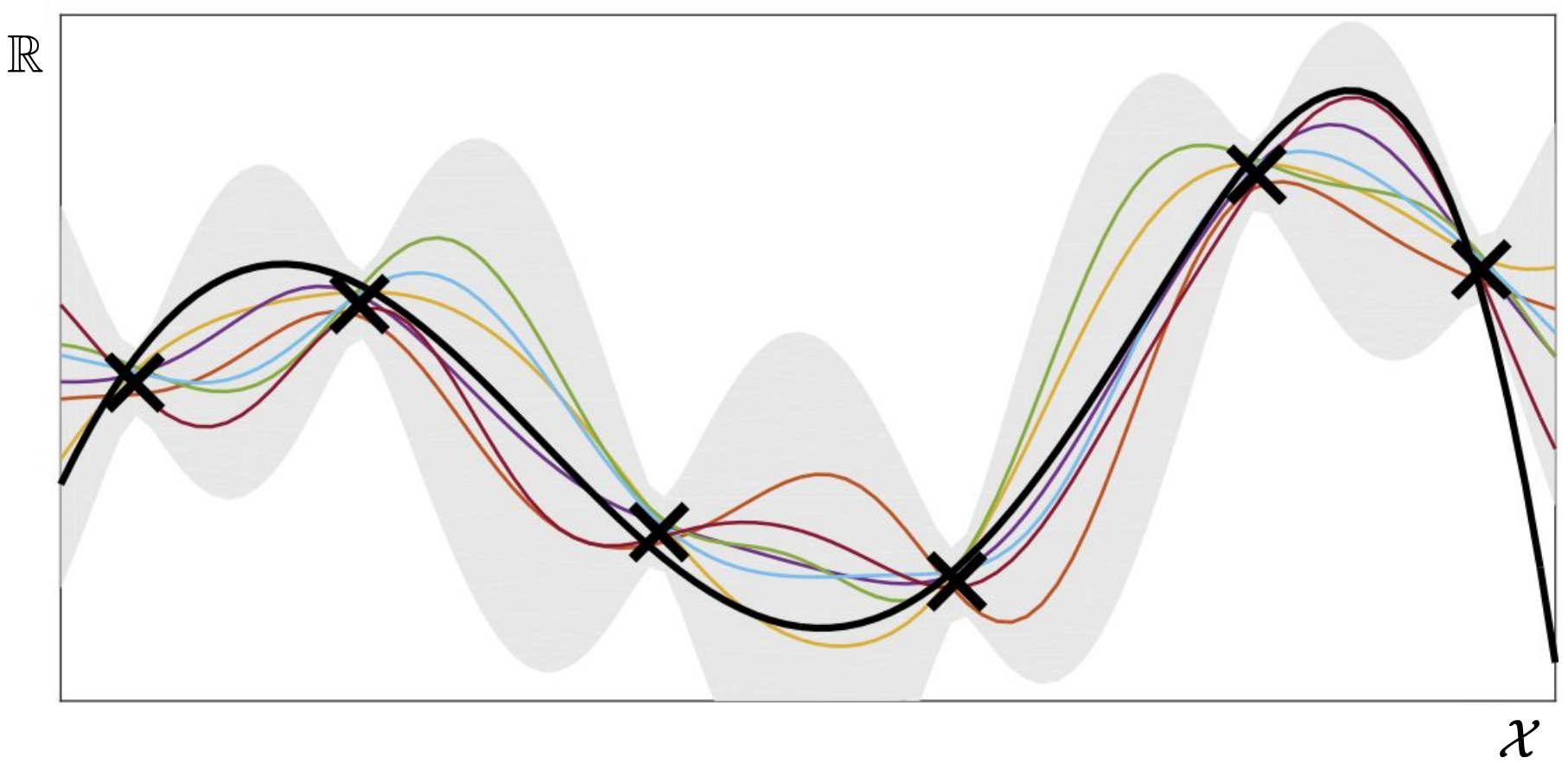

Define **acquisition function** using model.

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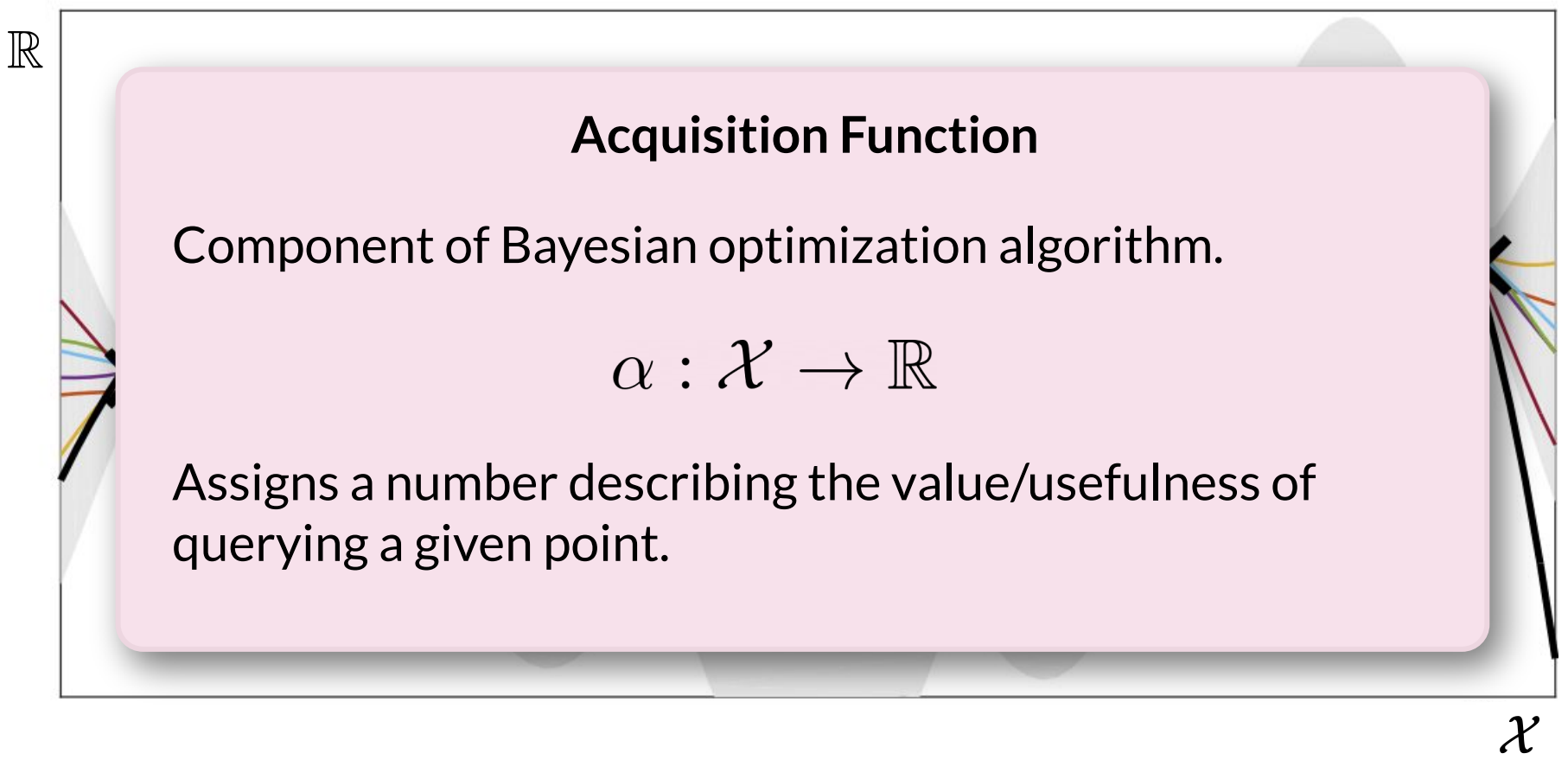

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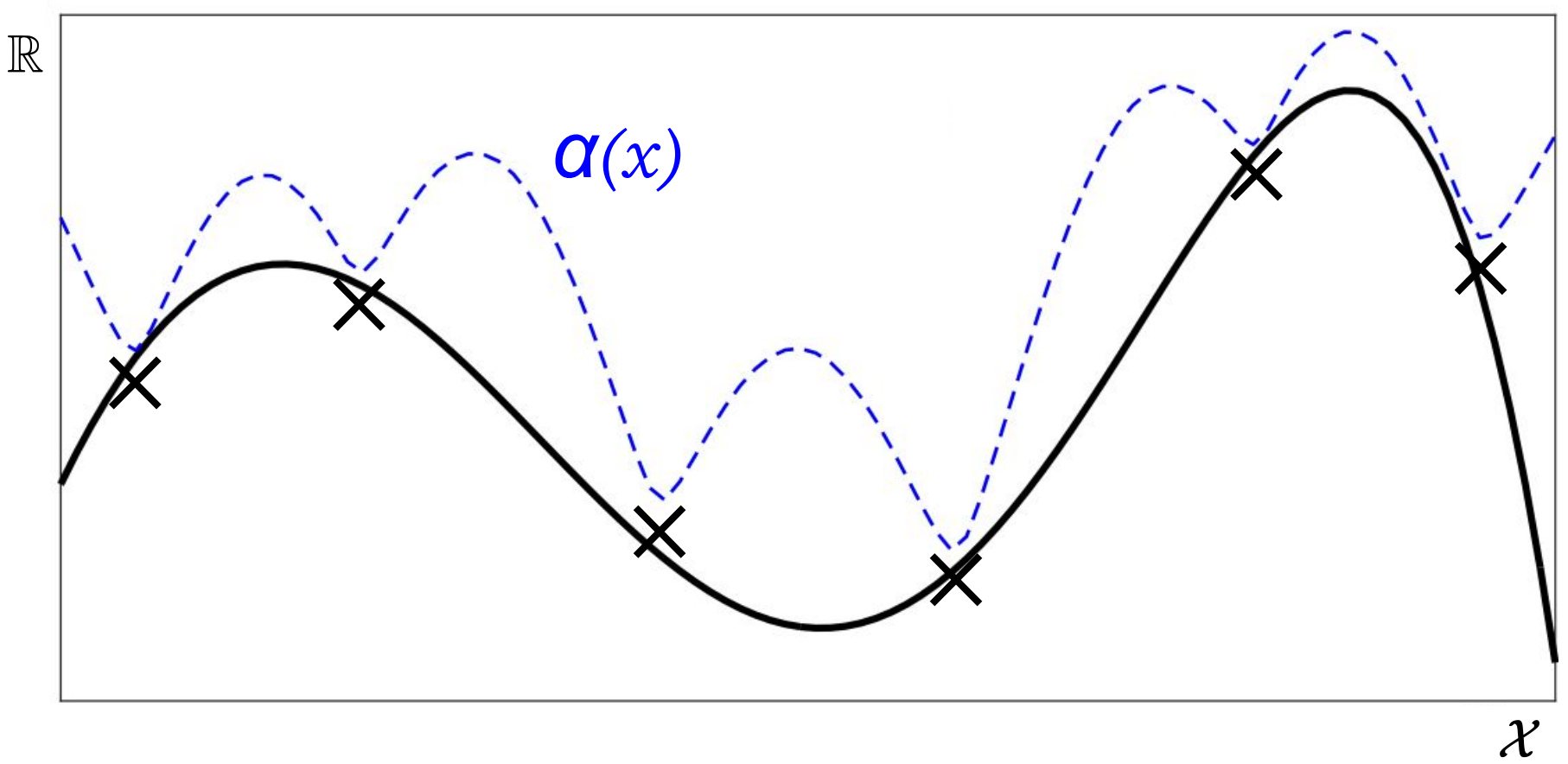

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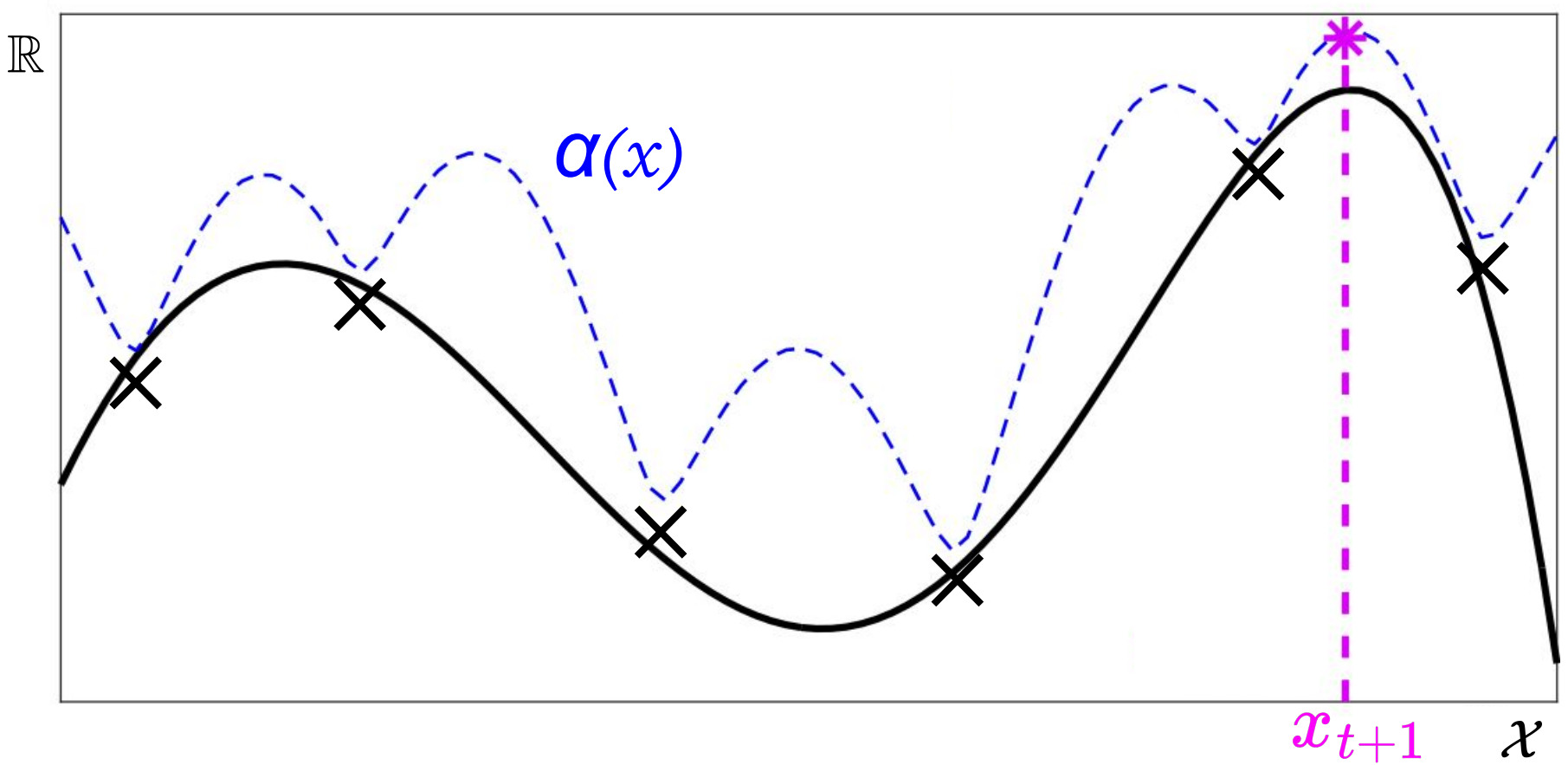

Optimize acquisition function ⇒ yields next point to query.

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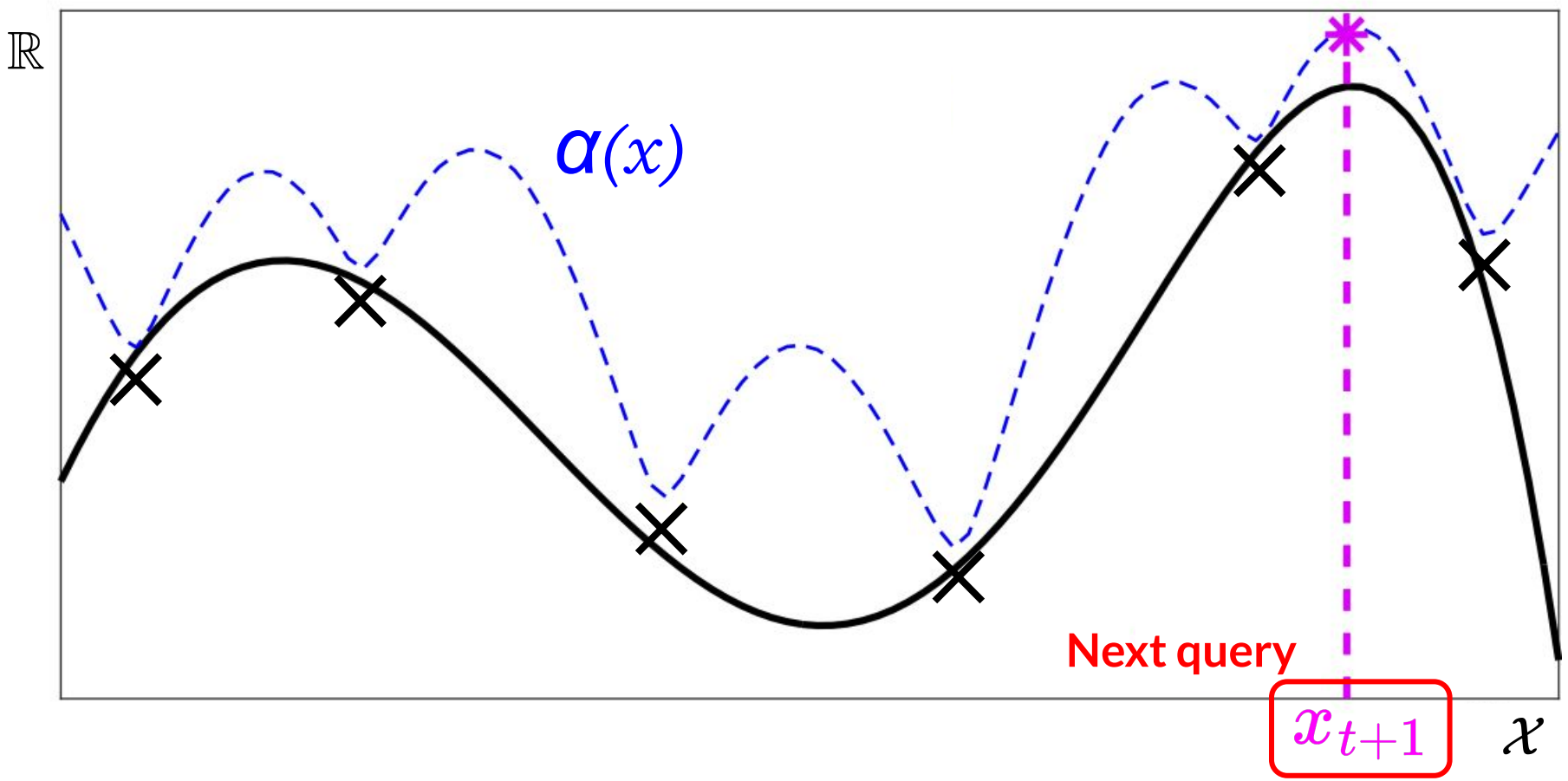

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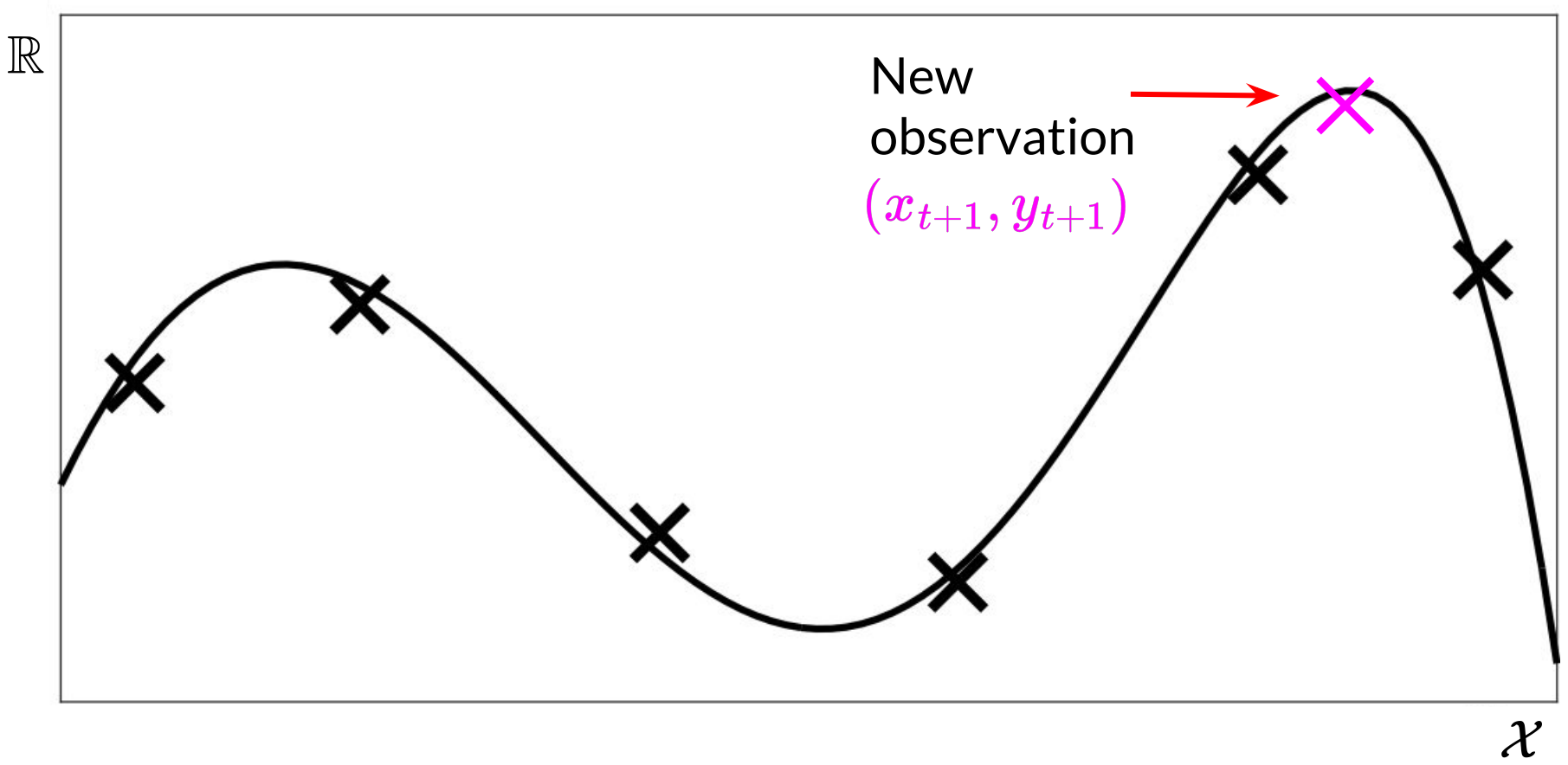

Query black-box f at x, observe y, and update dataset.

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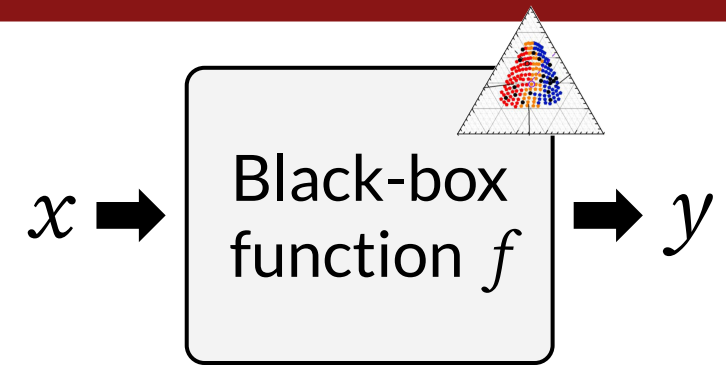

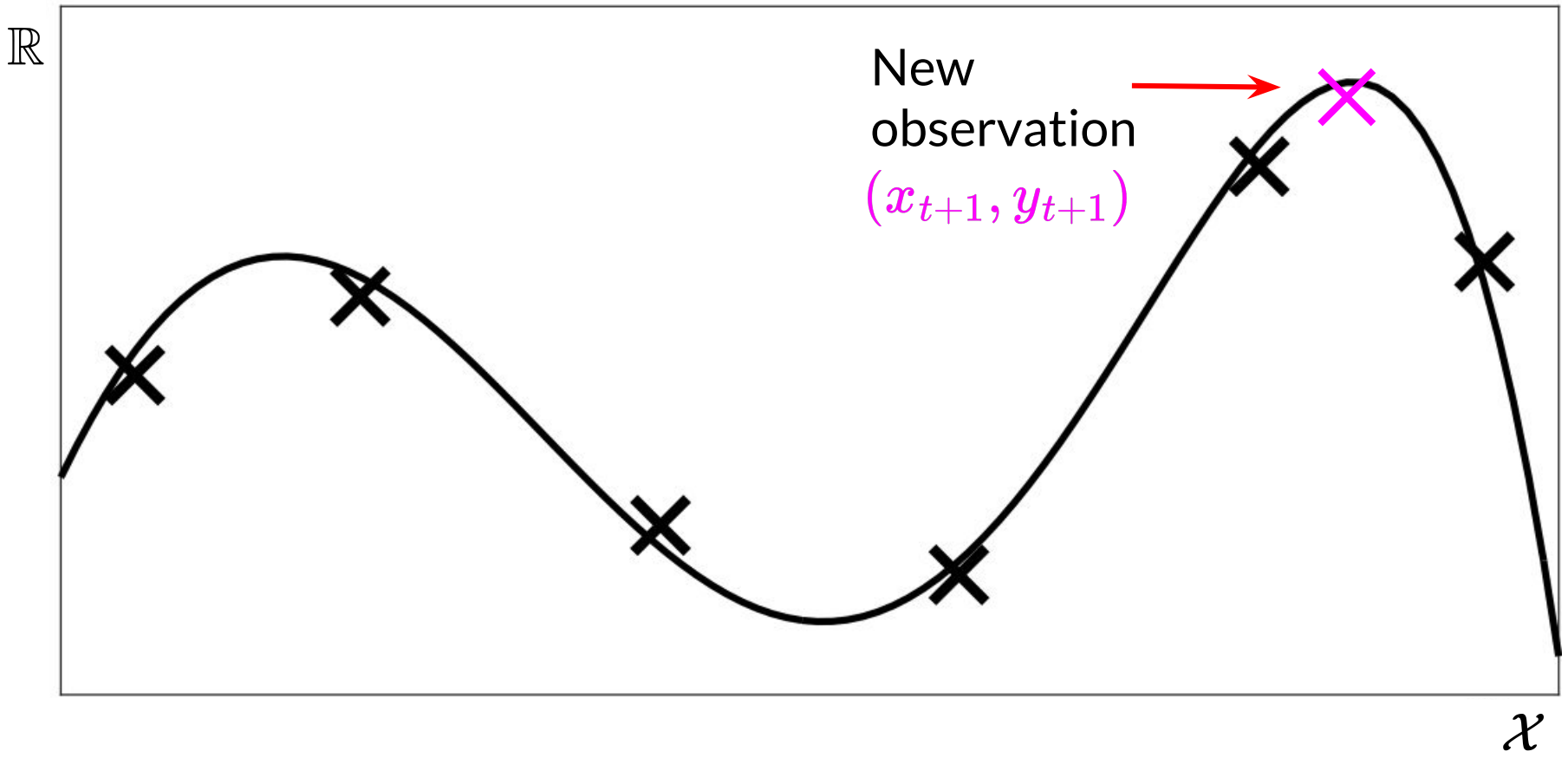

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Goal when designing acquisition functions:

- Want to be “optimal” in some sense; to choose the point that is *most informative*.
- And/or: most-likely to accomplish goals of algorithm, *e.g.*, carry out optimization.

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***But first*, a quick discussion on terminology!**

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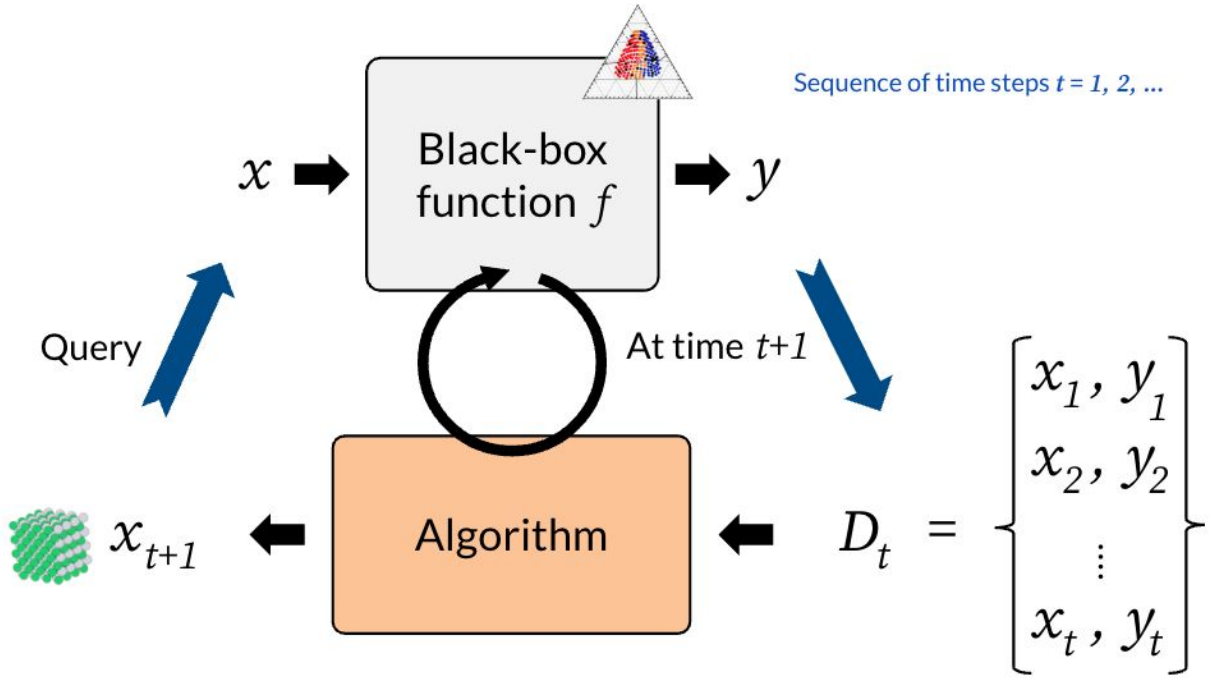

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Bayesian Optimization

Originally from operations research (among other fields).

Can view as: a special case of active learning, aiming to carry out the task of optimization.

(Which could potentially use an experimental design strategy, *e.g.*, in *entropy search*).

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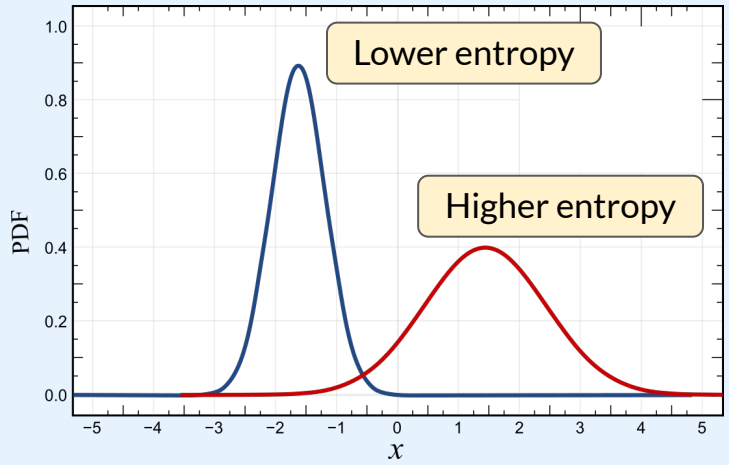
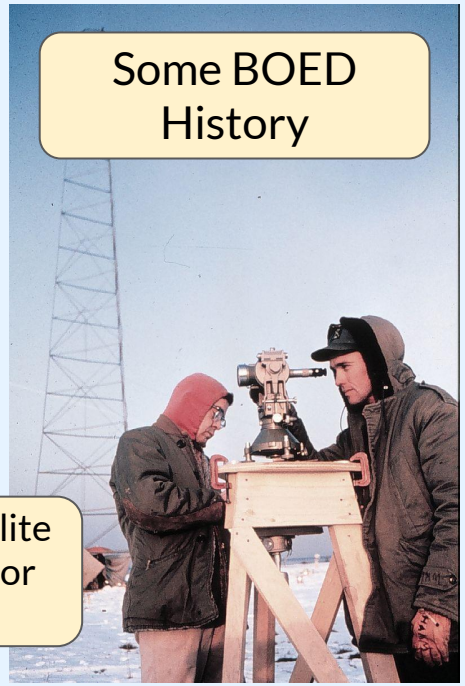
BOED: have model with an (unknown) parameter of interest.

- Choose experiments that most reduce uncertainty about parameter.
- *Uncertainty*: **entropy** of posterior distribution over parameter.





Terminology — Active Learning, Bayes Opt, Experimental Design, etc.

A bit more on experimental design: often referred to as *information-based experimental design* (if it involves reducing posterior entropy), or *Bayesian optimal experimental design (BOED)*.

Relatedly — there is *information-based Bayesian optimization*:

Info-based BO: entropy search (ES)[1], predictive ES[2], max-value ES[3].

- Rooted in **Bayesian optimal experimental design (BOED)**.

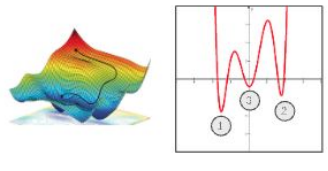
Which we will talk about a little later…

Terminology — Active Learning, Bayes Opt, Experimental Design, etc.

Side note: there are many other potential special cases of active learning beyond global optimization, as in BO…

Terminology — Active Learning, Bayes Opt, Experimental Design, etc.

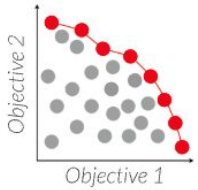
Optimization Variants
(global, local, top-k optima)



Applications

- *ML model training*
- *HPO / NAS*
- *Systems tuning*

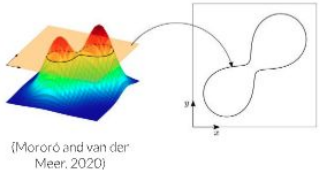
Multi-objective Opt.
(Pareto frontiers)



Applications

- *Process optimization*
- *Portfolio optimization*
- *Laboratory equipment / machines*

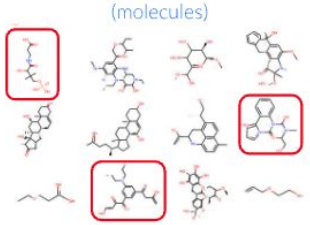
Level Set Estimation
(superlevel set, sublevel set)



Applications

- *Catalyst design*
- *Active learning / weak supervision*
- *Environmental monitoring*

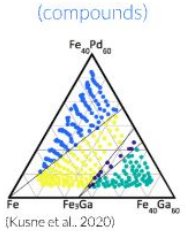
Search
(subset matching criteria)



Applications

- *Drug discovery*
- *Fraud detection*
- *Targeted opinion polling*

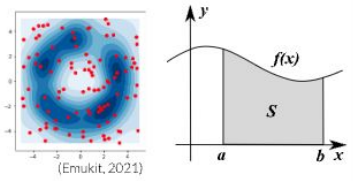
Phase Identification
(boundaries, partitions)



Applications

- *High throughput materials design/discovery*

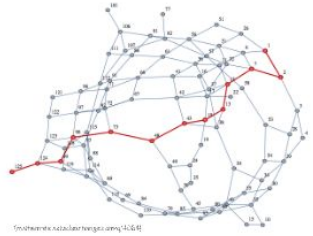
Quadrature, Integration
(integrals, expectations)



Applications

- *Probabilistic modeling (marginal distributions, normalization constants)*
- *Estimating center of mass (and centroids)*

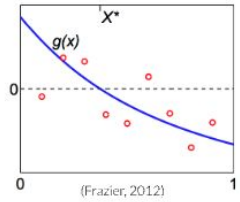
Graph Algorithms
(shortest paths)



Applications

- *Transportation networks*
- *Shipping networks*
- *Social networks*

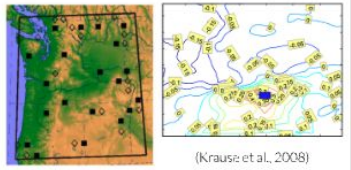
Root Finding, Bisection
(roots)



Applications

- *Target localization (airborne radar)*
- *Edge detection (computer vision)*
- *Biology / microbiology (phase shifts)*

Sensor Placement
(function value at locations)



Applications

- *Water distribution systems*
- *Outbreak detection in networks*
- *Weather monitoring*

Acquisition Functions — Back to Acquisition Functions

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Acquisition Function

Component of Bayesian optimization algorithm.

$$\alpha : \mathcal{X} \to \mathbb{R}$$

Assigns a number describing the value/usefulness of querying a given point.

Acquisition Functions — Upper Confidence Bound (UCB)

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The UCB acquisition function is often written:

$$\alpha_t(x) = \mu(x) + \beta_t \sigma(x)$$

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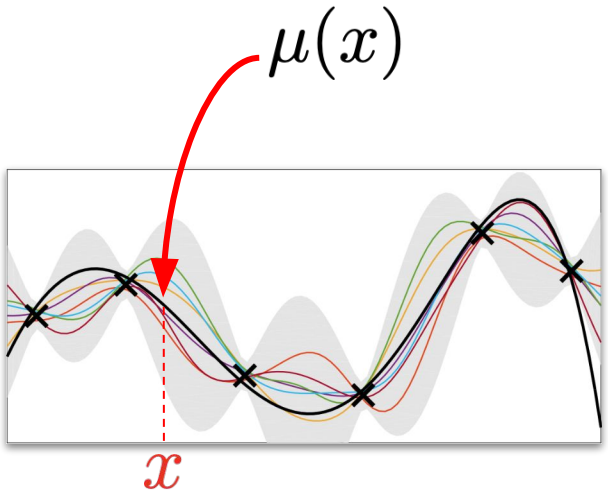
where:

$\mu(x)$ - Mean of *marginal posterior* at input x.



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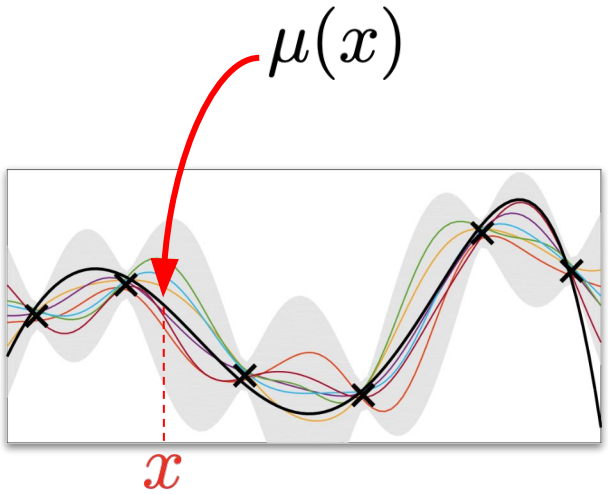

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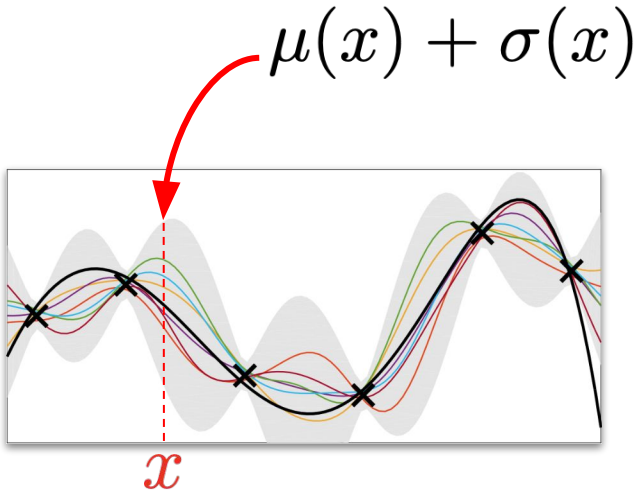

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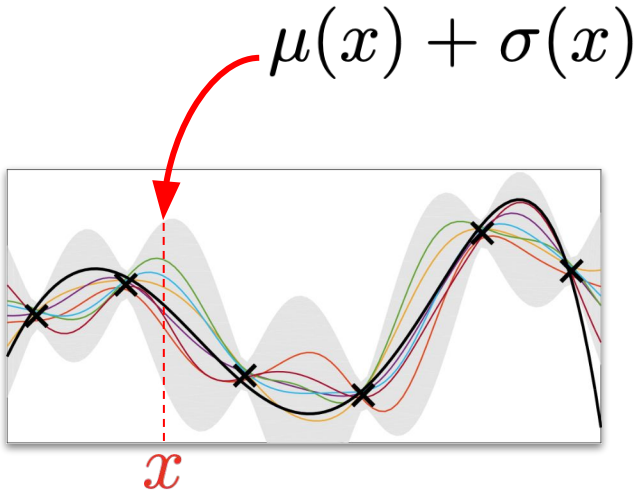
β_t - Hyperparameter controlling tradeoff between exploration and exploitation.



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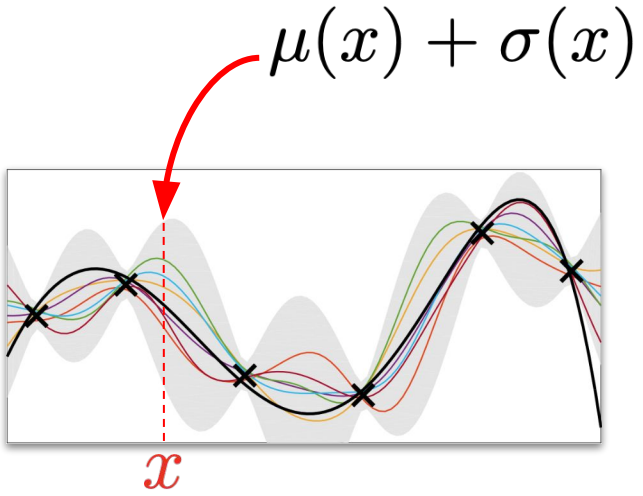

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Maximizing variance → queries *most unknown* part of function
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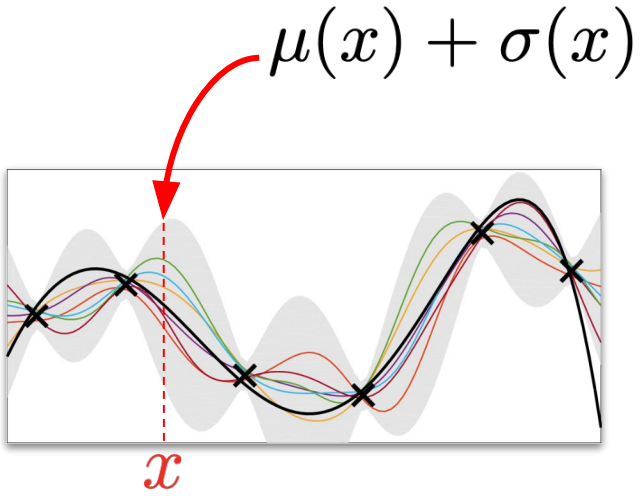

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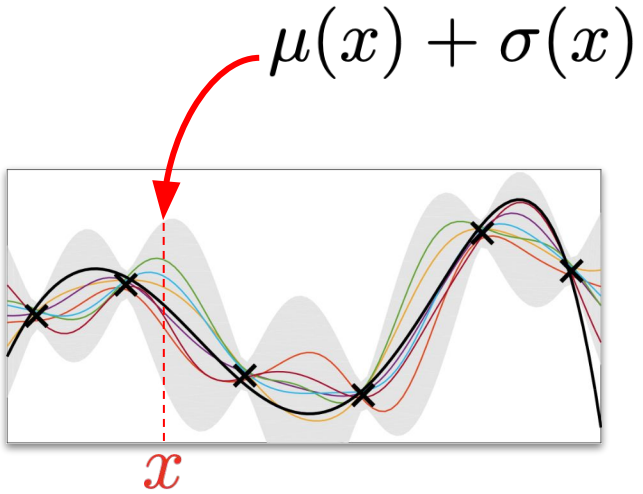

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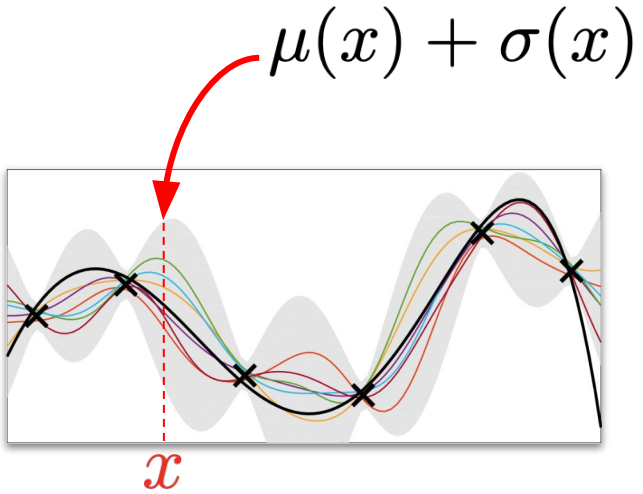

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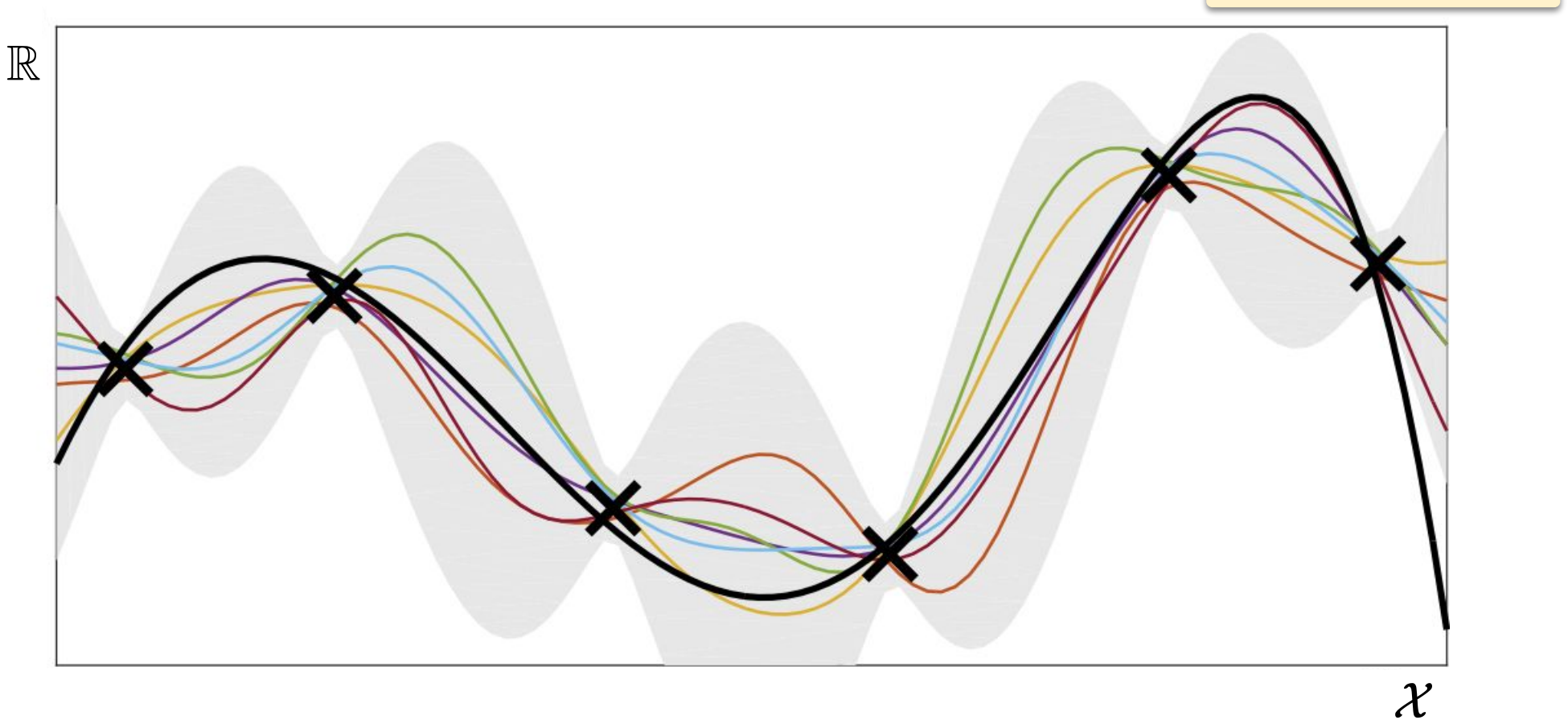
We want to trade off between these two quantities.

Acquisition Functions — Upper Confidence Bound (UCB)

Visualizing UCB



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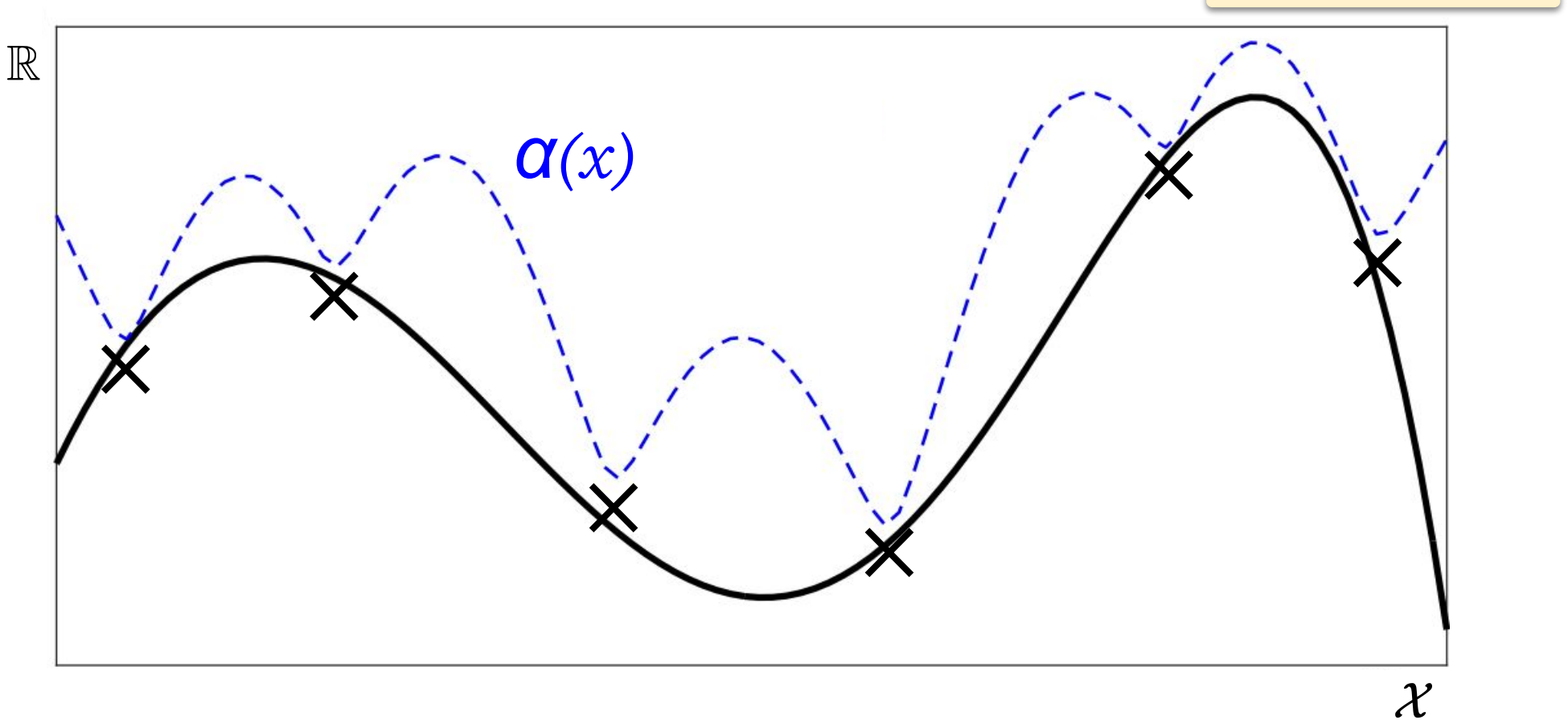

… define the **UCB acquisition function**.

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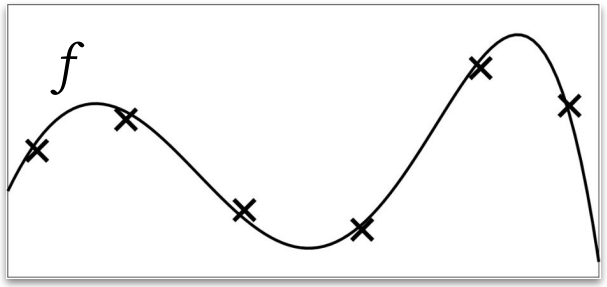

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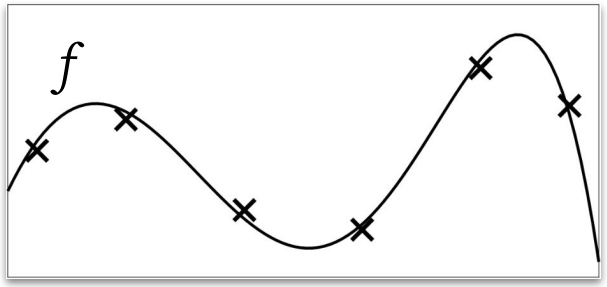

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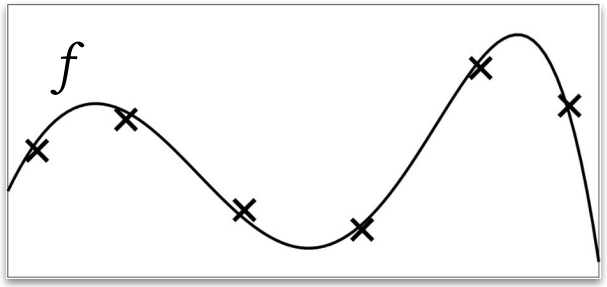

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(This is equivalently also commonly called: *expected information gain*, or *EIG*, *about* f.)

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You can prove (at least for GP models) that maximally reducing posterior entropy is equivalent to querying point with maximum standard deviation (of posterior marginal).

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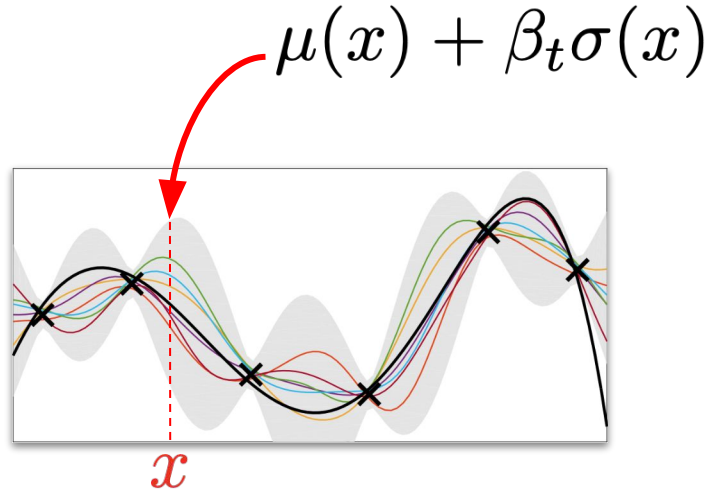
So in **UCB** ⇒

The second term (standard deviation term) is in fact balancing exploration (EIG about f) with exploitation (best expected input x).



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You can prove this is equal to …

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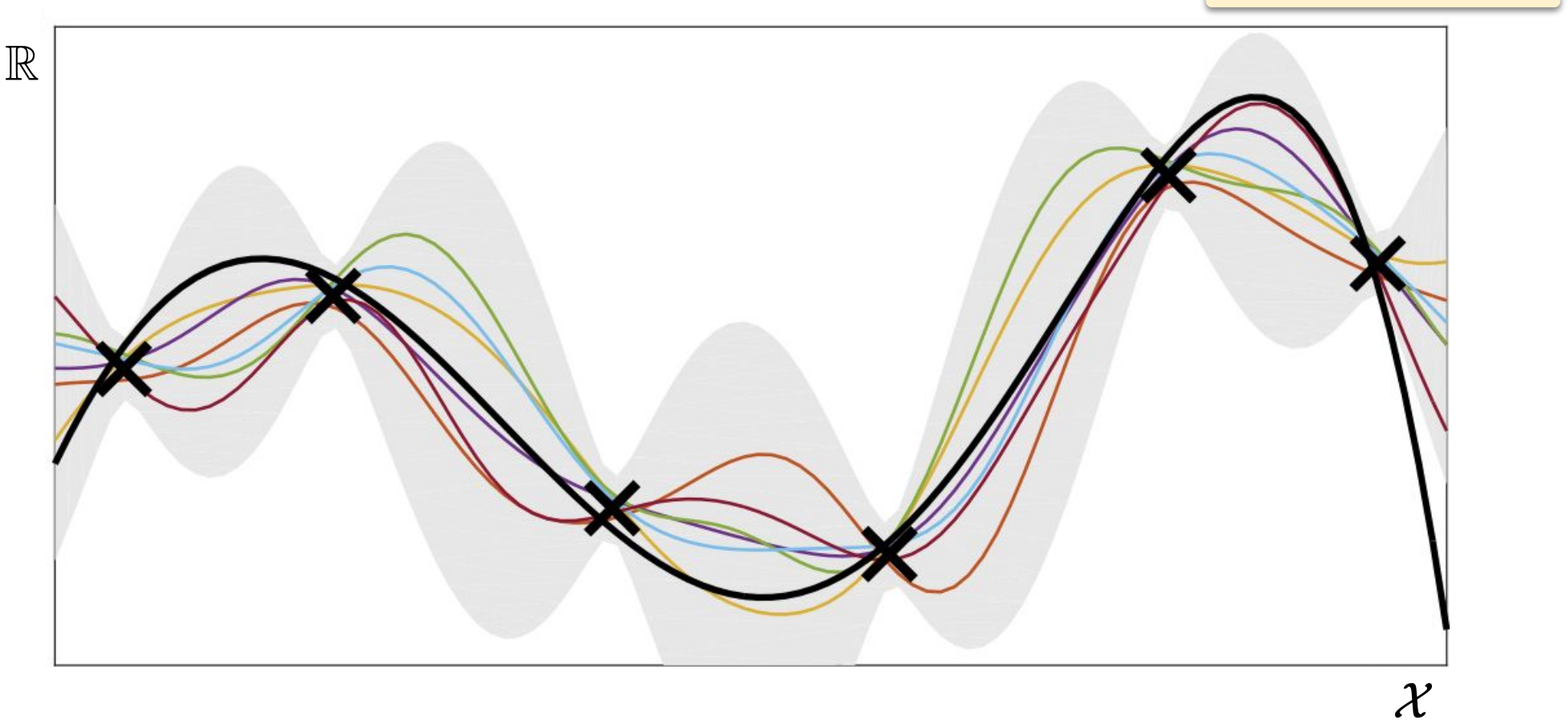
where $\Phi(\cdot)$ denotes the CDF of the standard normal distribution.

(And, as before, $\mu(x)$ and $\sigma(x)$ are the mean and SD of marginal posterior at x.)

Acquisition Functions — Probability of Improvement (PI)

Visualizing PI



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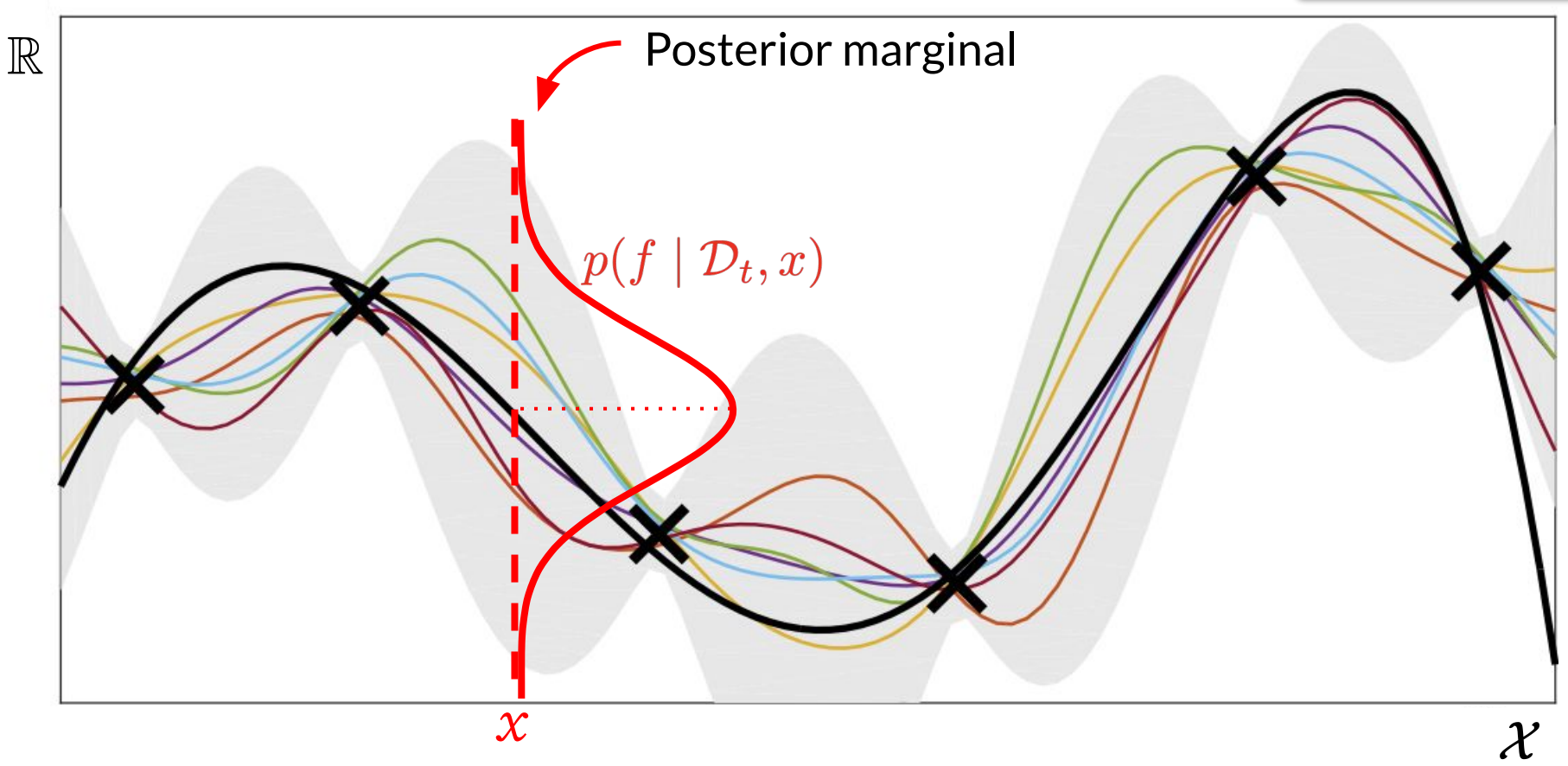

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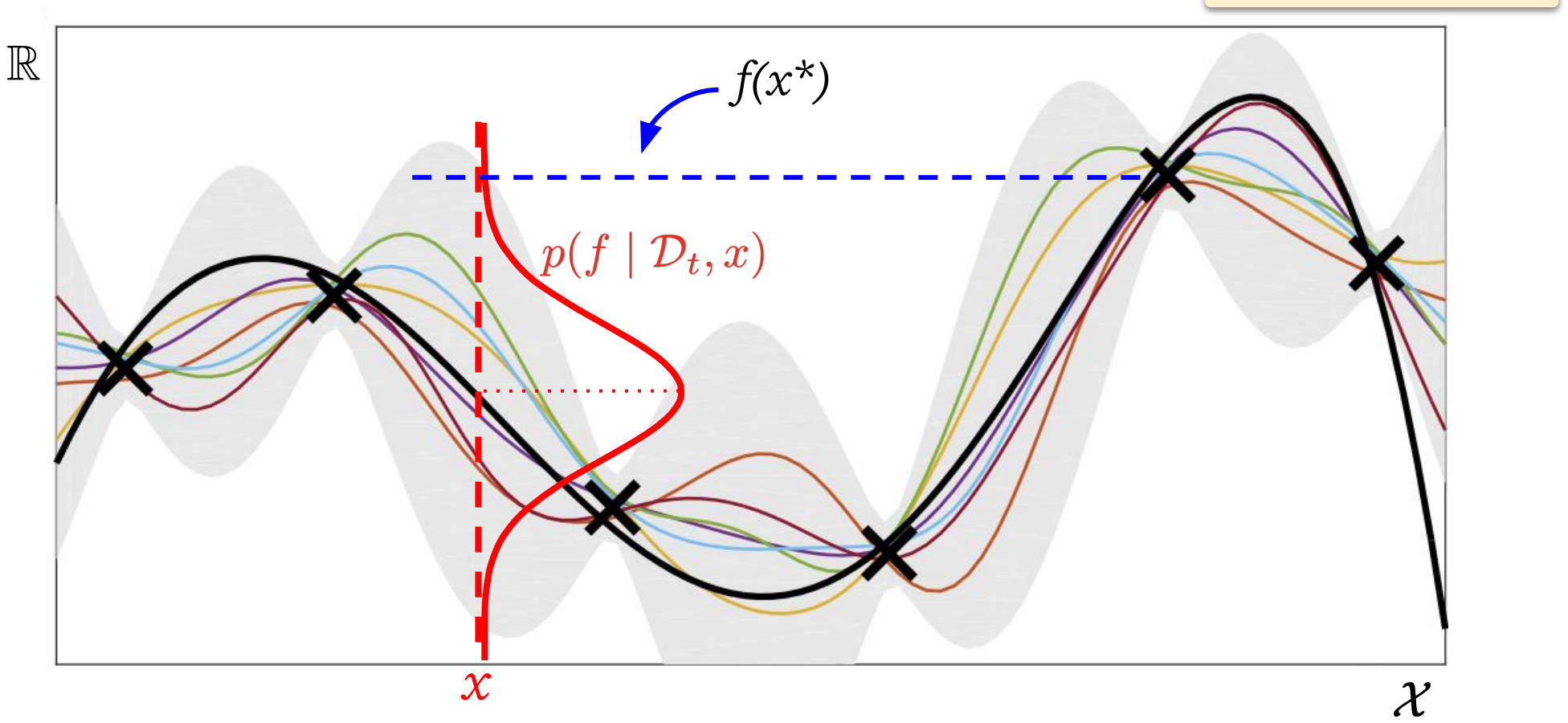

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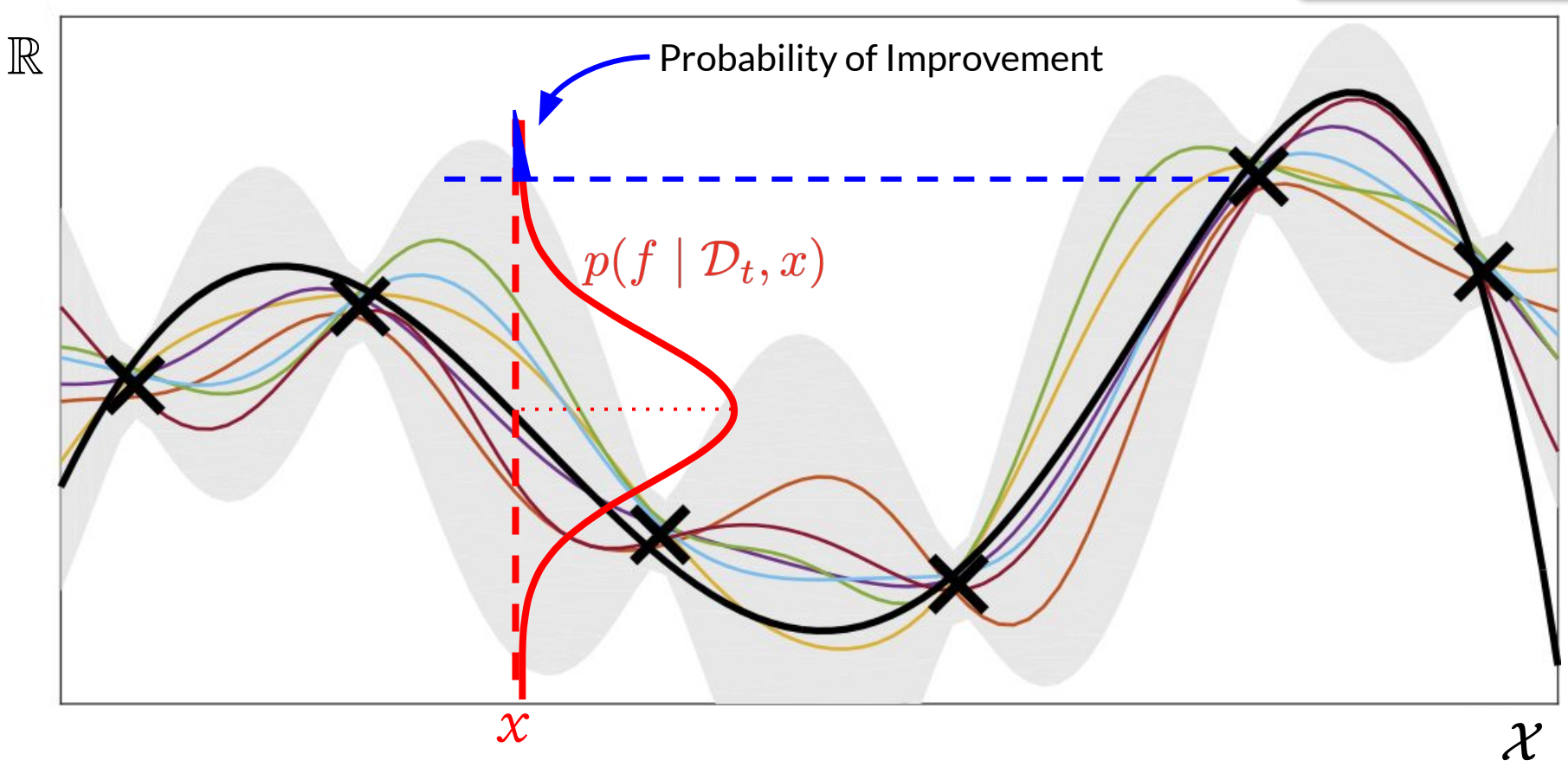

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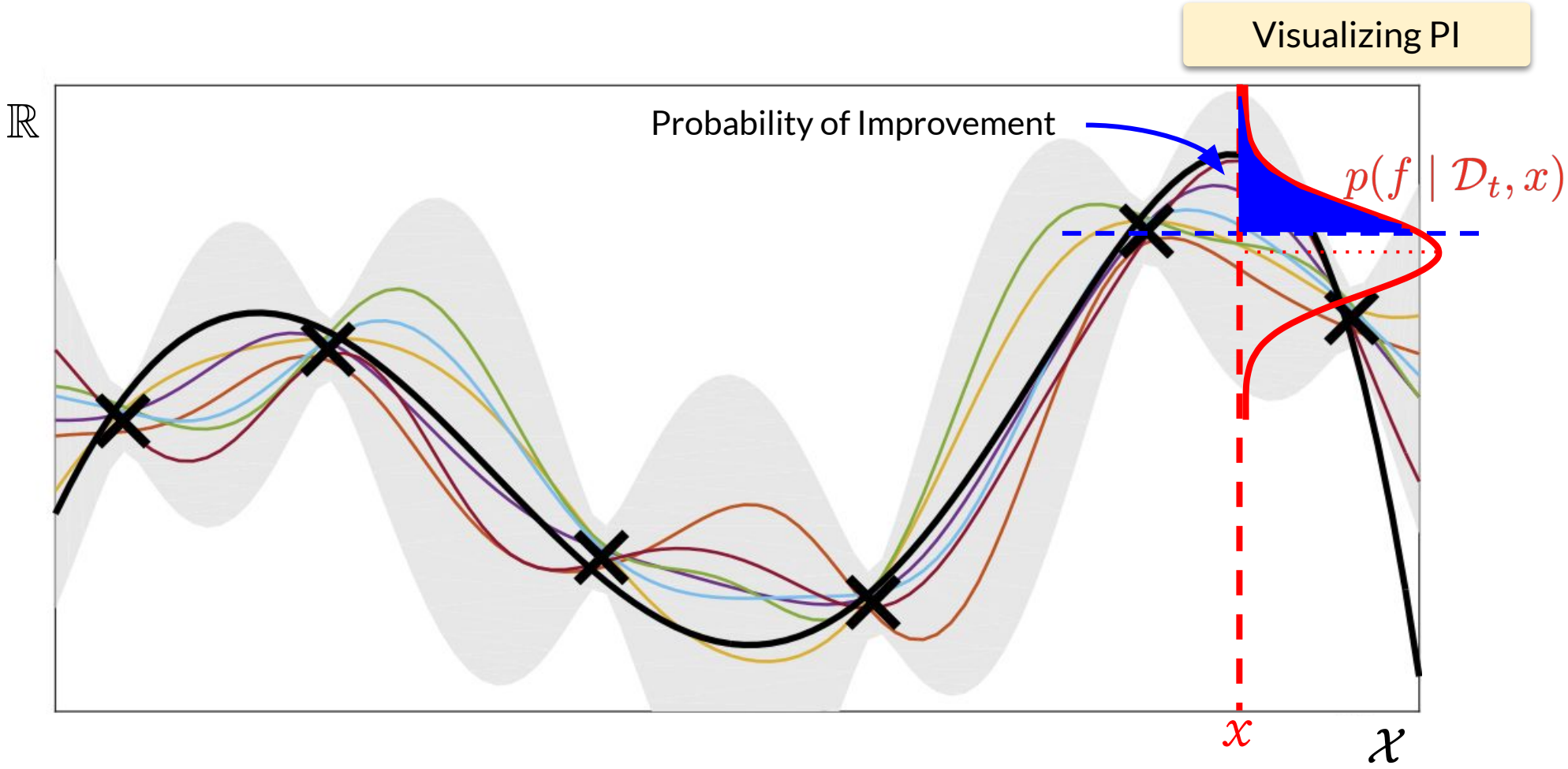

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PI maximizes the **probability** that $f(x)$ is greater than then best point so far.

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Visualizing this…

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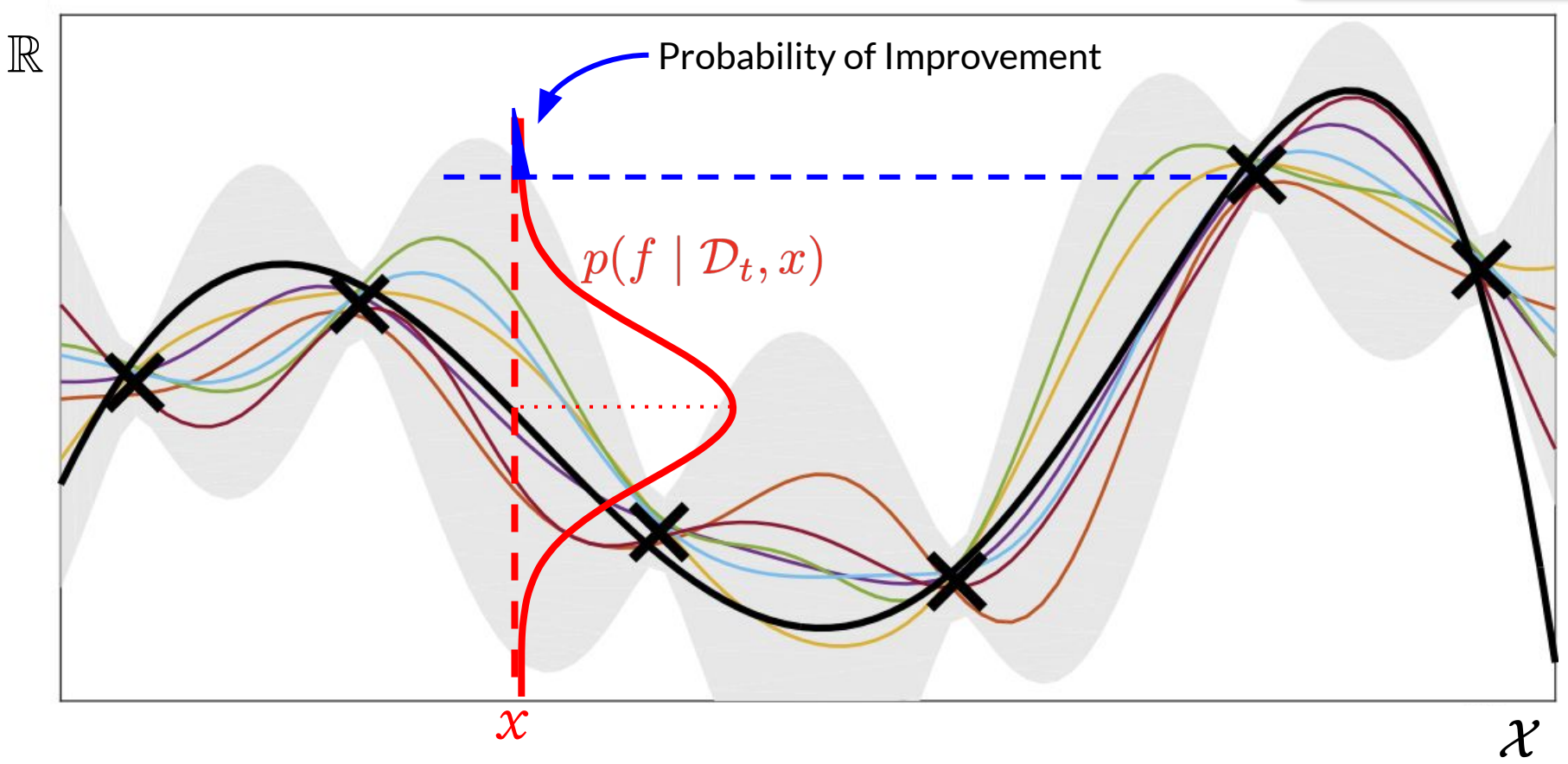

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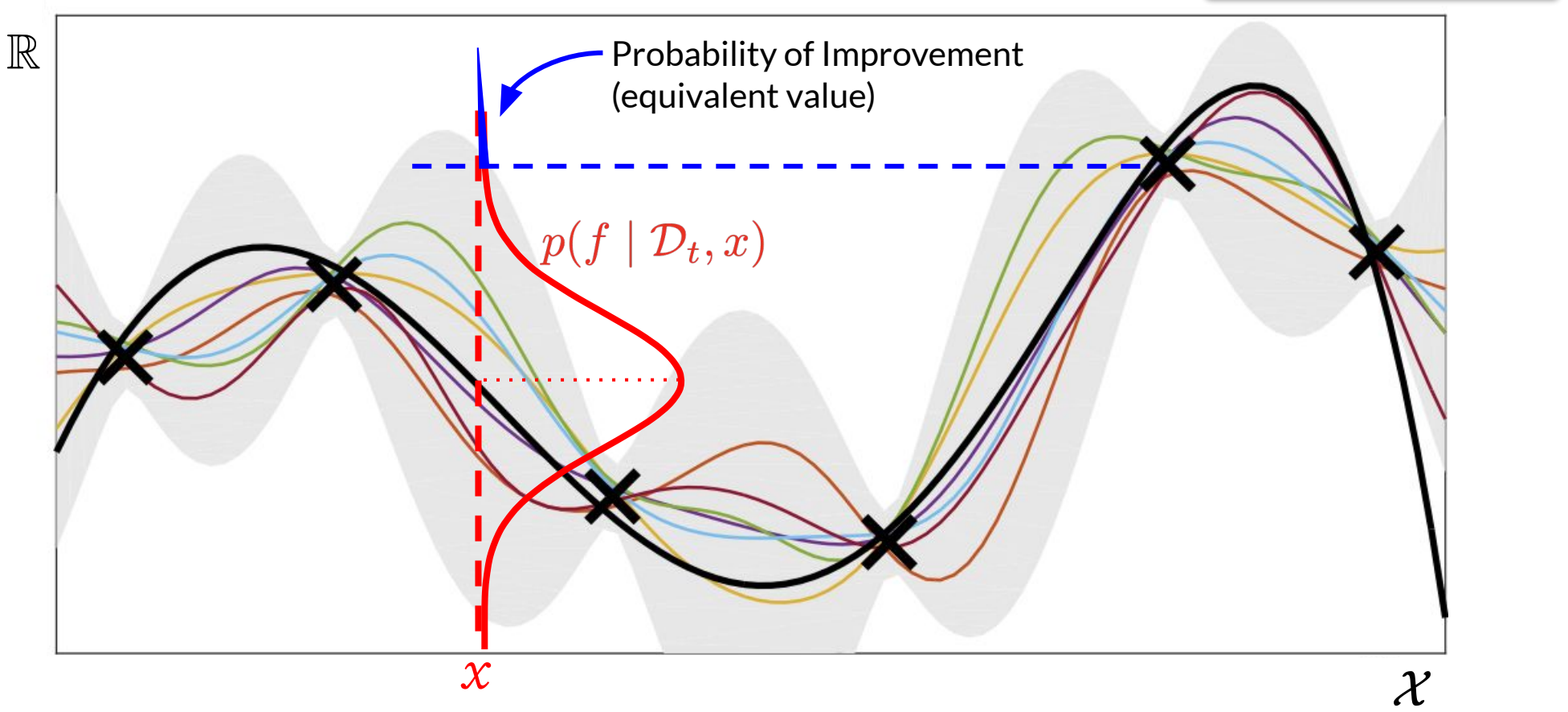
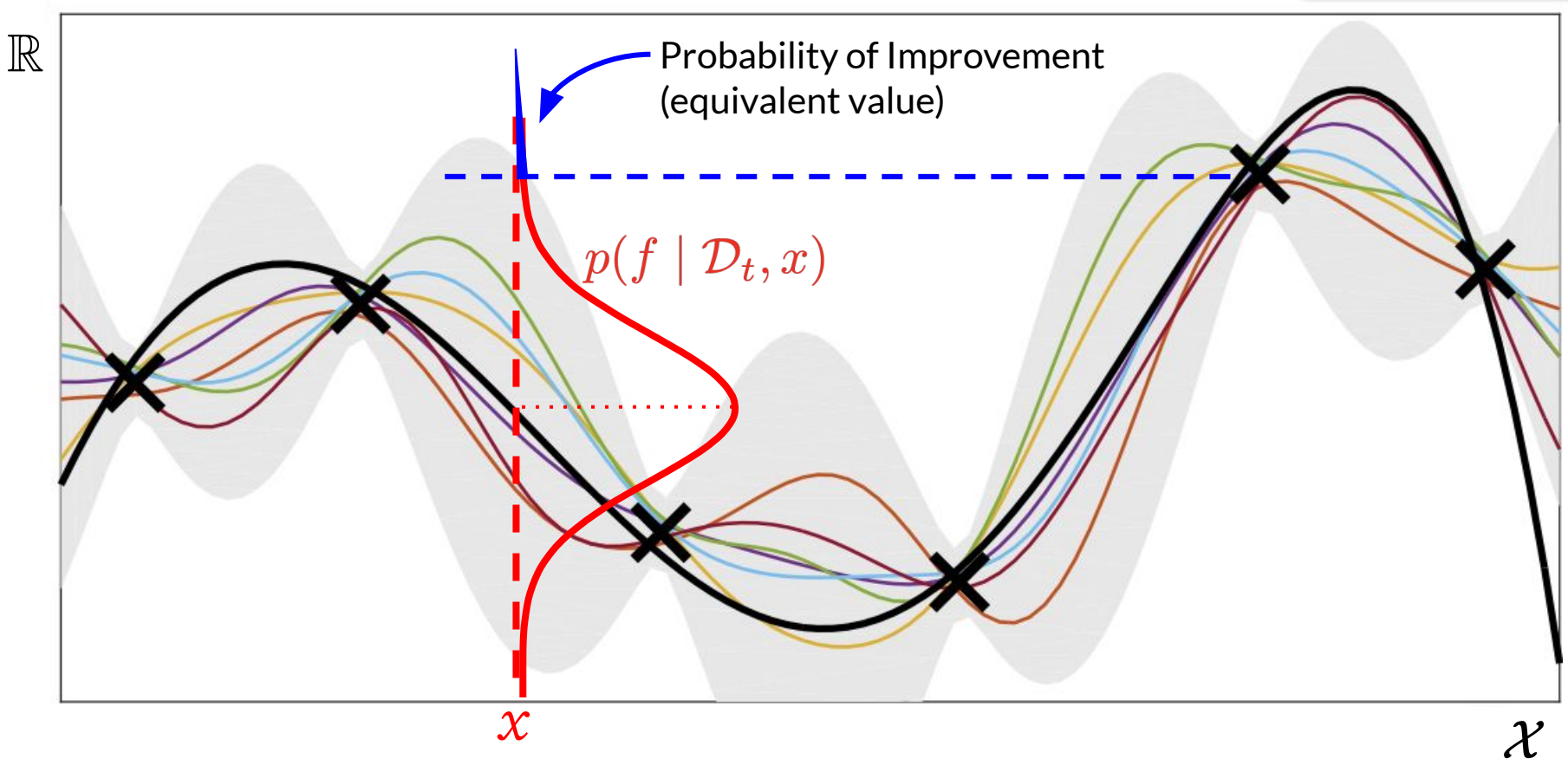


Acquisition Functions — Probability of Improvement (PI)

Visualizing PI



In contrast, we could try to maximize the *expected **amount** of improvement* over the best point so far…

Acquisition Functions — Expected Improvement (EI)

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You can prove this is equal to …

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where $\Phi(\cdot)$ denotes the CDF of the standard normal distribution and $\phi(\cdot)$ denotes the PDF of the standard normal distribution.

(And, as before, $\mu(x)$ and $\sigma(x)$ are the mean and SD of marginal posterior at x.)

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Nice visual comparing UCB *vs.* PI *vs.* EI:

Source: M. O. Ahmed, S. Prince, “Bayesian optimization”

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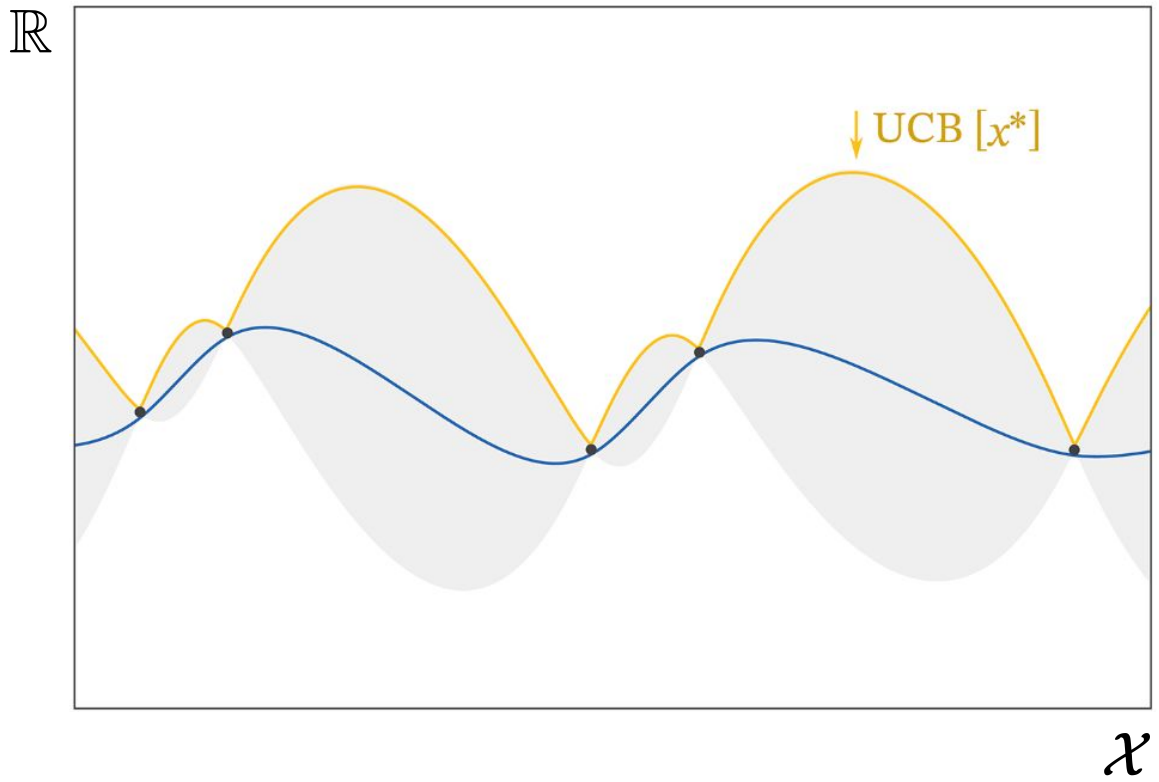

UCB: upper confidence bound of posterior

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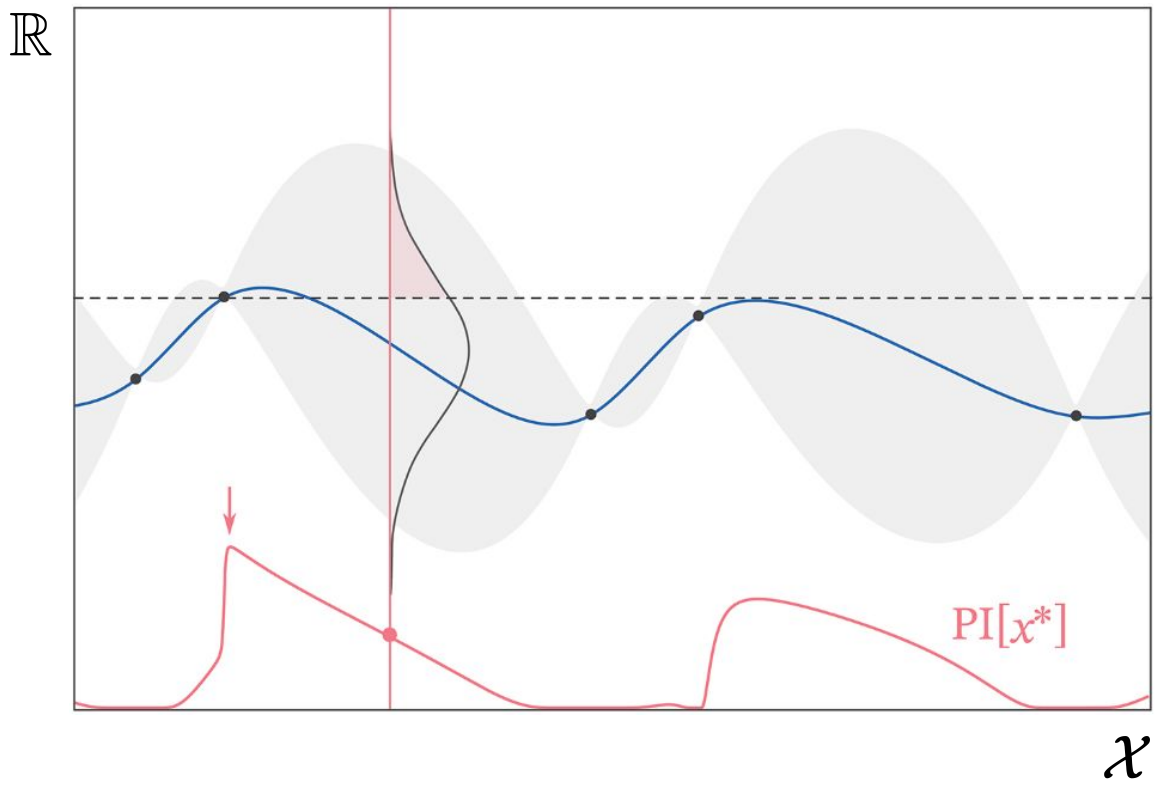

PI: probability that $f(x)$ is greater than best point

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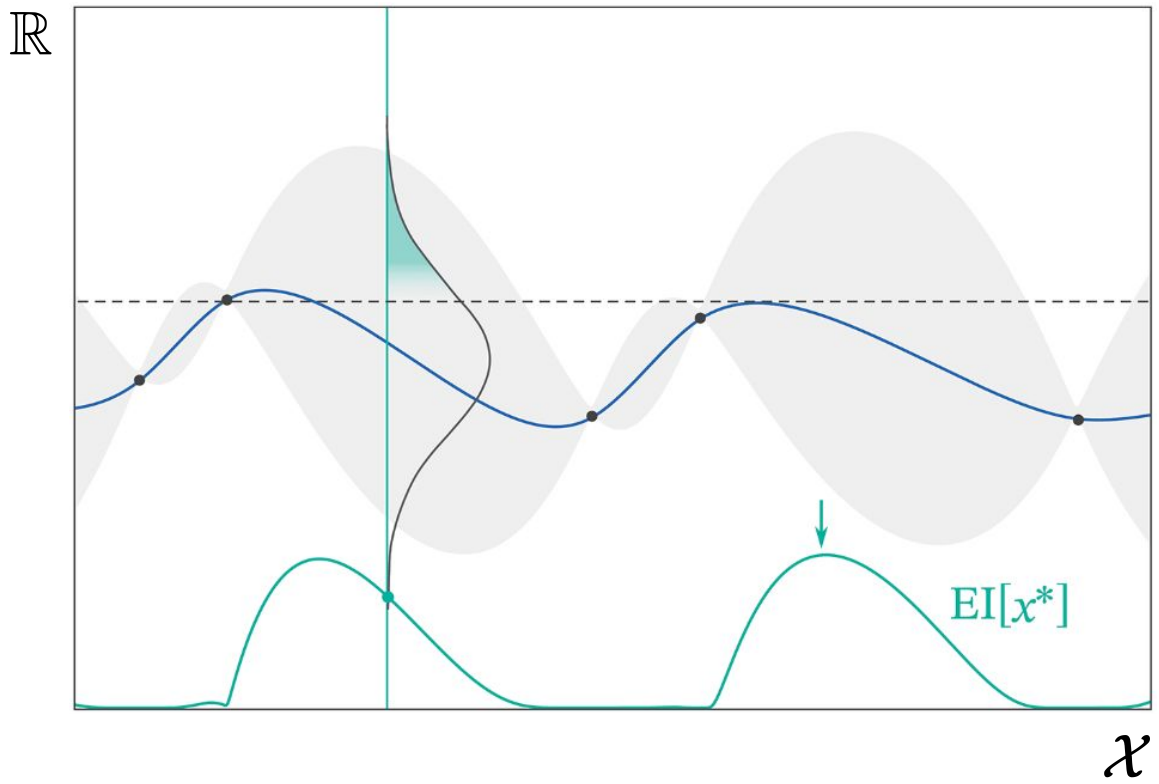

EI: *expected amount* $f(x)$ is greater than best point

(and ignoring amount that it's less than best point)

Acquisition Functions — Entropy Search (ES)

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Why would you want to use this acquisition function?

⇒ Intuitively: if you get rewarded for *how good your guess of* x^* *is* — rather than, the value of the maximizer, $f(x^*)$ — ES should be more optimal.

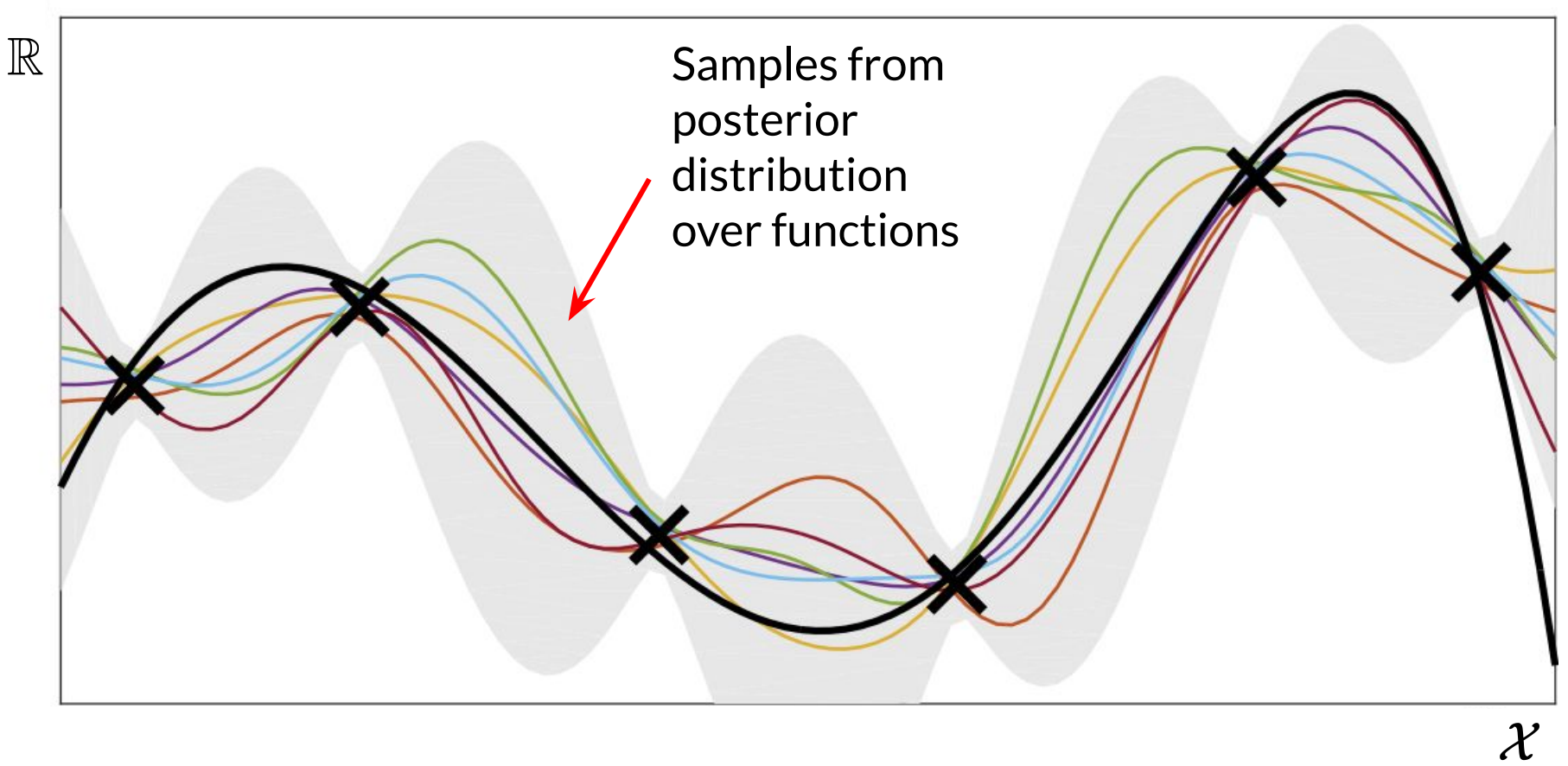
Acquisition Functions — Entropy Search

Visualizing ES

To explain this acquisition function, let's visualize…

Acquisition Functions — Entropy Search

Visualizing ES



Probabilistic model of f, given dataset.

Acquisition Functions — Entropy Search

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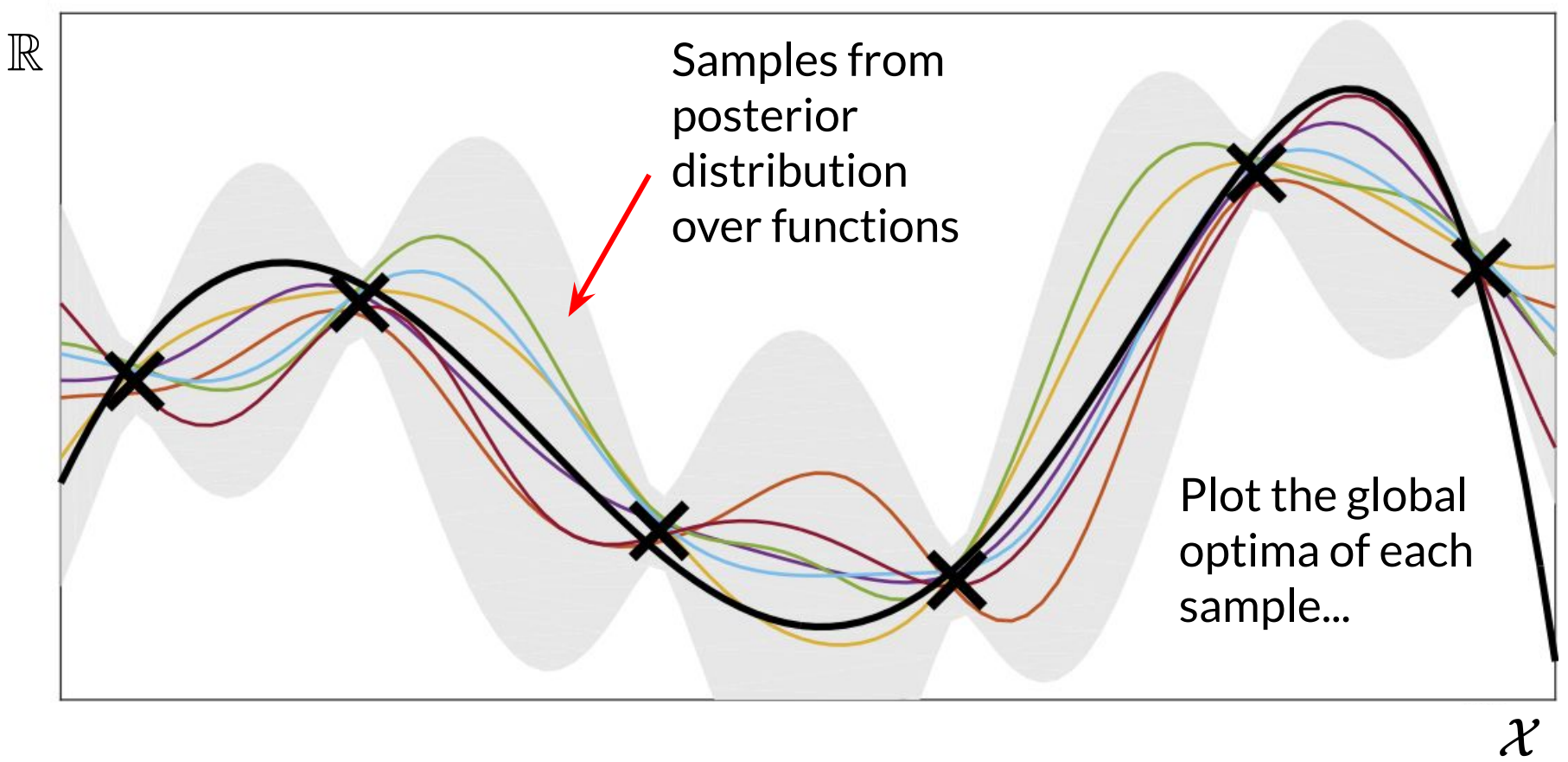

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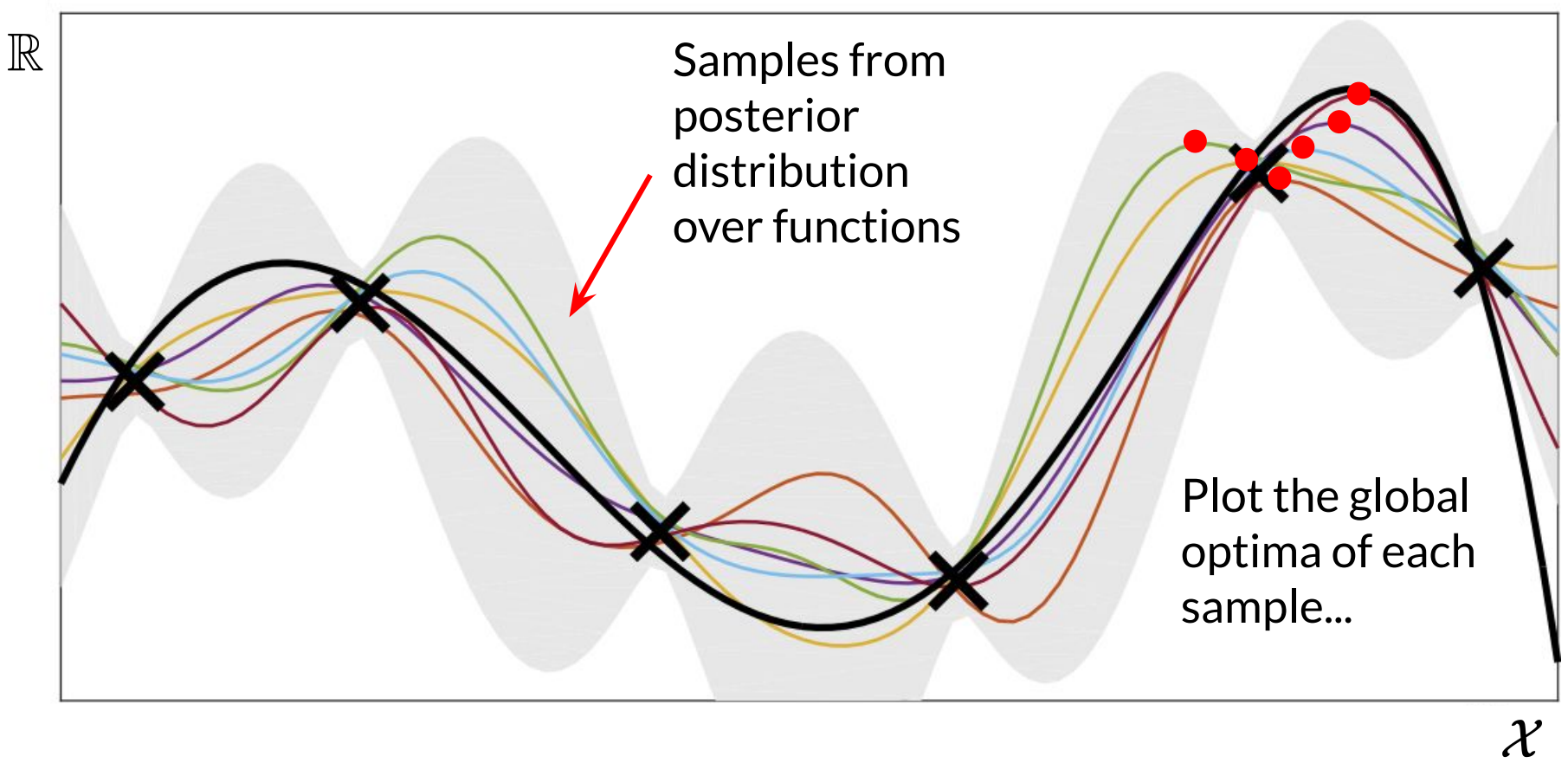

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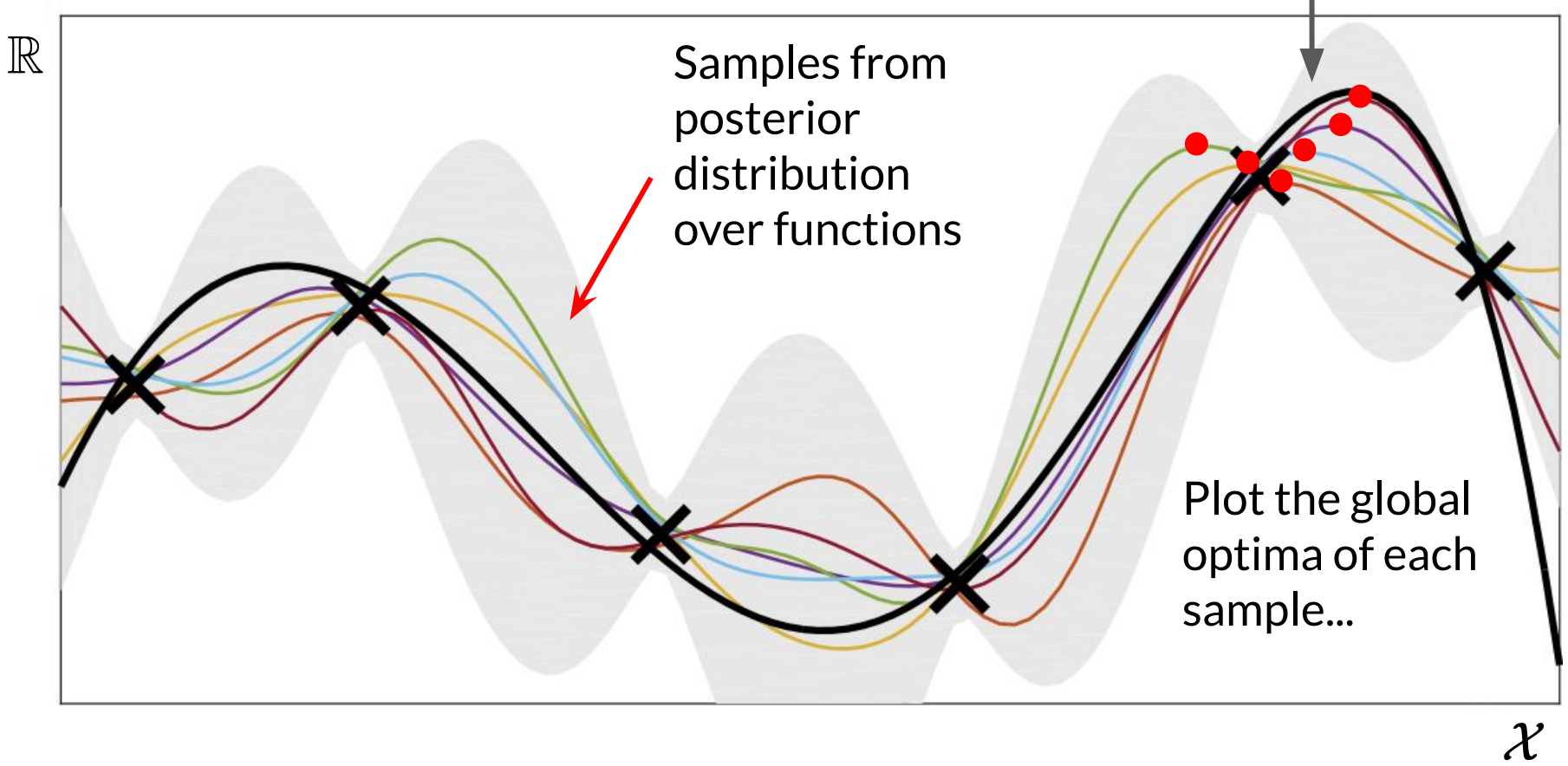
Acquisition Functions — Entropy Search

There is a posterior distribution over global optima induced by probabilistic model: $p(x^* \mid \mathcal{D}_t)$



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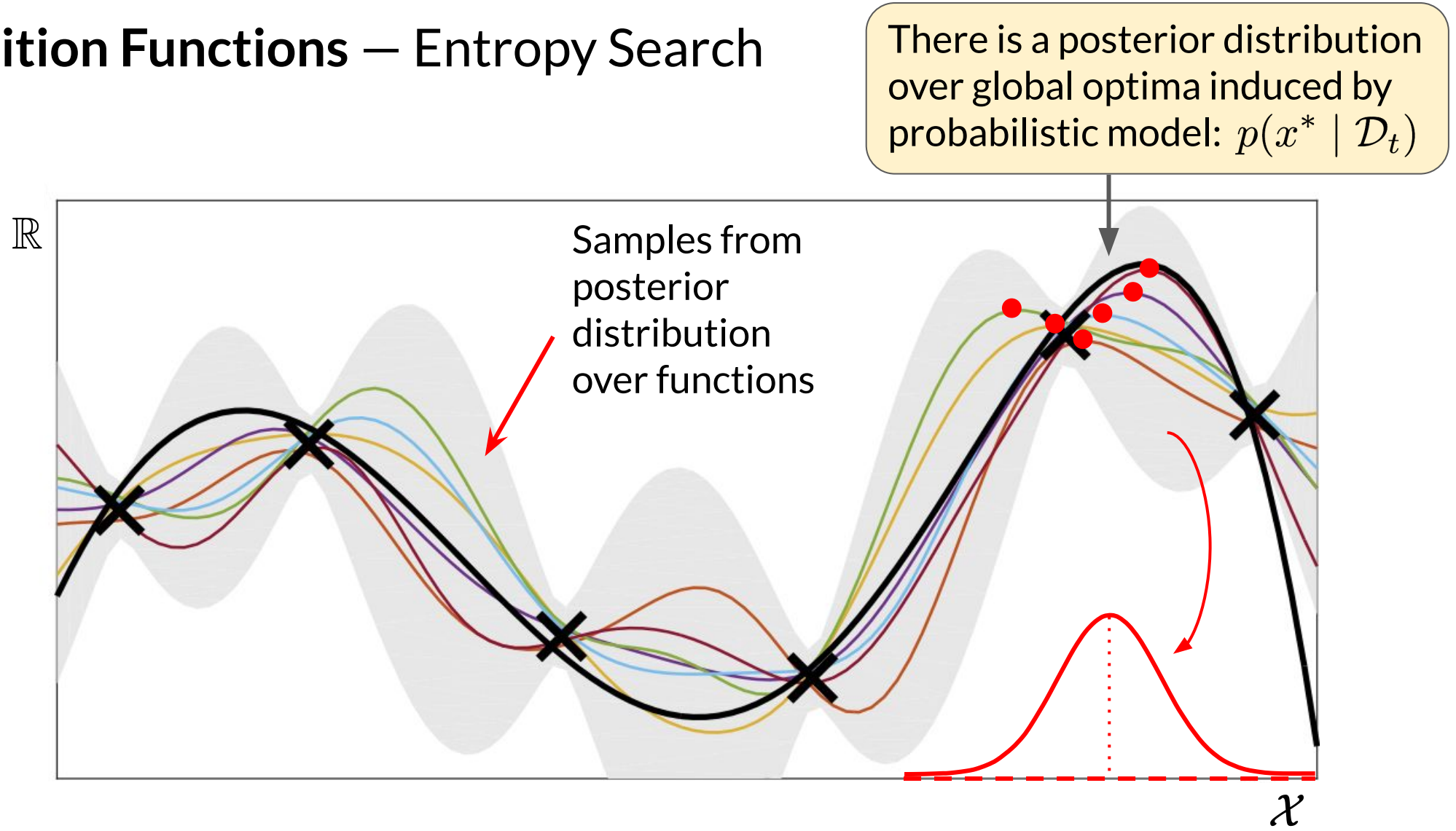

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This leads us to the acquisition function:

e.g. used in entropy search (ES), predictive entropy search (PES)

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Expected information gain (EIG) — expected decrease in entropy if we were to query f at x.

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- **Thompson sampling** — a stochastic acquisition function (*i.e.*, draw one posterior, and use it within an acquisition function)
- **Non-BO acq fns.** — acquisition functions for non-optimization tasks, such as level sets, quadrature, phase boundaries, and more-general tasks.

Next Time

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Finish up our discussion of active learning methods!