Probabilistic methods for Machine Learning

September
27 2022

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Topics For Today

- **Probability recap**
- Naïve Bayes
- Gaussian process
- Bayesian hyperparameter optimization

Probability: definitions

Sample Space Ω:
The set of all outcomes of a random experiment
Event space $\mathcal{F}$ **:**
A set whose elements $A \in \mathcal{F}$ (called events) are subsets of Ω (i.e., $A \subseteq \Omega$ is a collection of possible outcomes of an experiment)
Probability measure:
A function $P : \mathcal{F} \to \mathbb{R}$ that satisfies the following properties:

- $P(A) \geq 0$, for all $A \in \mathcal{F}$
- $P(\Omega)=1$
- If $A_1, A_2, \ldots$ are disjoint events (i.e., $A_i \cap A_j = \emptyset$ for $i \neq j$), then $P(\cup_i A_i) = \sum_i P(A_i)$

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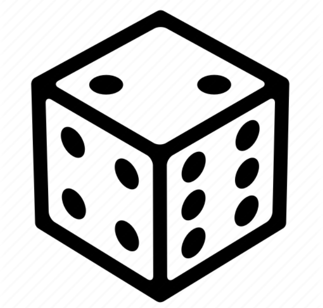


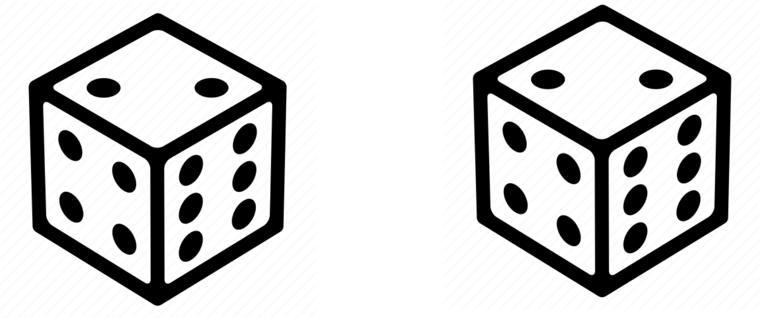
Example: Tossing a six-sided die
$\Omega = \{1, 2, 3, 4, 5, 6\}$
$\mathcal{F} = \{\emptyset, \Omega\} = \{\emptyset, 1, 2, 3, 4, 5, 6\}$
$P(\emptyset) = 0$, $P(\Omega) = 1$
$P(\{1\}) = \frac{1}{6}$
$P(\{1,2,3,4\}) = \frac{4}{6}$
$P(\{2,4,6\}) = \frac{3}{6}$

Probability: Conditional probability and independence

The conditional probability of any event A given B is

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

Example: tossing two 6-sided die.
A = {We got same digits on first and second die}
B = {Sum of digits on first and second die more than 8}



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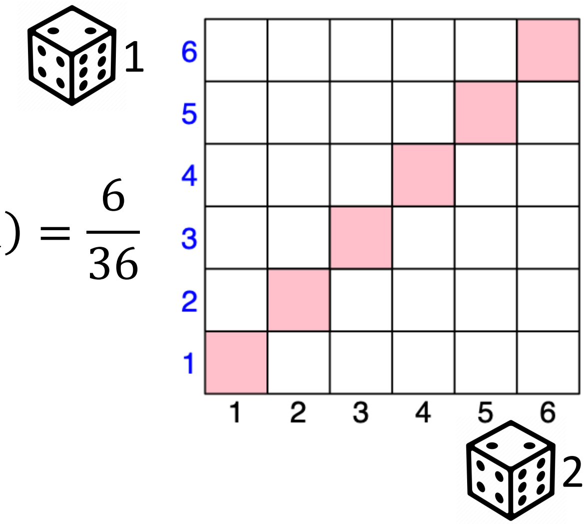
$$P(A) = \frac{6}{36}$$



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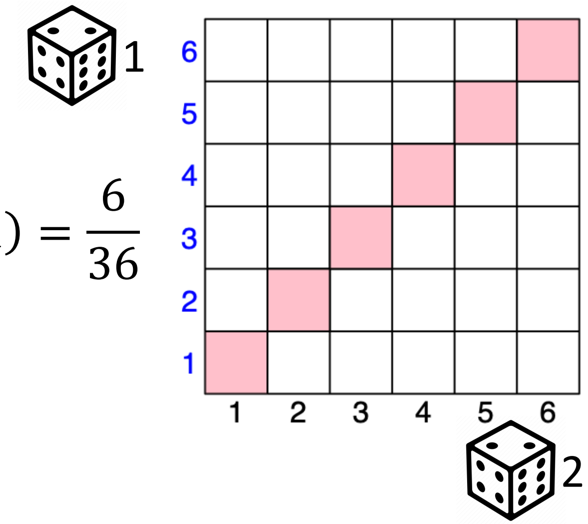
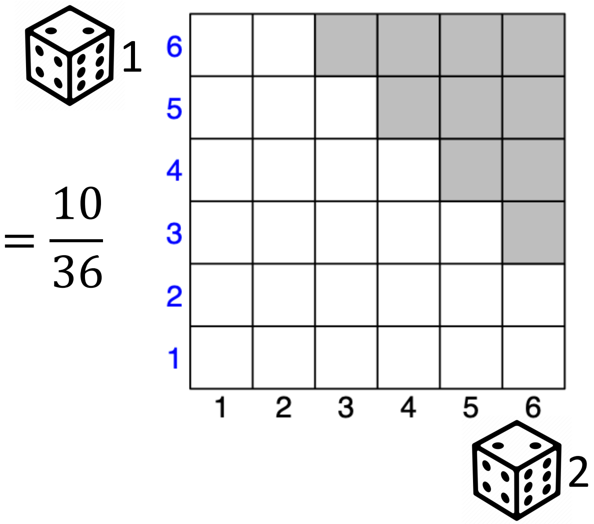


$$P(B) = \frac{10}{36}$$



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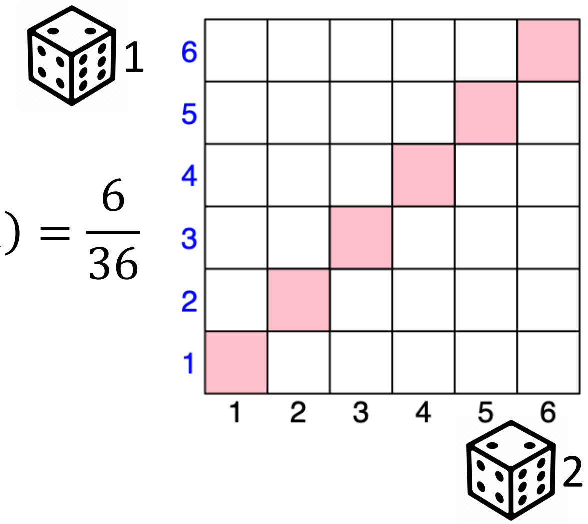

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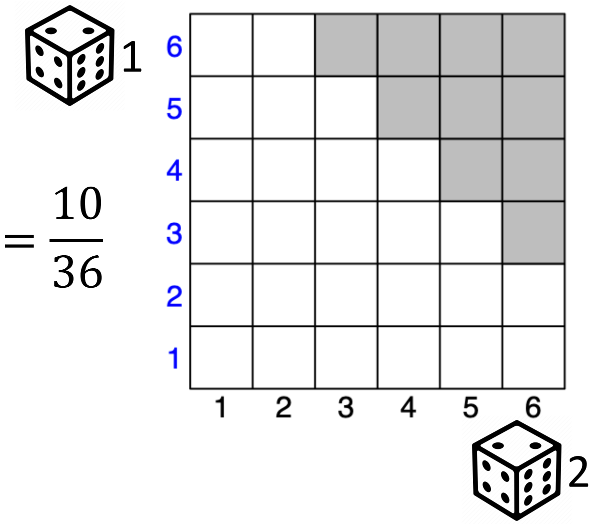
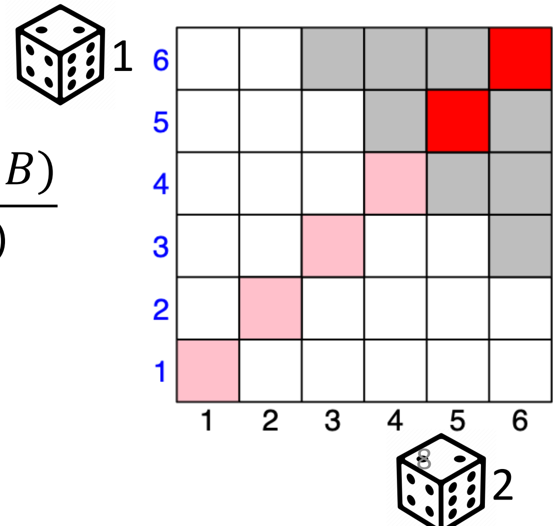


$$P(A|B) = \frac{P(A \ \cap B)}{P(B)}$$

$$= \frac{2/36}{10/36} = \frac{1}{5}$$



Probability: Conditional probability and independence

The conditional probability of any event A given B is

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

In other words, P (A|B) is the probability measure of the event A after observing the occurrence of event B.

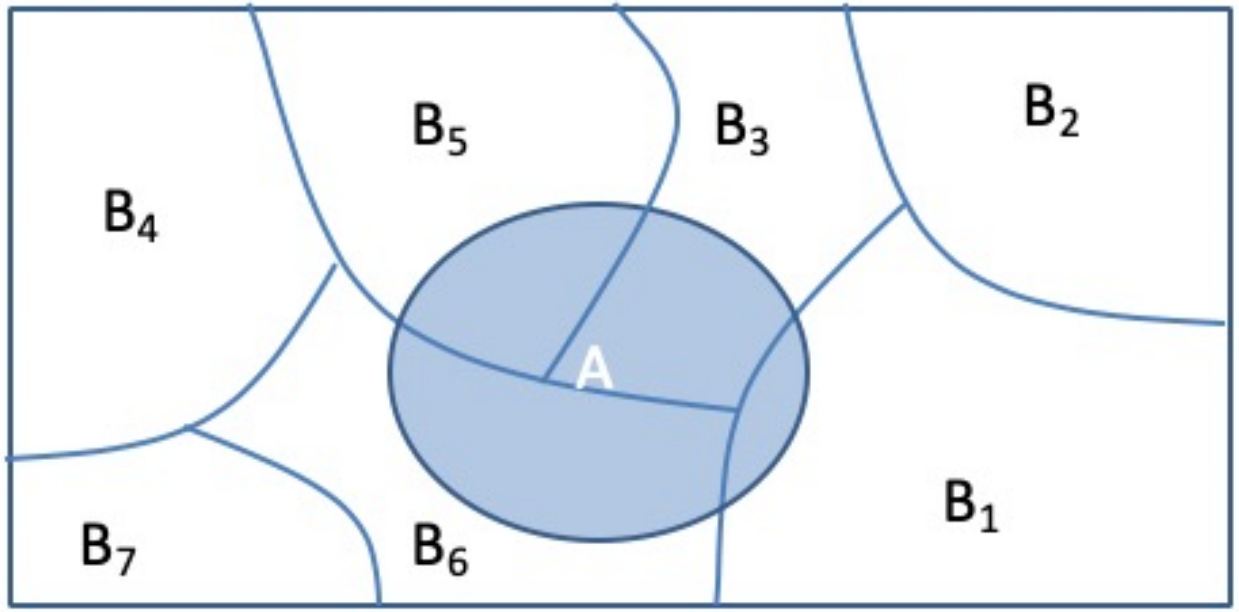
Two events are called **independent** if and only if

$$P(A \ \cap B) = P(A)\text{x}P(B)$$

Independence is equivalent to saying that **observing B does not have any effect on the probability of A**.

Probability: Law of total probability

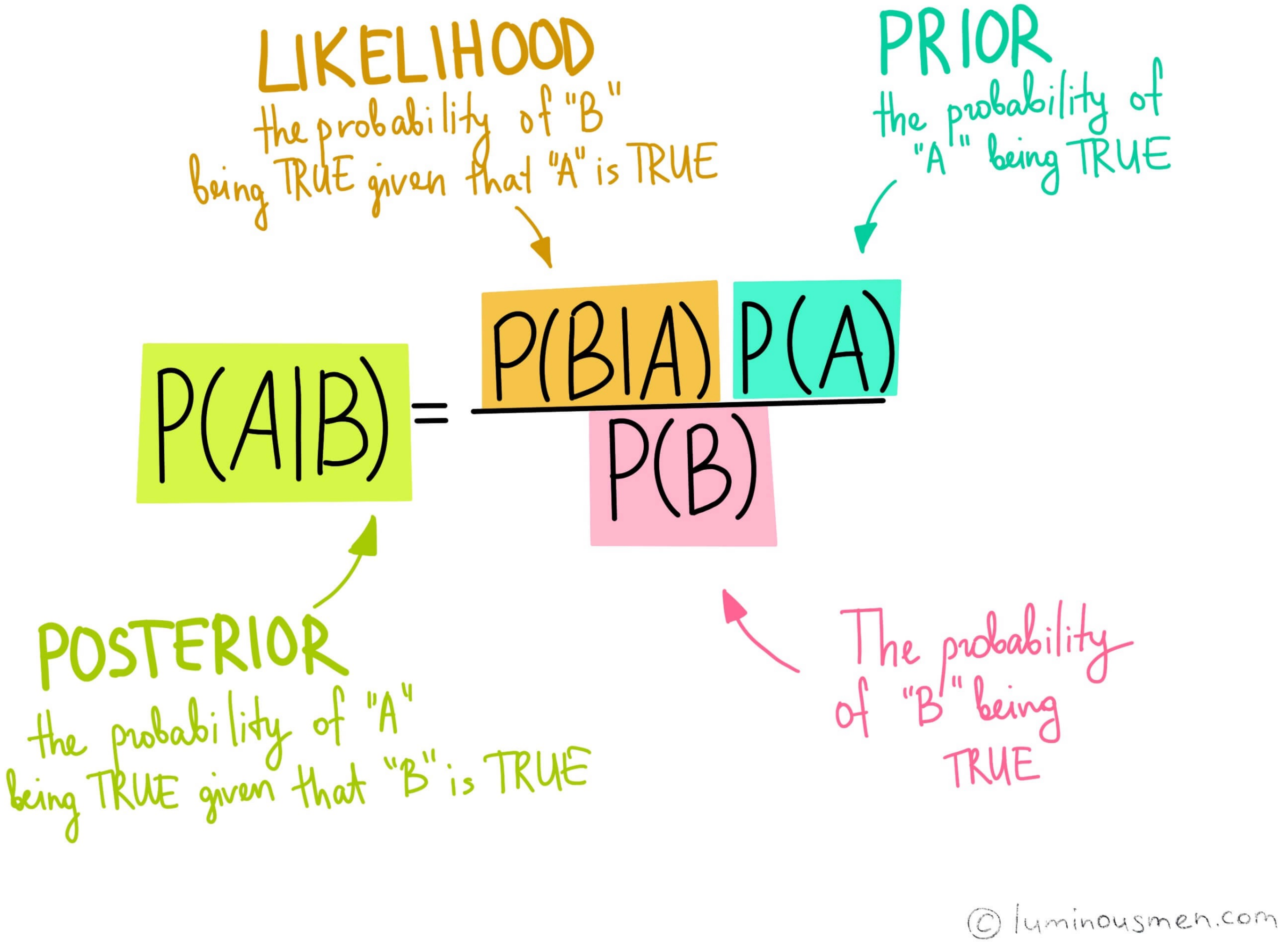
$$P(A) = \sum_{i=1}^{n} P(A \cap B_i) = \sum_{i=1}^{n} P(A|B_i)P(B_i)$$



Probability: Bayes' theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

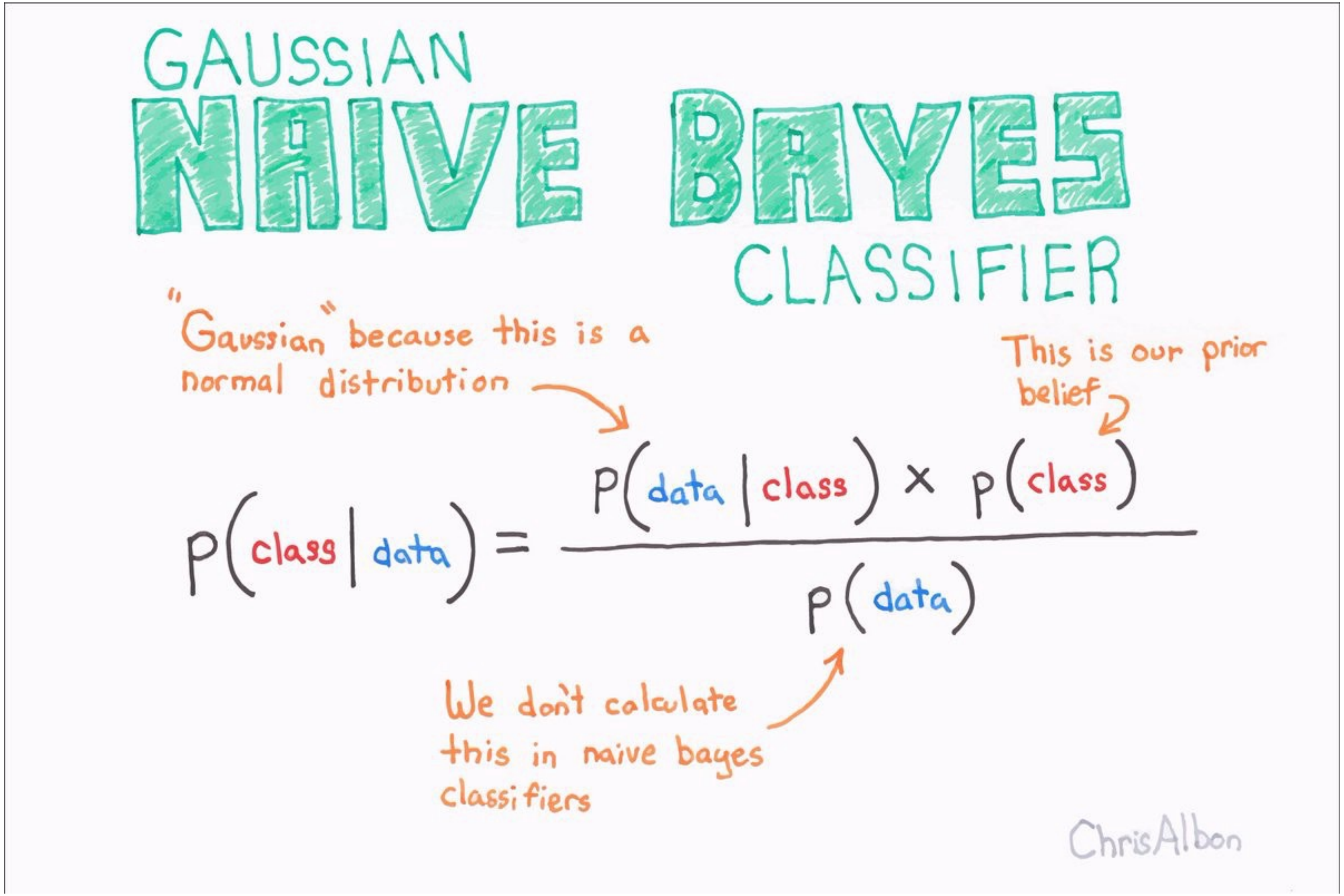
Probability: Bayes' theorem



Topics

- Probability recap
- **Naïve Bayes**
- Gaussian process
- Bayesian hyperparameter optimization

Naïve Bayes: introduction

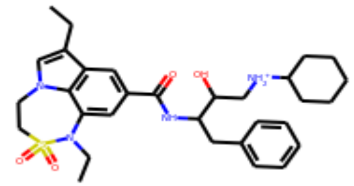
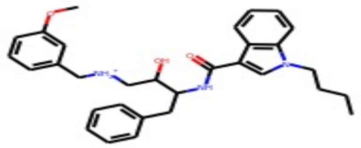


Naïve Bayes: introduction

Problem statement:

- Given features $X_1, X_2, \ldots, X_n$
- Given assumption about feature distribution
- Predict a label Y
- And give level of [un]certainty in prediction

Naïve Bayes: classification example [2 classes]

ROMol	MW	AMW	Sv	Se	Sp	H%	C%	N%		Class
	565.75	6.98	49.03	81.24	51.69	49.38	39.51	3.70	…	1
…										
	521.75	6.60	46.69	78.56	49.93	51.90	37.97	5.06	…	0

$\underbrace{\hspace{5em}}_{X_1,\ldots,X_n \in \mathbb{R} \text{ (features)}}$

$\underbrace{\hspace{2em}}_{Y \in \{1,0\}}$ **(predict whether molecule active or inactive)**

Naïve Bayes: Why "Bayes"?

Use Bayes Rule:

$$P(Y|X_1,\ldots,X_n) = \frac{\overbrace{P(X_1,\ldots,X_n|Y)}^{\text{Likelihood}}\overbrace{P(Y)}^{\text{Prior}}}{\underbrace{P(X_1,\ldots,X_n)}_{\text{Normalization Constant}}}$$

- Why did this help?
  Well, we think that we might be able to specify how features are "generated" by the class label

Naïve Bayes: Why "Bayes"? [cont.]

For our example

$$P(Y=0|X_1,\ldots,X_n) = \frac{P(X_1,\ldots,X_n|Y=0)P(Y=0)}{P(X_1,\ldots,X_n)} = \frac{P(X_1,\ldots,X_n|Y=0)P(Y=0)}{P(X_1,\ldots,X_n|Y=1)P(Y=1)+P(X_1,\ldots,X_n|Y=0)P(Y=0)}$$

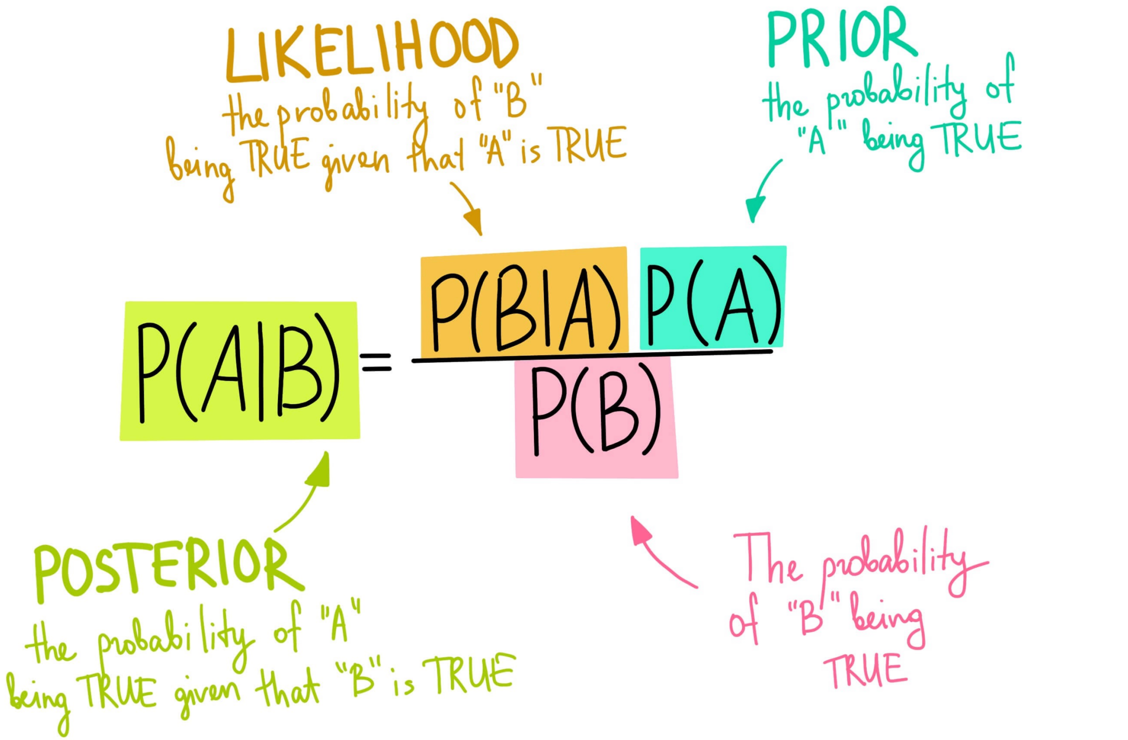
$$P(Y=1|X_1,\ldots,X_n) = \frac{P(X_1,\ldots,X_n|Y=1)P(Y=1)}{P(X_1,\ldots,X_n)} = \frac{P(X_1,\ldots,X_n|Y=1)P(Y=1)}{P(X_1,\ldots,X_n|Y=1)P(Y=1)+P(X_1,\ldots,X_n|Y=0)P(Y=0)}$$

To classify, we'll simply compute these two probabilities and predict based on which one is greater

Naïve Bayes: Why “Naïve”?

For the Bayes classifier, we need to “learn” two functions, the **likelihood** and the **prior**

But:



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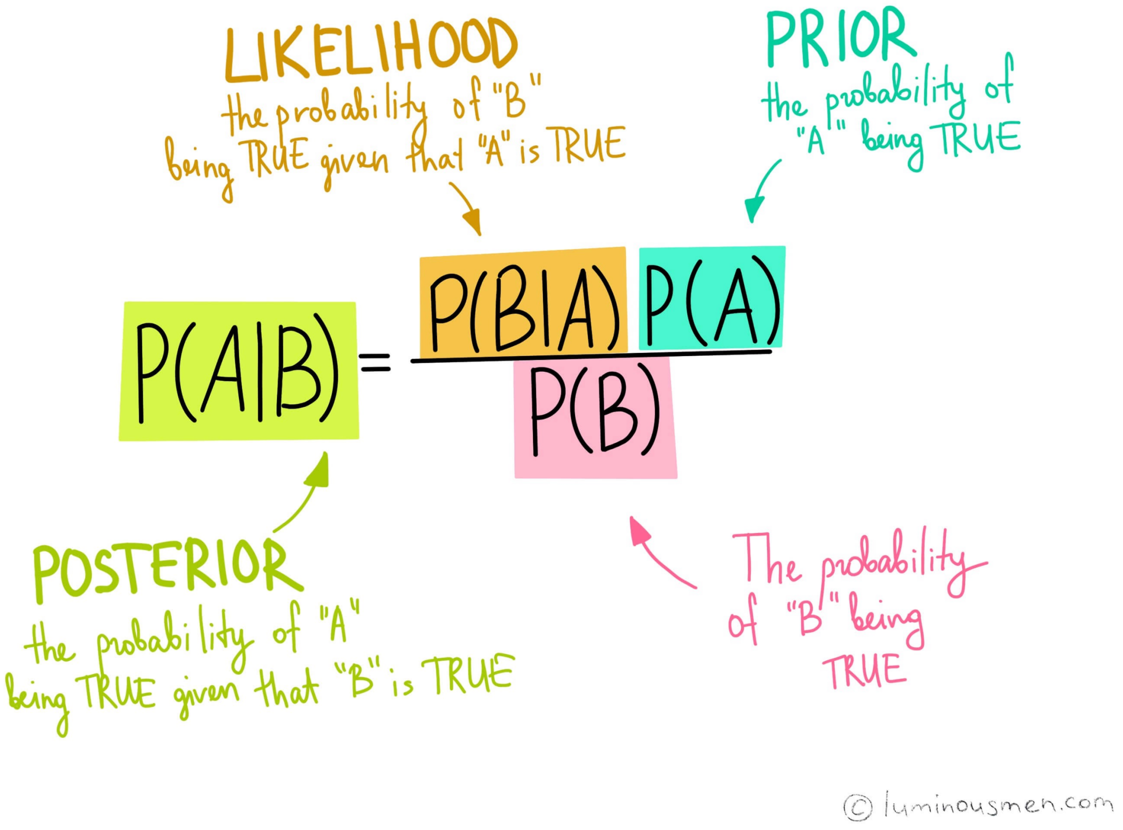

Naïve Bayes: Why "Naïve"? [cont.]

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Likelihood

Prior

$$P(Y|X_1,\ldots,X_n) = \frac{P(X_1,\ldots,X_n|Y)P(Y)}{P(X_1,\ldots,X_n)}$$

Normalization Constant

But: How many parameters are required to specify the prior for our example?

# of parameters for modeling $P(X_1,\ldots,X_n|Y)$: $\mathbf{2(2^n-1)}$

Naïve Bayes: Why "Naïve"? [cont. 2]

The *Naïve Bayes Assumption*:

Assume that all features are *conditionally independent* **given the class label Y**

$$P(X_1, \ldots, X_n | Y) = \prod_{i=1}^{n} P(X_i | Y)$$

Likelihood

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Naïve Bayes: Why "Naïve"? [And why **2n**]

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Gaussian naive Bayes

assumption: features distributed normally :

$$p(x = v \mid C_k) = \frac{1}{\sqrt{2\pi\sigma_k^2}}\, e^{-\frac{(v-\mu_k)^2}{2\sigma_k^2}}$$

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Naïve Bayes: Training

Training in Naïve Bayes is **easy :**

we have to select **feature distribution** (aka likelihood function)
[usually Gaussian distribution]

and **estimate parameters** of model of feature distribution

This corresponds to Maximum Likelihood estimation of model parameters.

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Is there other than Gaussian Naïve Bayes?

Sure, as a likelihood function, we could select different distributions.

In Scikit-learn there is implementation for Gaussian, Multinomial, Bernoulli etc.

Topics

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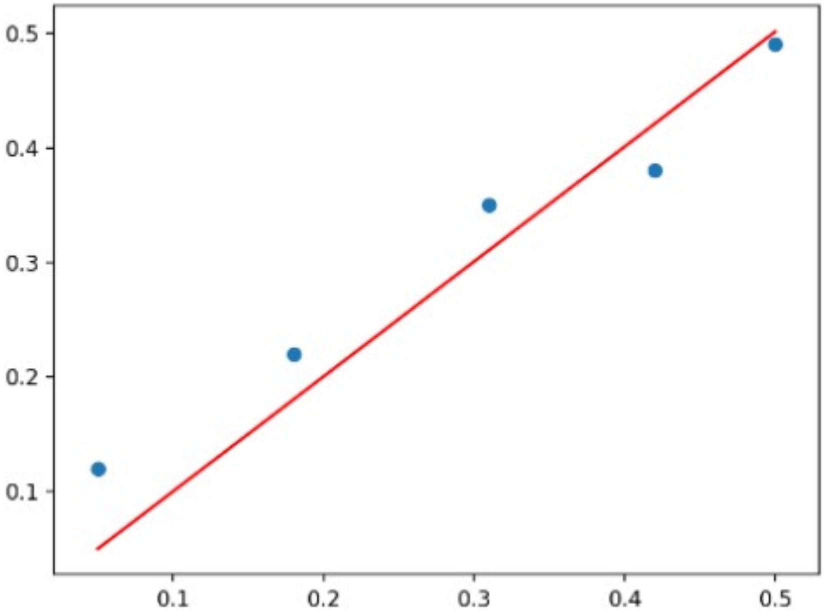
- Naïve Bayes
- **Gaussian process**
- Bayesian hyperparameter optimization

Gaussian Process: ML perspective



Gaussian Process: Definition

Continuous stochastic process — random functions — a set of random variables indexed by a continuous variable: $f(x)$

Set of 'inputs' $\mathbf{X} = \{x_1, x_2, \ldots, x_N\}$; corresponding set of random function variables $\mathbf{f} = \{f_1, f_2, \ldots, f_N\}$

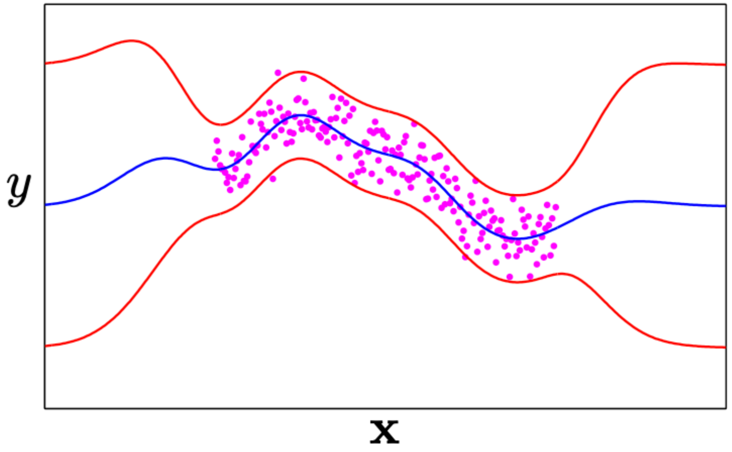
GP: Any set of function variables $\{f_n\}_{n=1}^{N}$ has joint (zero mean) Gaussian distribution:

$$p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{0}, \mathbf{K})$$

Gaussian Process: ML perspective

Consider the problem of nonlinear regression:

You want to learn a function f with error bars from data $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$



A Gaussian process is a prior over functions $p(f)$ which can be used for Bayesian regression:

$$p(f|\mathcal{D}) = \frac{p(f)p(\mathcal{D}|f)}{p(\mathcal{D})}$$

Gaussian Process: vs Gaussian distributions

Gaussian distributions
$\mathcal{N}(\mu, \Sigma)$

Distribution over vectors.
Fully specified by a mean and covariance.
The position of the random variable in the vector plays the role of the index.

Gaussian processes
$\mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$

Distribution over functions.
Fully specified by a mean function and covariance function.
The argument of the random function plays the role of the index.

Gaussian Process: covariance matrix

Gaussian processes are merely based on the good old Gaussian

$$\mathcal{N}\left(\mathbf{x} \middle| \boldsymbol{\mu}, \mathbf{K}\right) = \frac{1}{\sqrt{|2\pi \mathbf{K}|}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \mathbf{K}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right]$$

Covariance matrix or kernel matrix

Covariance matrix constructed from *covariance function*:

$$\mathbf{K}_{ij} = K(x_i, x_j)$$

Covariance function characterizes correlations between different points in the process:

$$K(x, x') = \mathcal{E}[f(x)f(x')]$$

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Gaussian Process: kernel examples

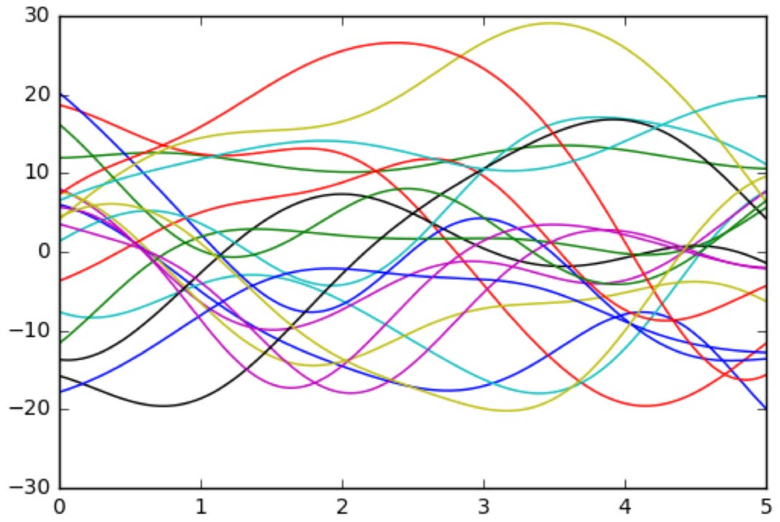
Kernels -- are a crucial ingredient of GPs which determine the shape of prior and posterior of the GP.
They **encode the assumptions** on the function being learned by defining the "similarity" of two datapoints combined with the assumption that similar datapoints should have similar target values.

Squared exponential (SE), RBF

$$K(x, x') = \sigma_0{}^2 \exp\left[-\frac{1}{2}\left(\frac{x - x'}{\lambda}\right)^2\right]$$

Intuition: function variables close in input space are highly correlated, whilst those far away are uncorrelated

λ, σ_0 — hyperparameters. λ: lengthscale, σ_0: amplitude



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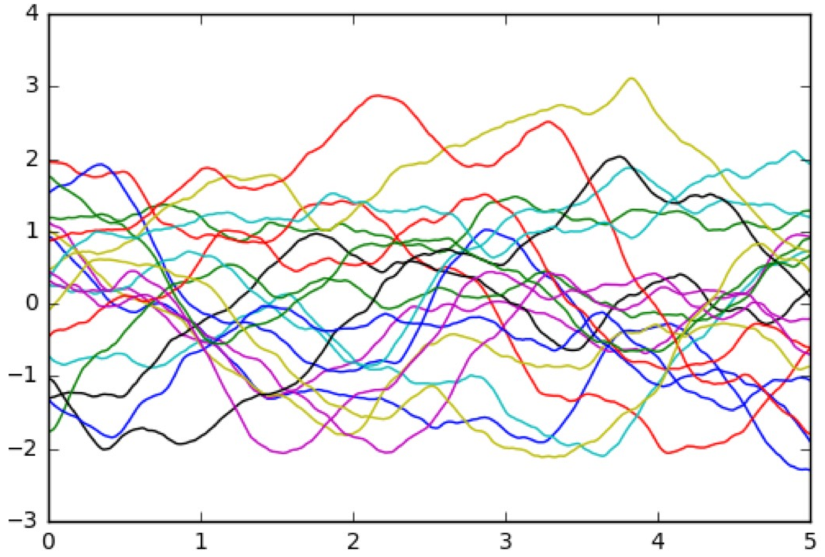
Mat́ern class [usually ν = 1/2 or 3/2]

$$K(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}|x - x'|}{\lambda} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}|x - x'|}{\lambda} \right)$$

where K_ν is a modified Bessel function.



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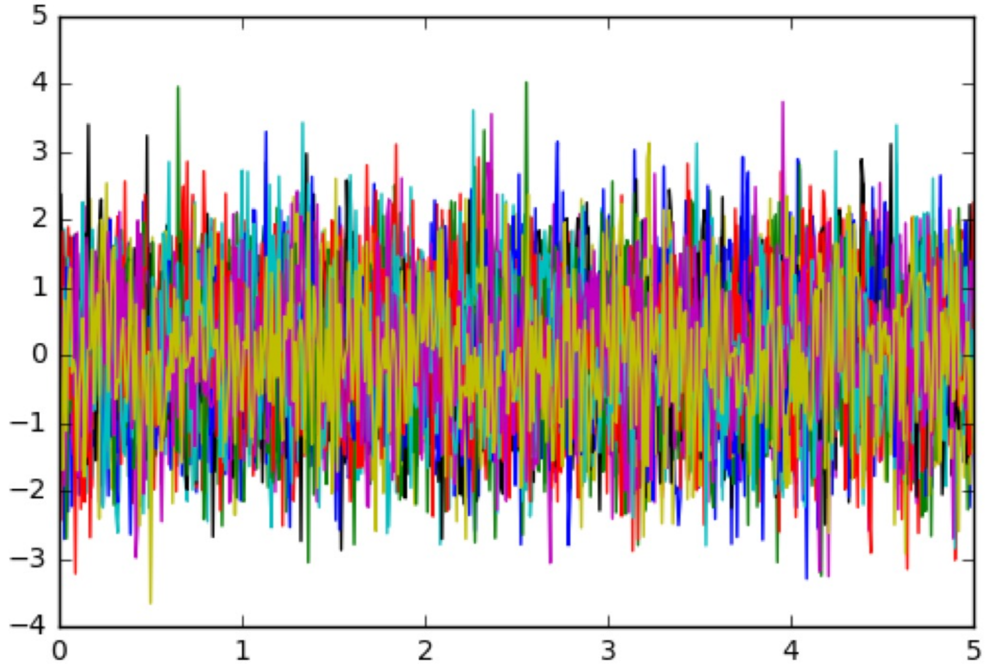
White noise

$$k(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$



Gaussian Process: most standard kernel

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We can make new kernels by summing or multiplying kernels

Most default kernel K=RBF+White_noise

Gaussian Process Regression: training

$\mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x'}))$

I) Select mean function *m*(x) [usually constant]
II) Select kernel function *k*(x,x’) [usually RBF + White_nise]

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III) Find parameters [fit GP to data]

Gaussian Process: as a regression [in 2 words]

Covariance function defines the properties in the function space.

Data points "anchor" the function as specific locations.

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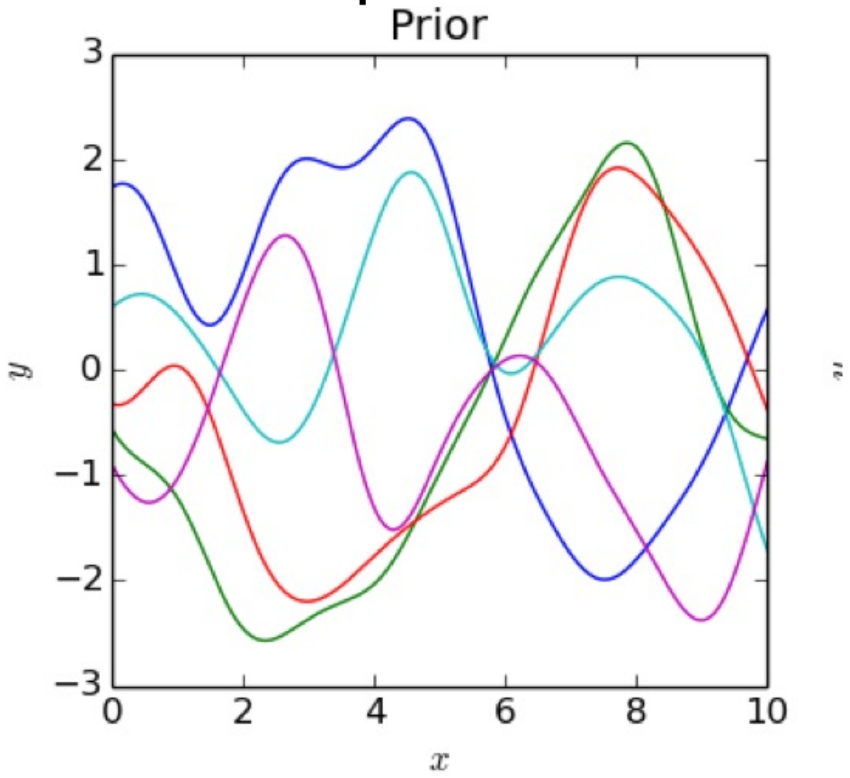

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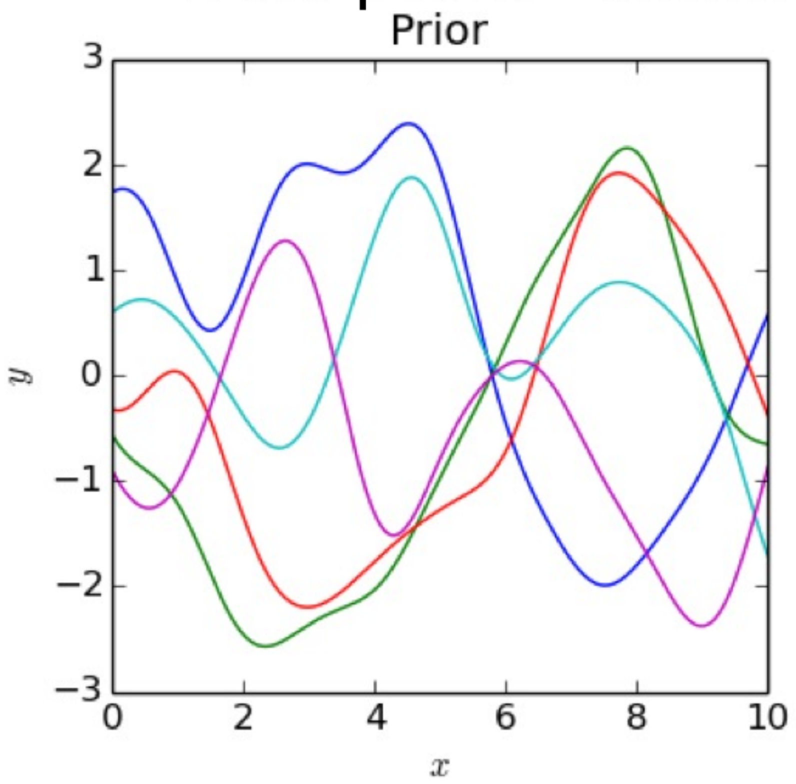

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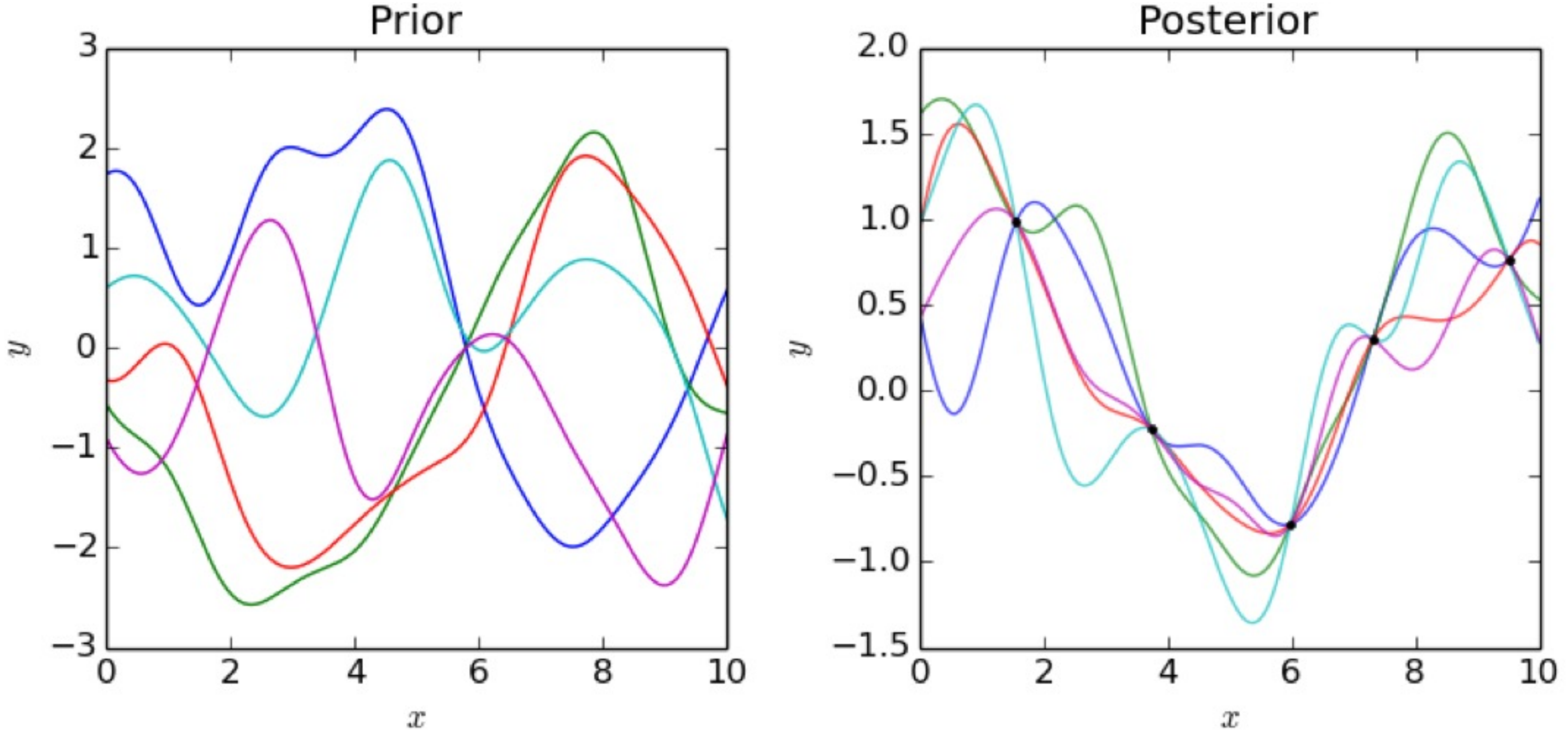

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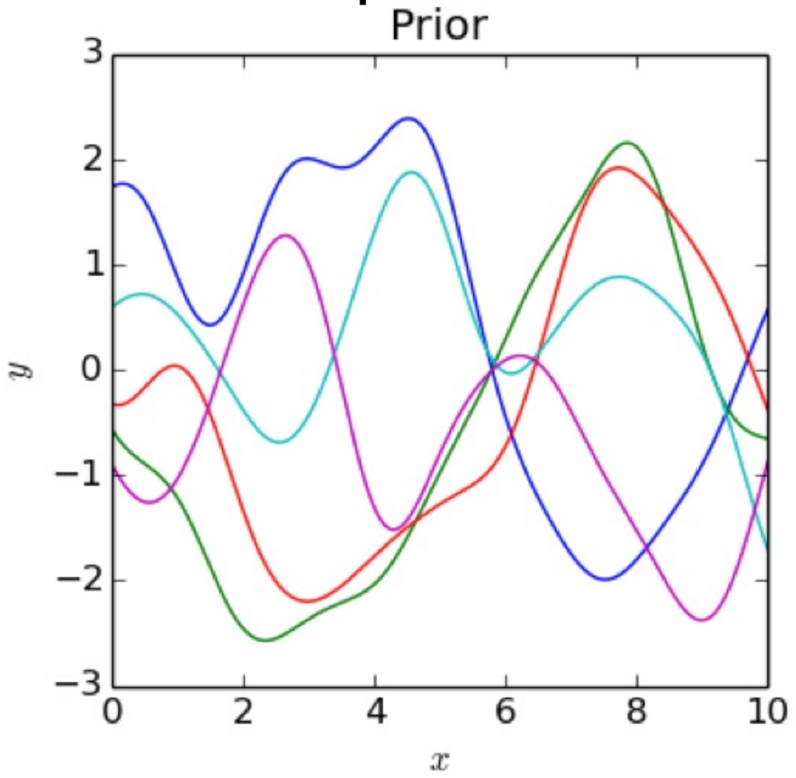

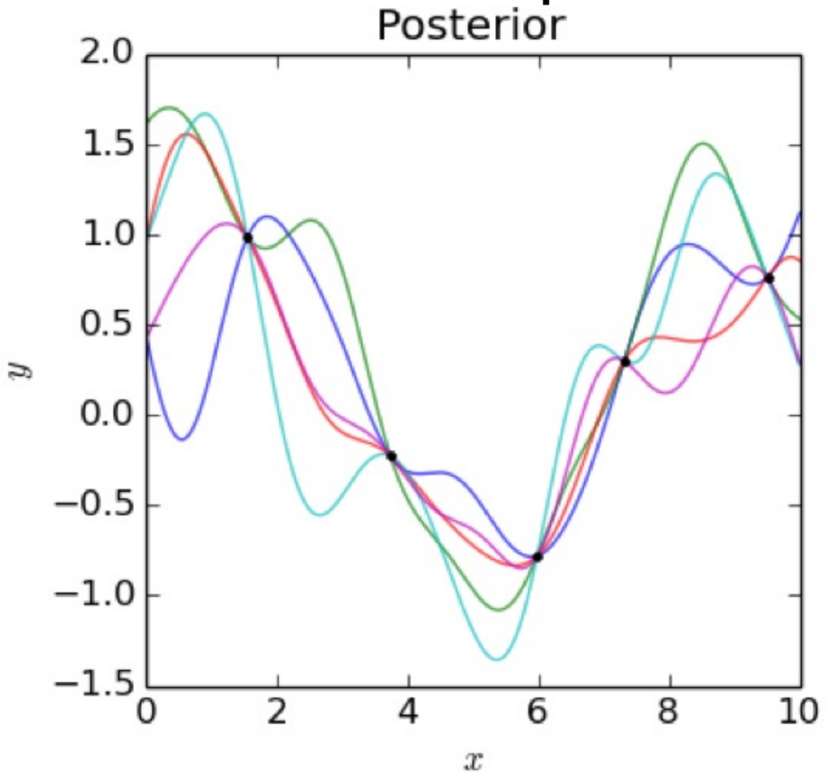

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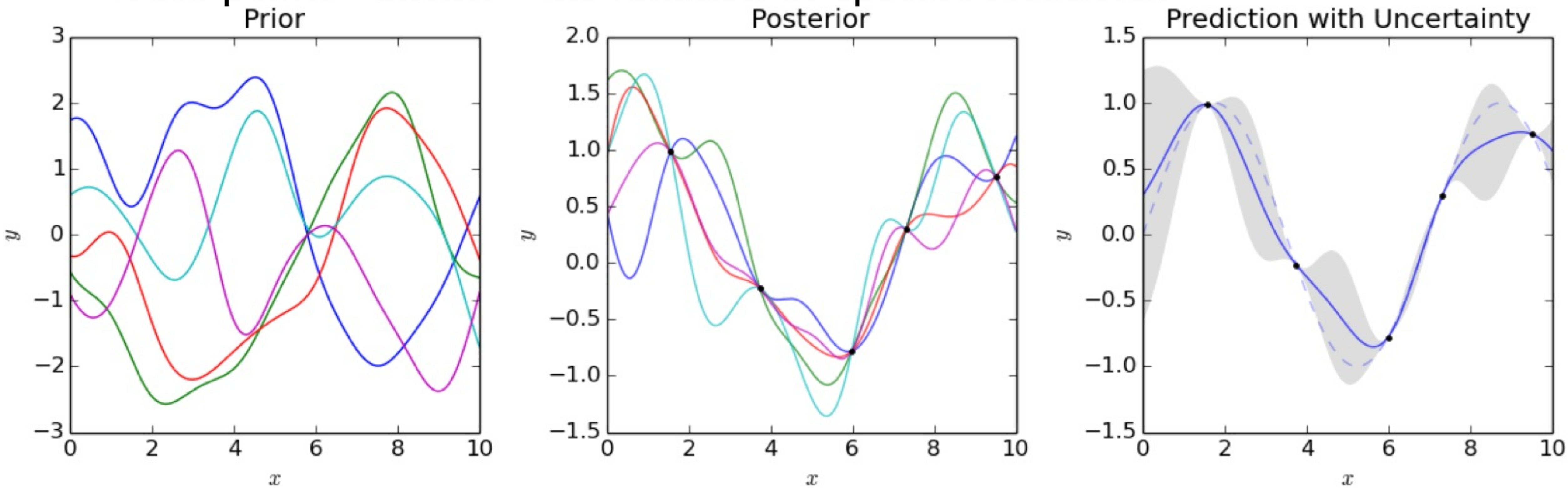

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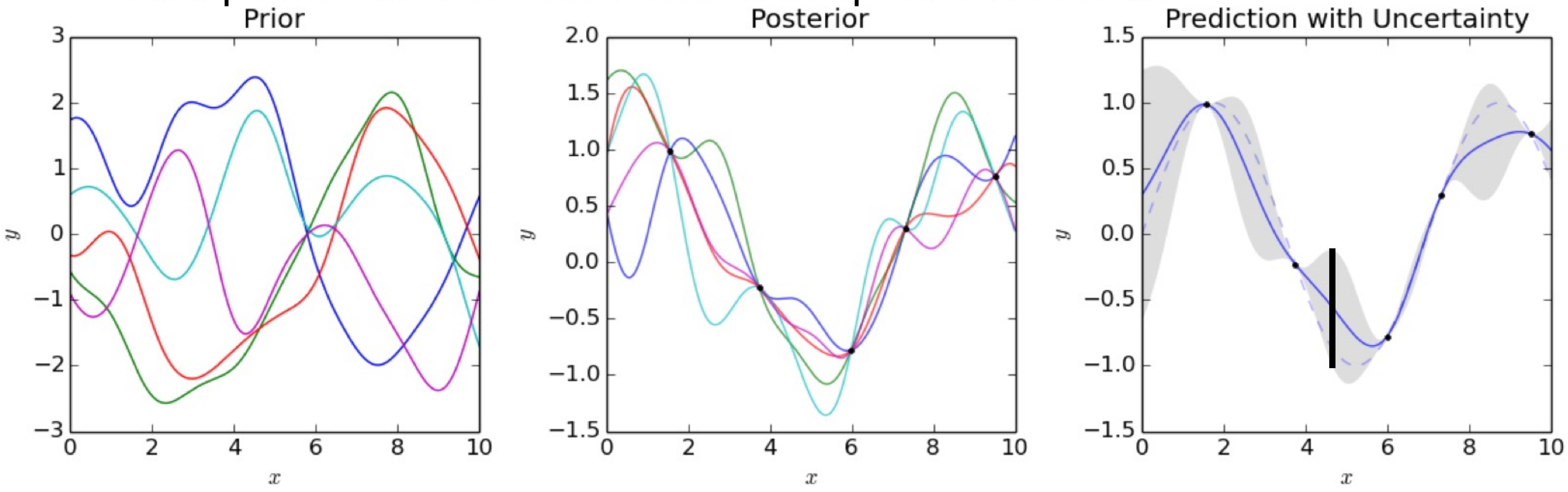
Data points "anchor" the function as specific locations.



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II) and than **sampling this functions from GP** and calculate values of those **sampled functions for particular input**

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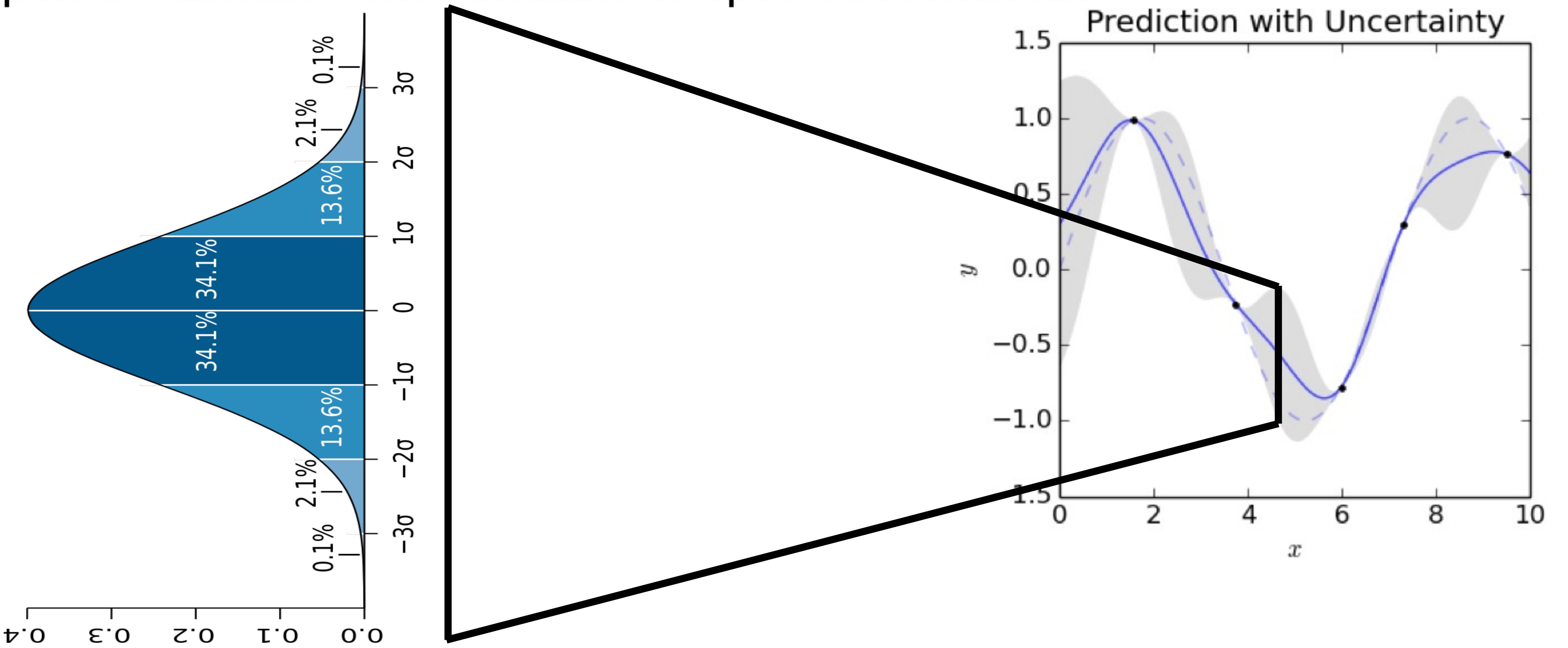

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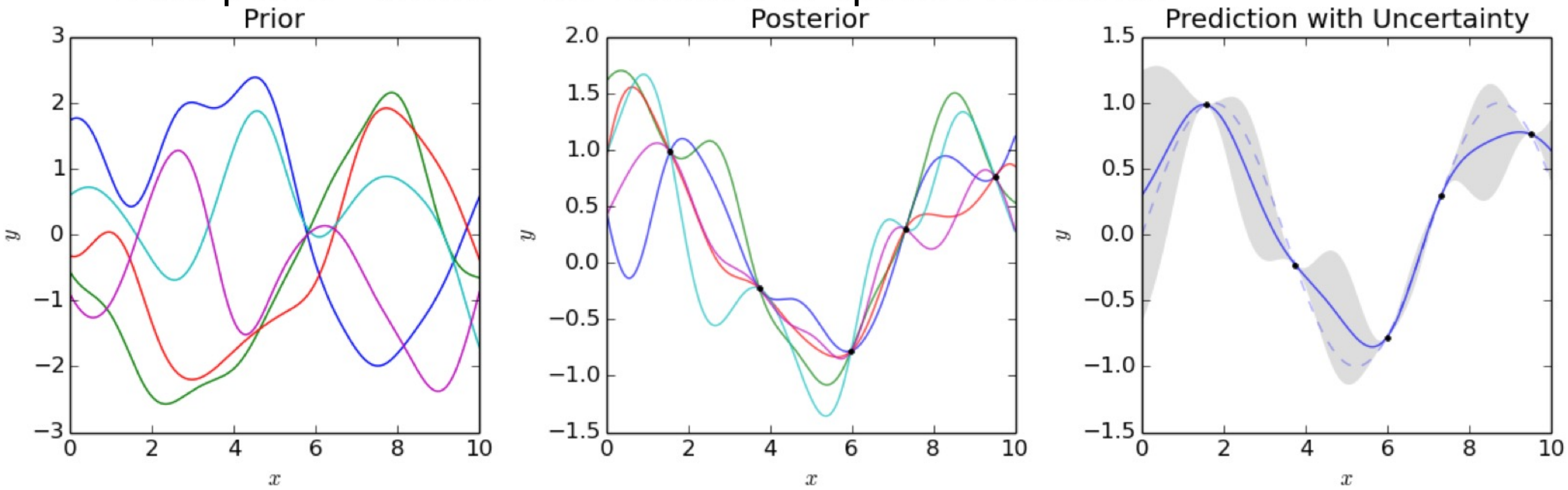

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Topics

- Probability recap
- Naïve Bayes
- Gaussian process
- **Bayesian hyperparameter optimization**

Bayesian hyperparameter optimization

If you have an **experiment** with **set of hyperparameters** and some **objective function,** then you can optimize those hyperparameters with GP.

An experiment could be:

- Actual wet-lab experiment
- Machine learning model with big set of hyperparameters, like neural network or xgboost

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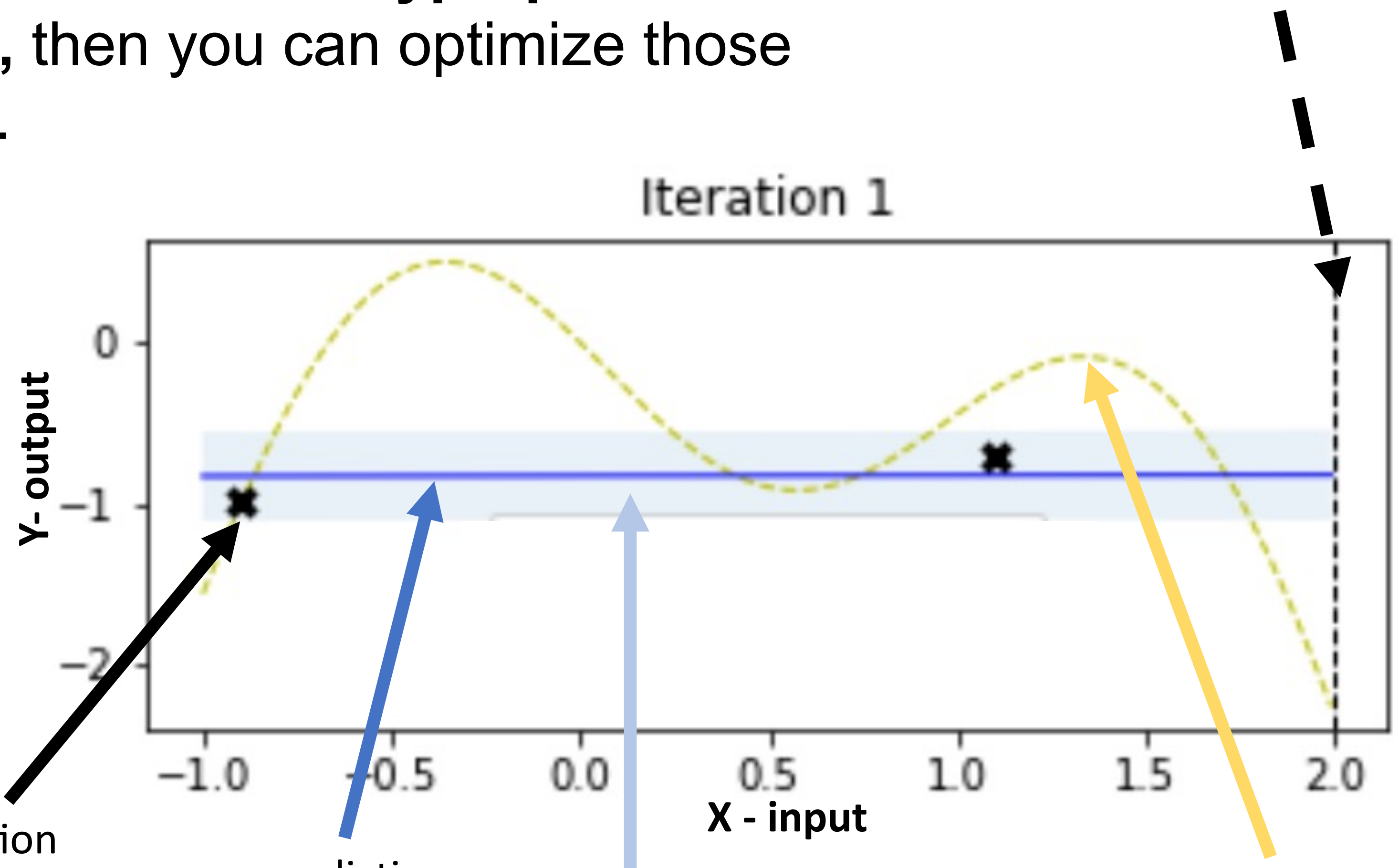

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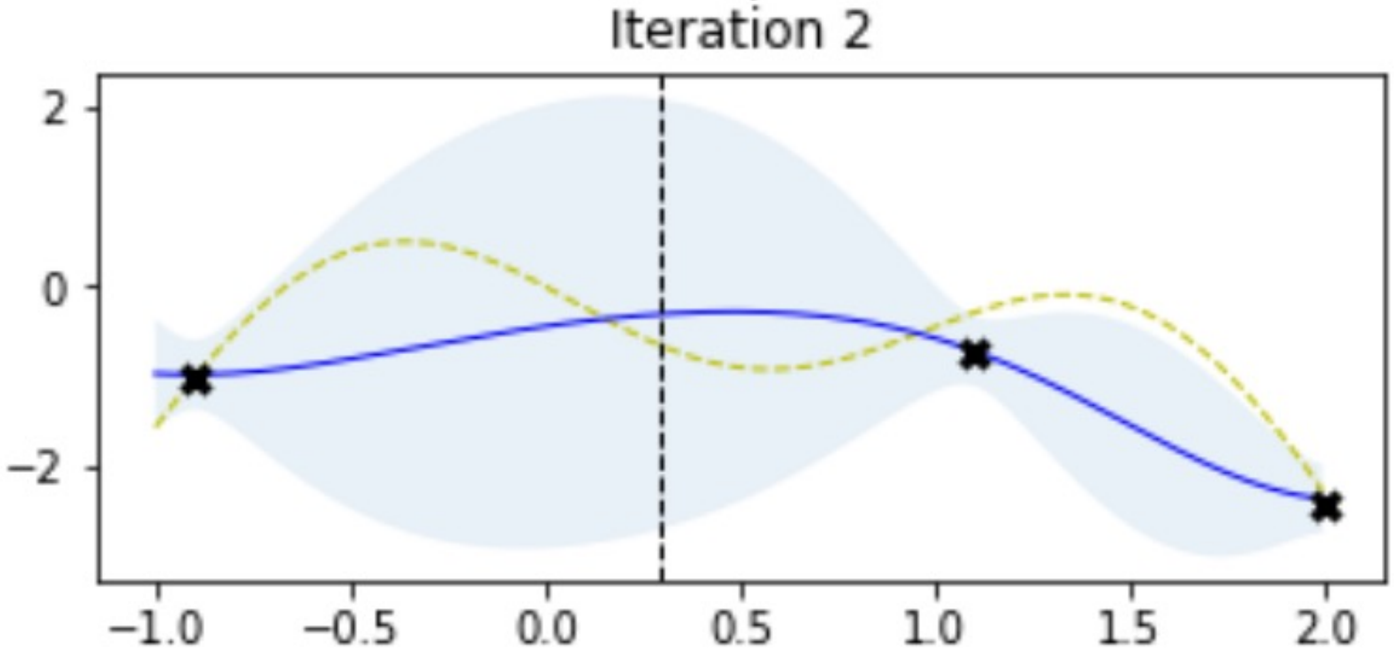

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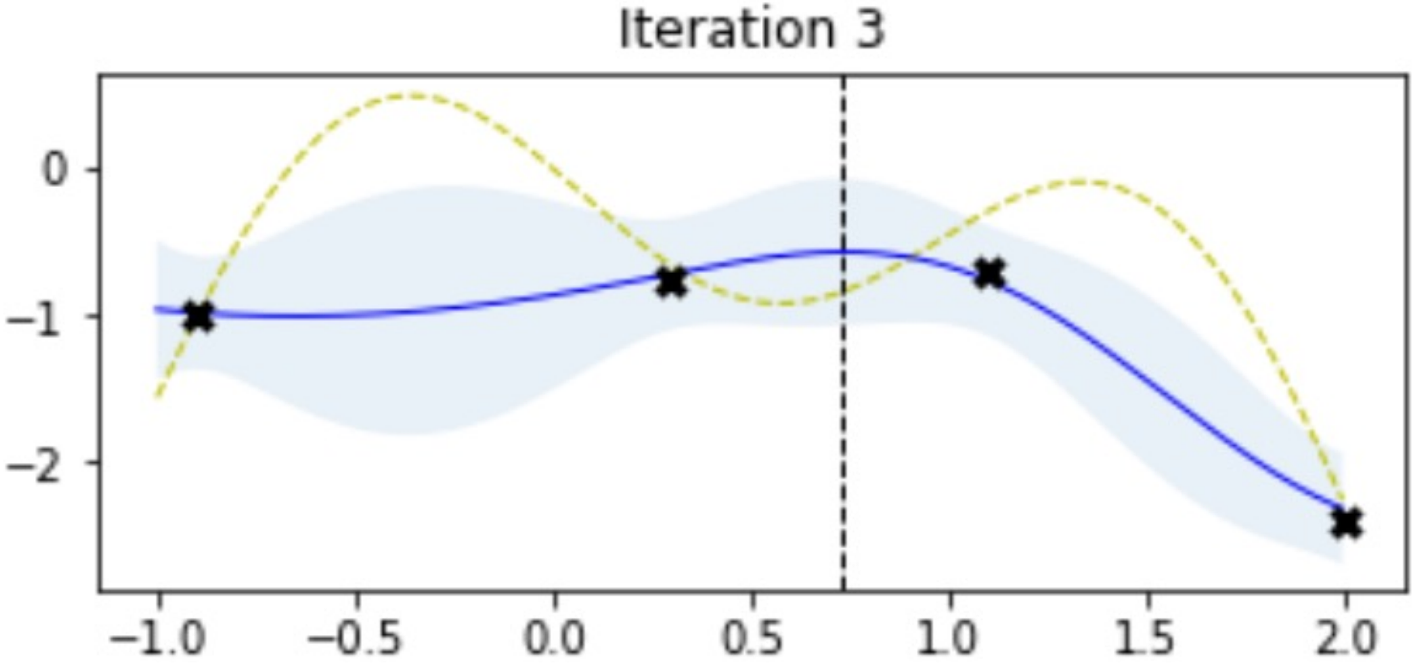

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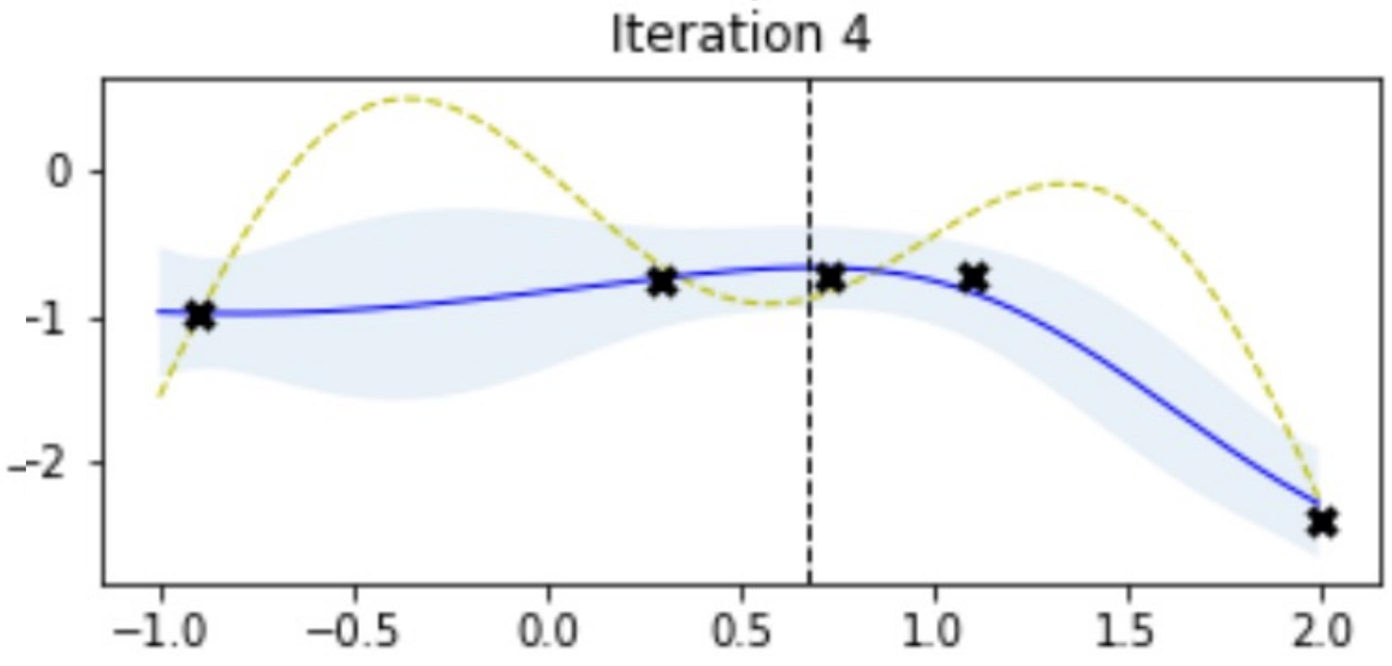

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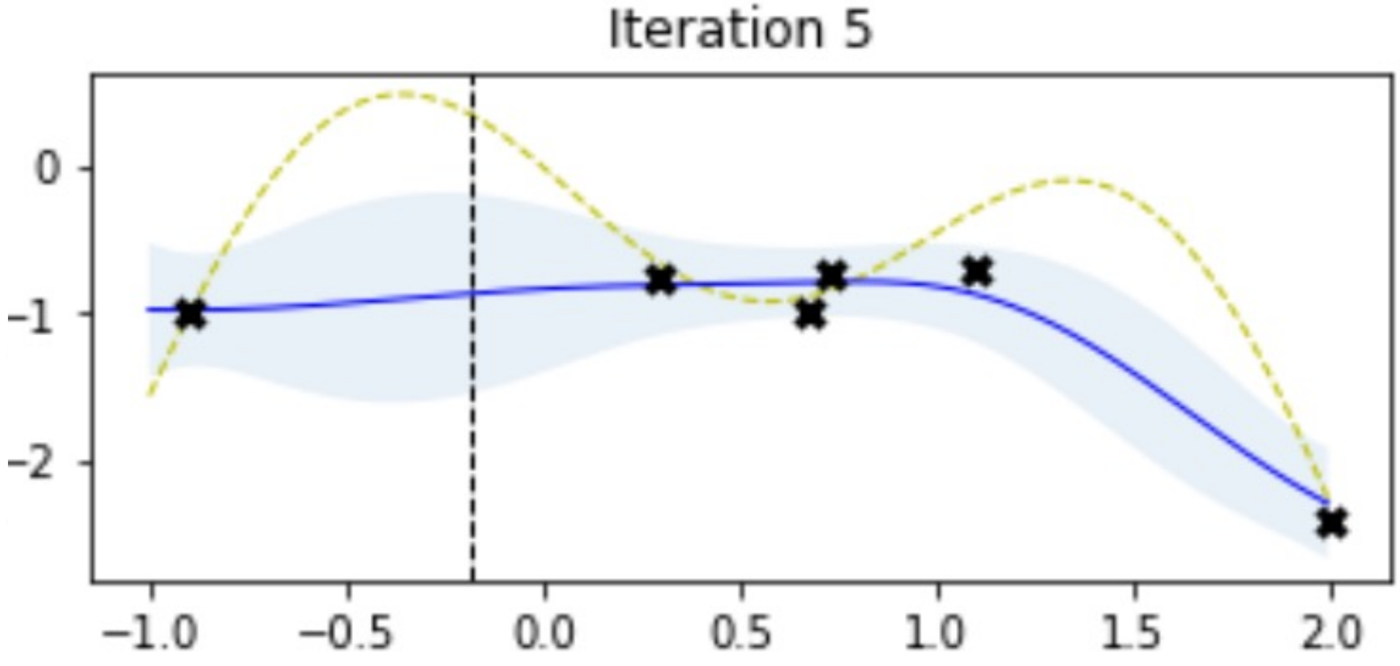

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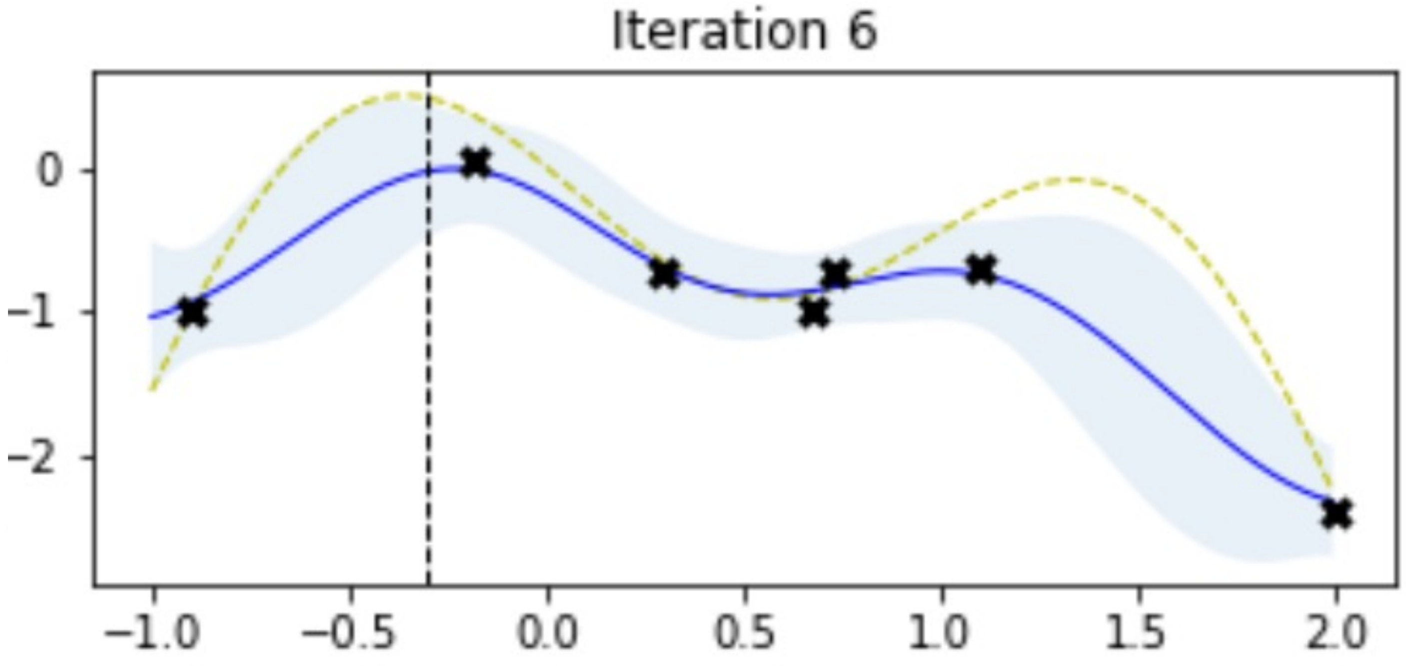

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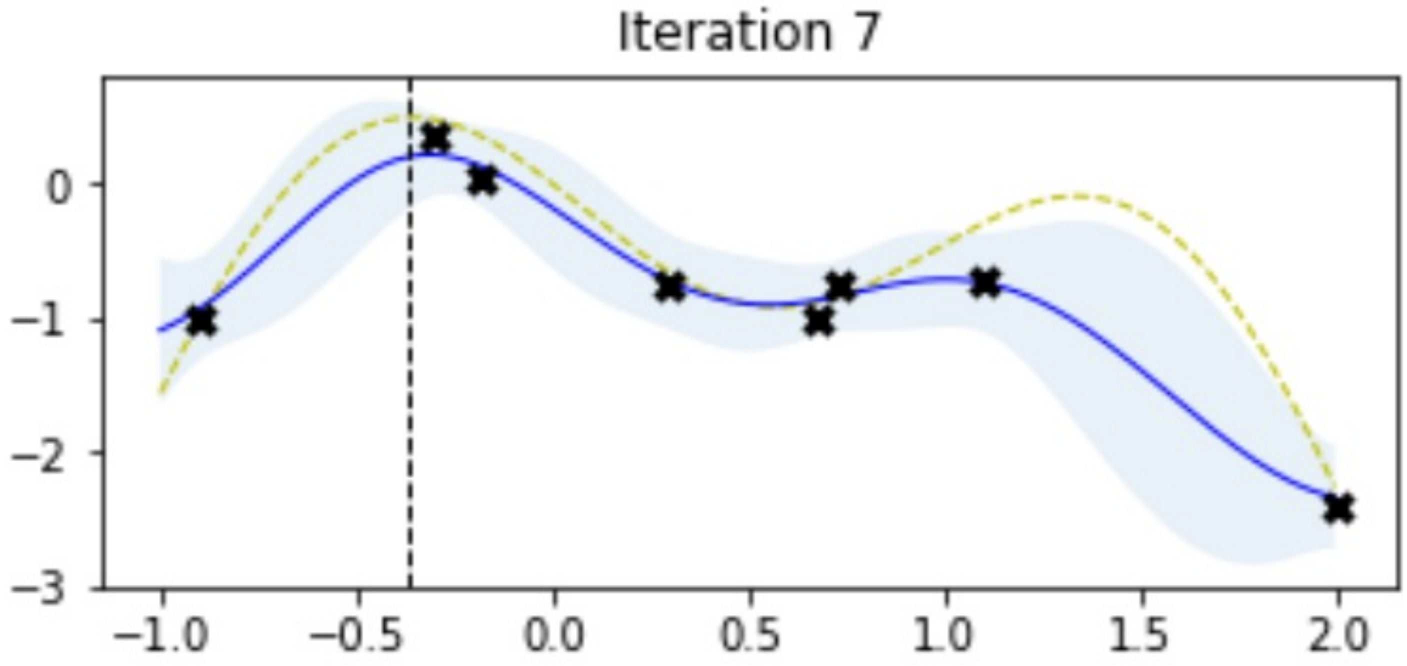

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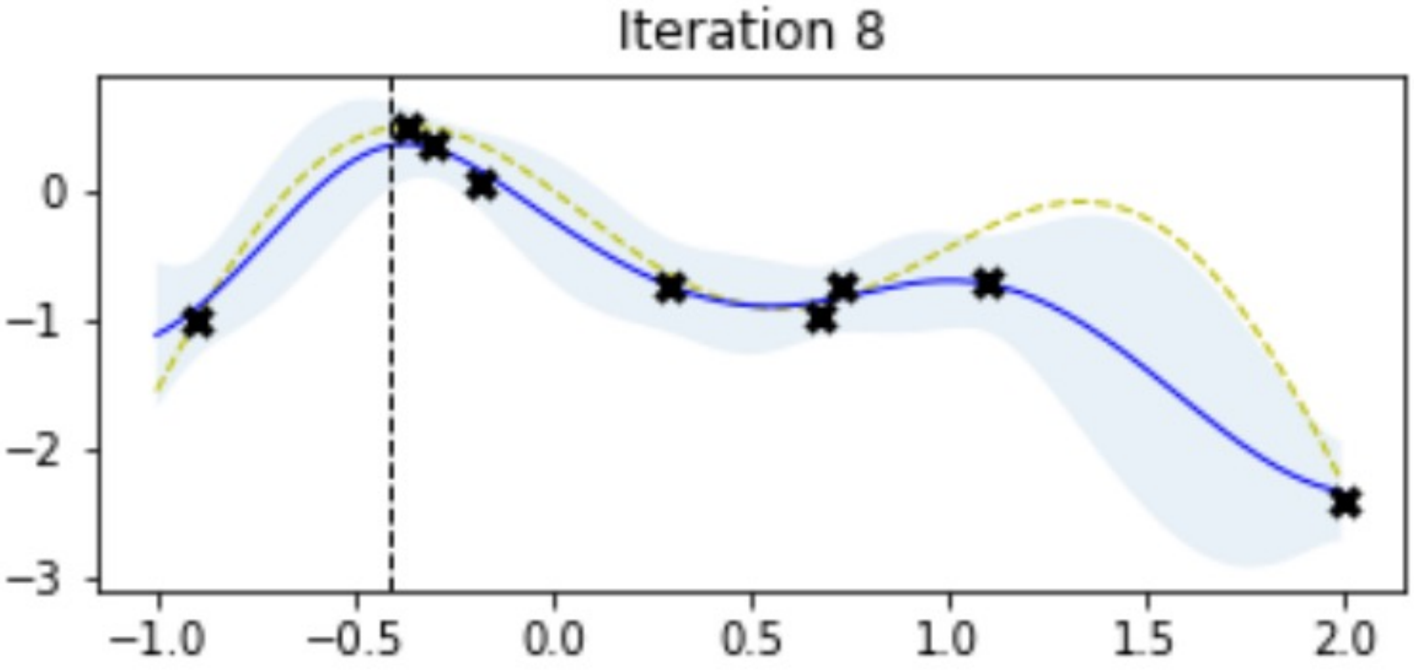

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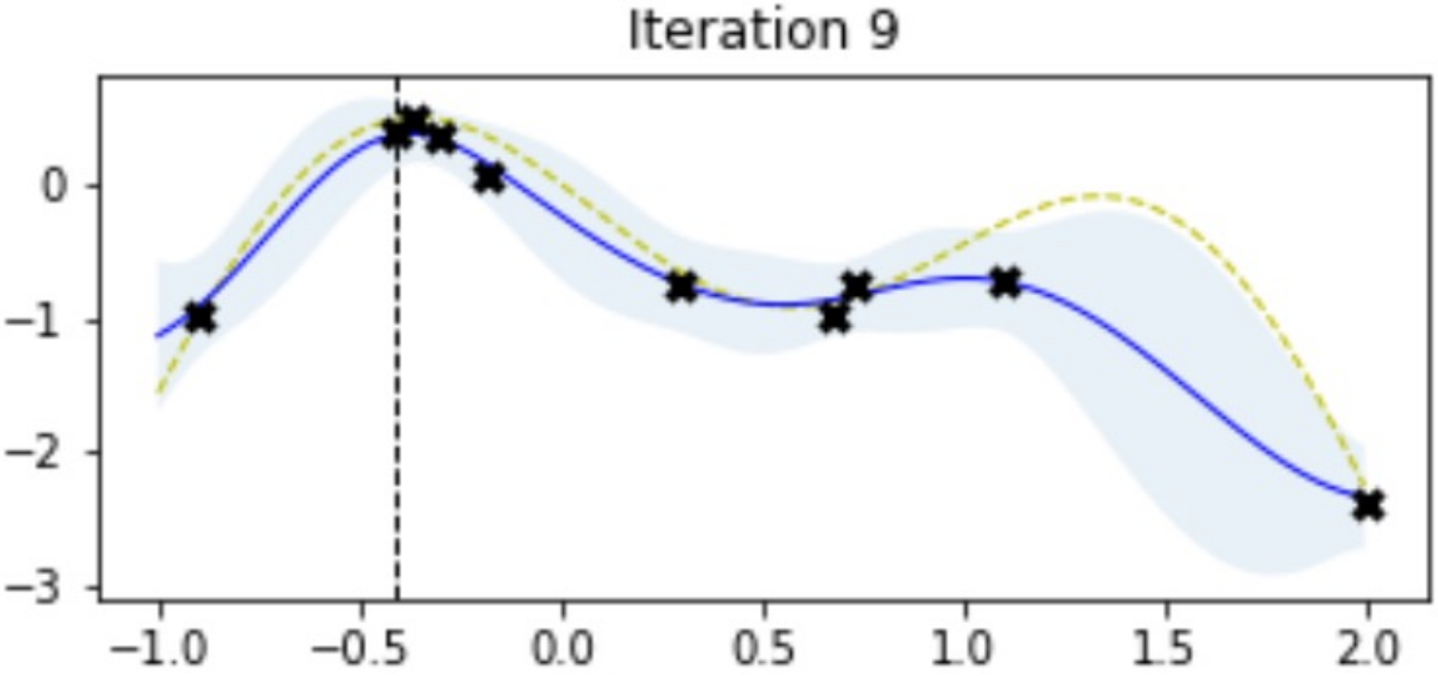

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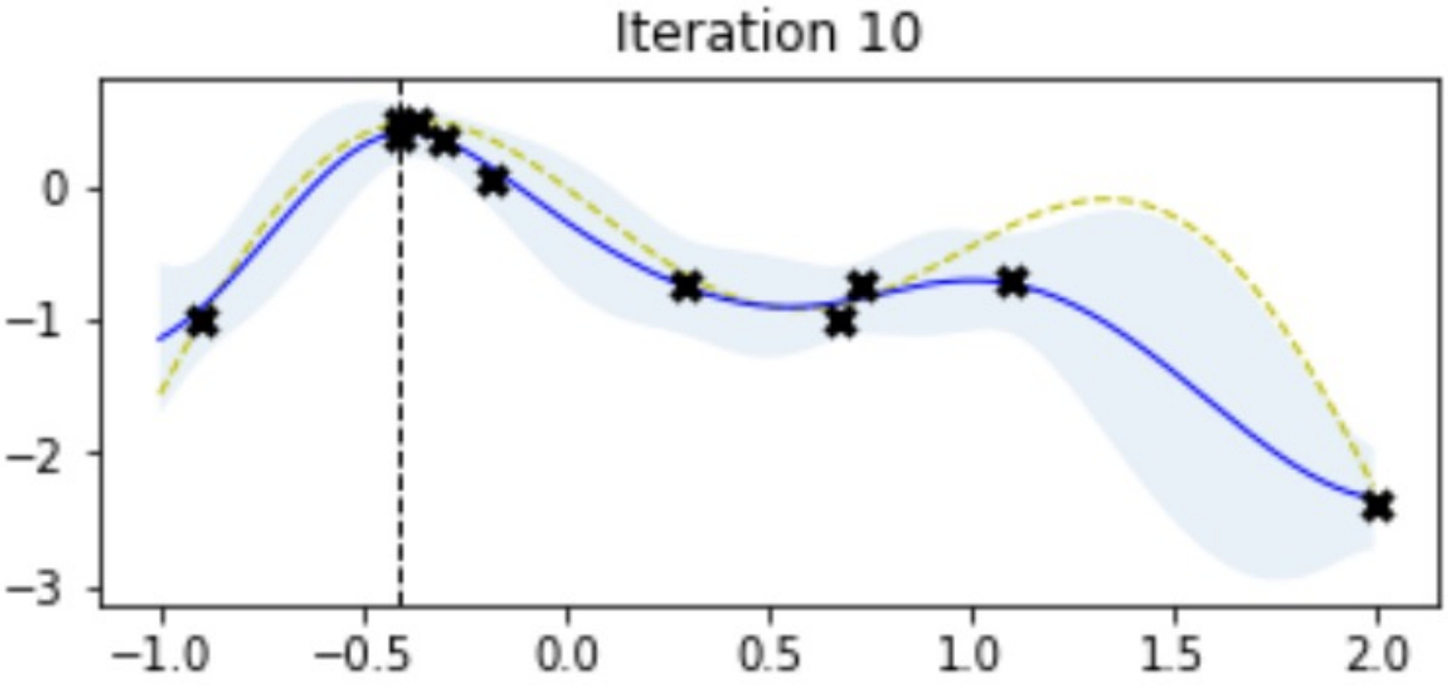
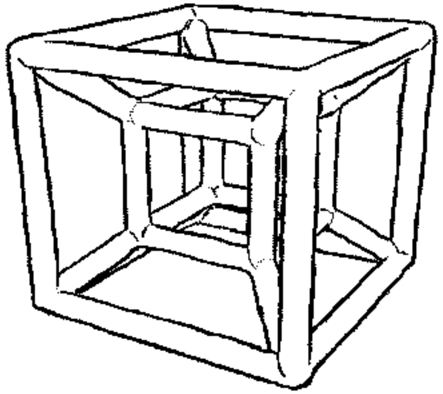
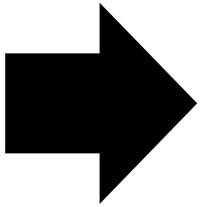


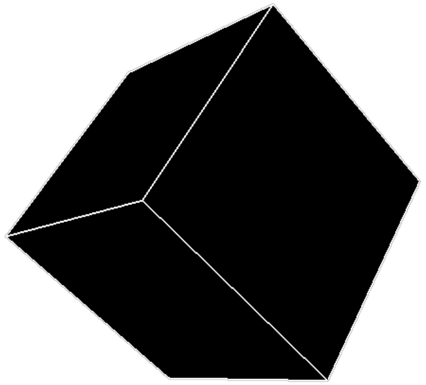
Bayesian hyperparameter optimization

Graduate student perspective



multidimensional
data





Machine learning
model

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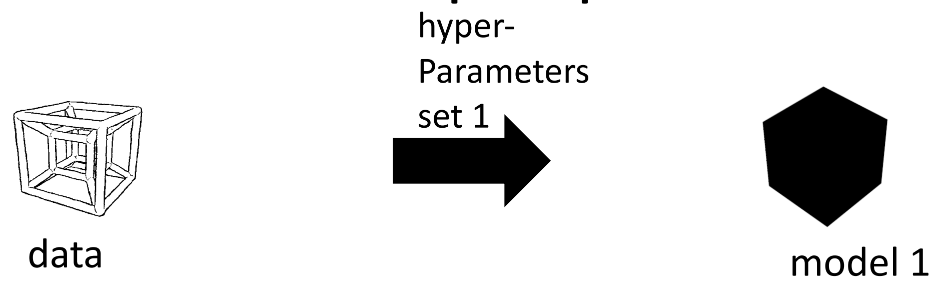

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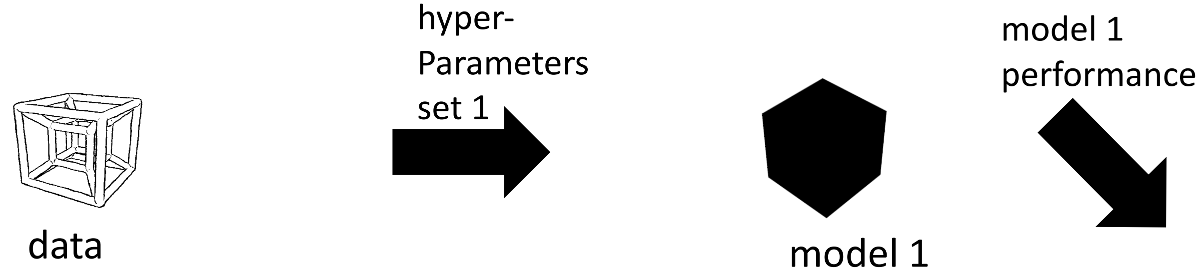

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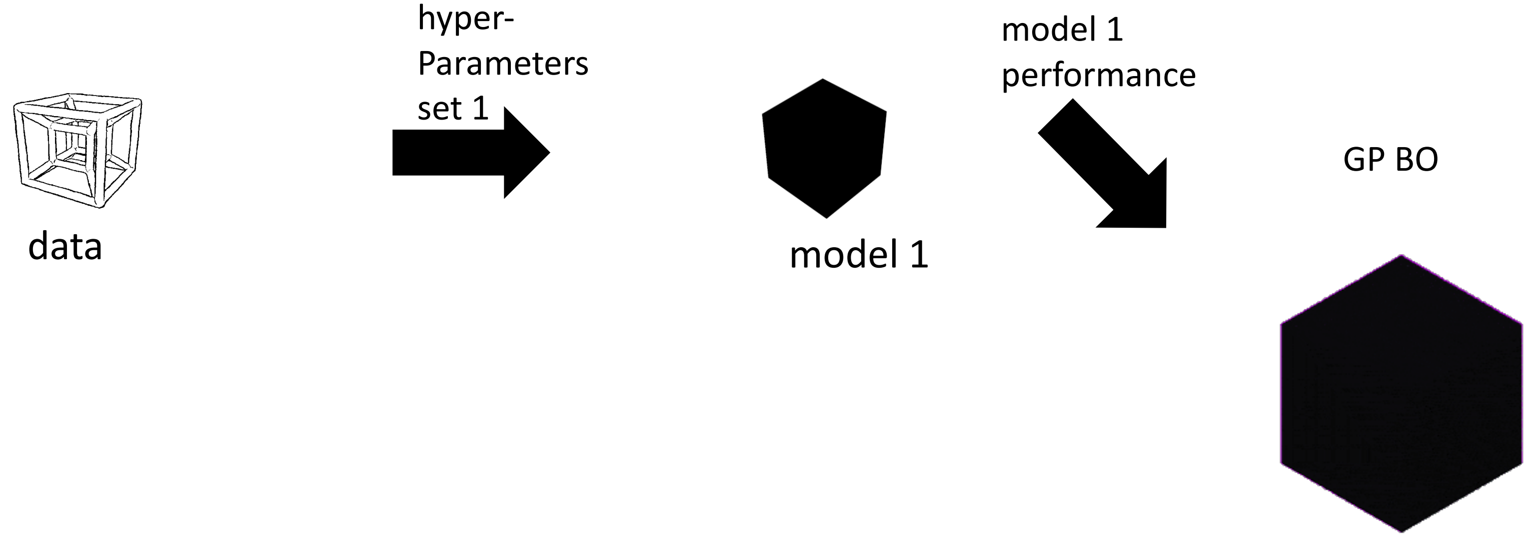

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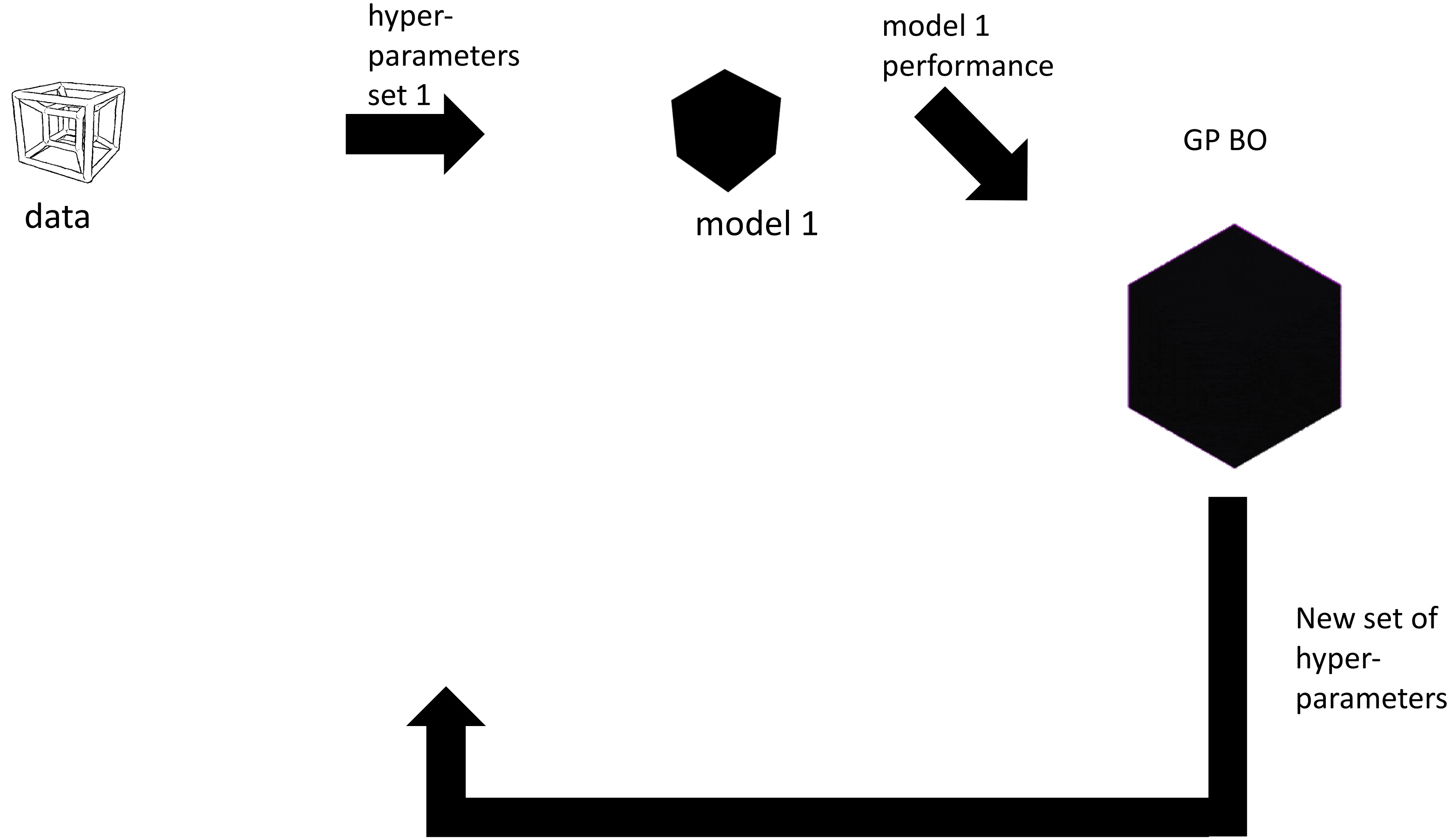

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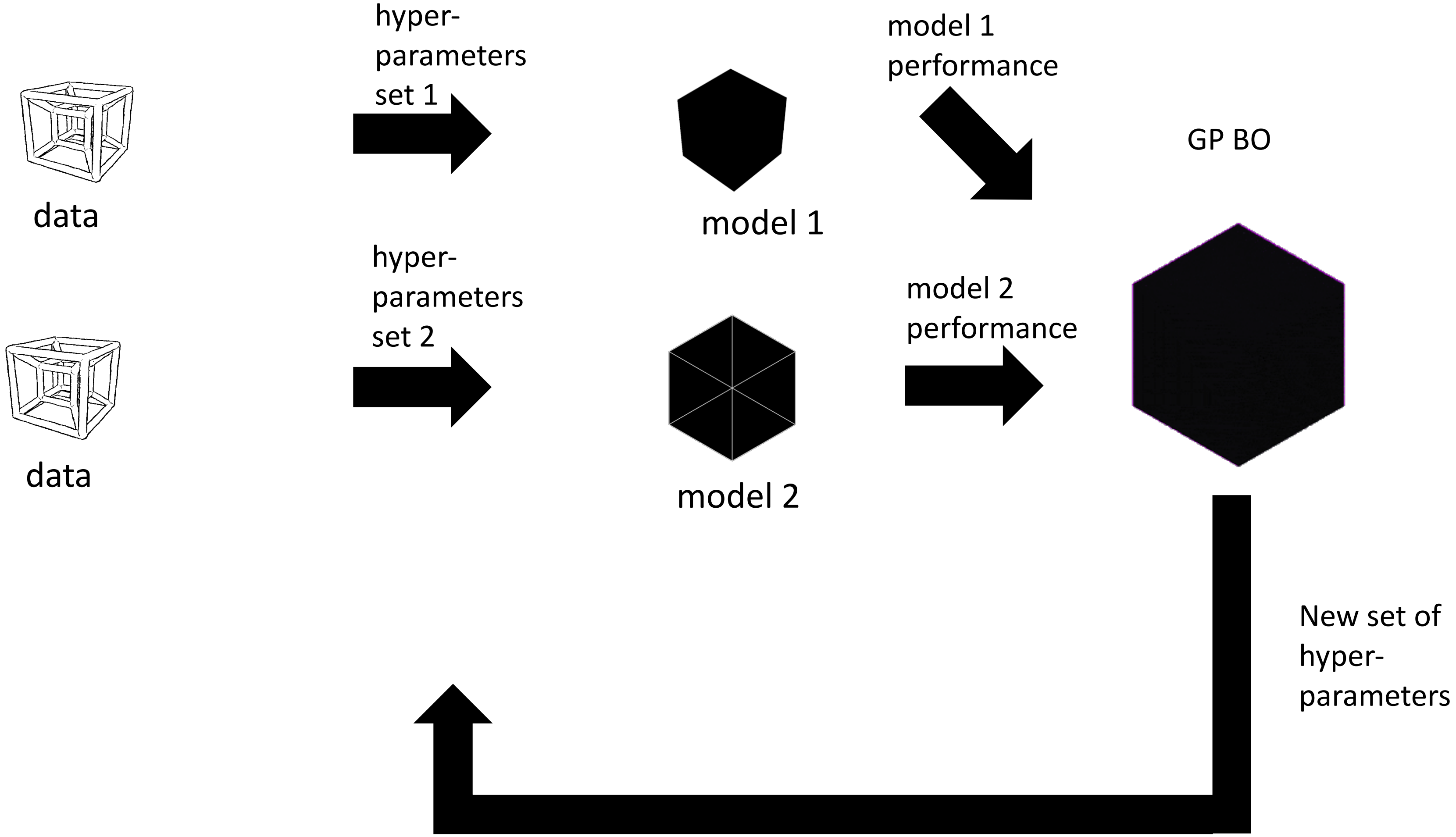

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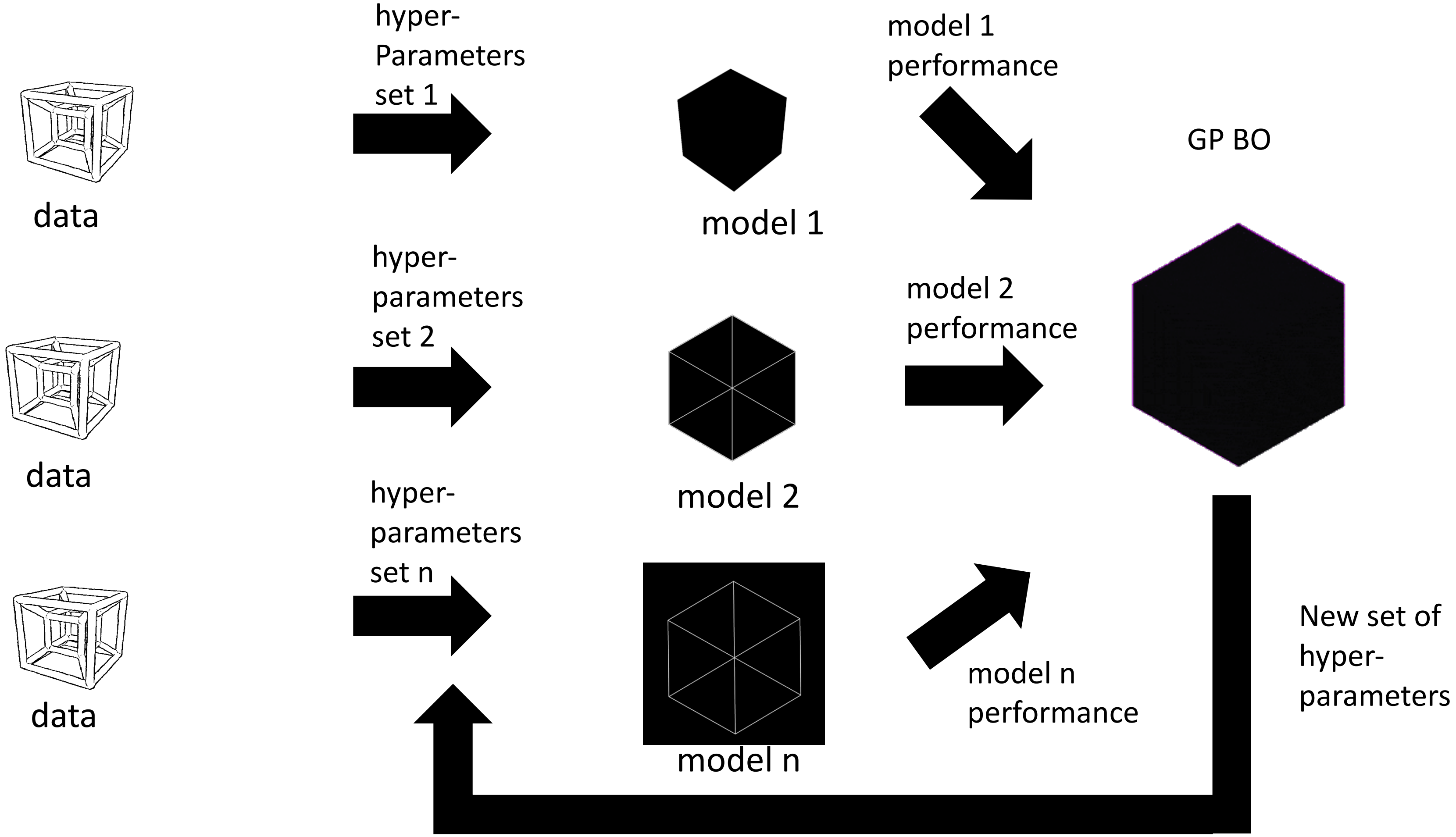

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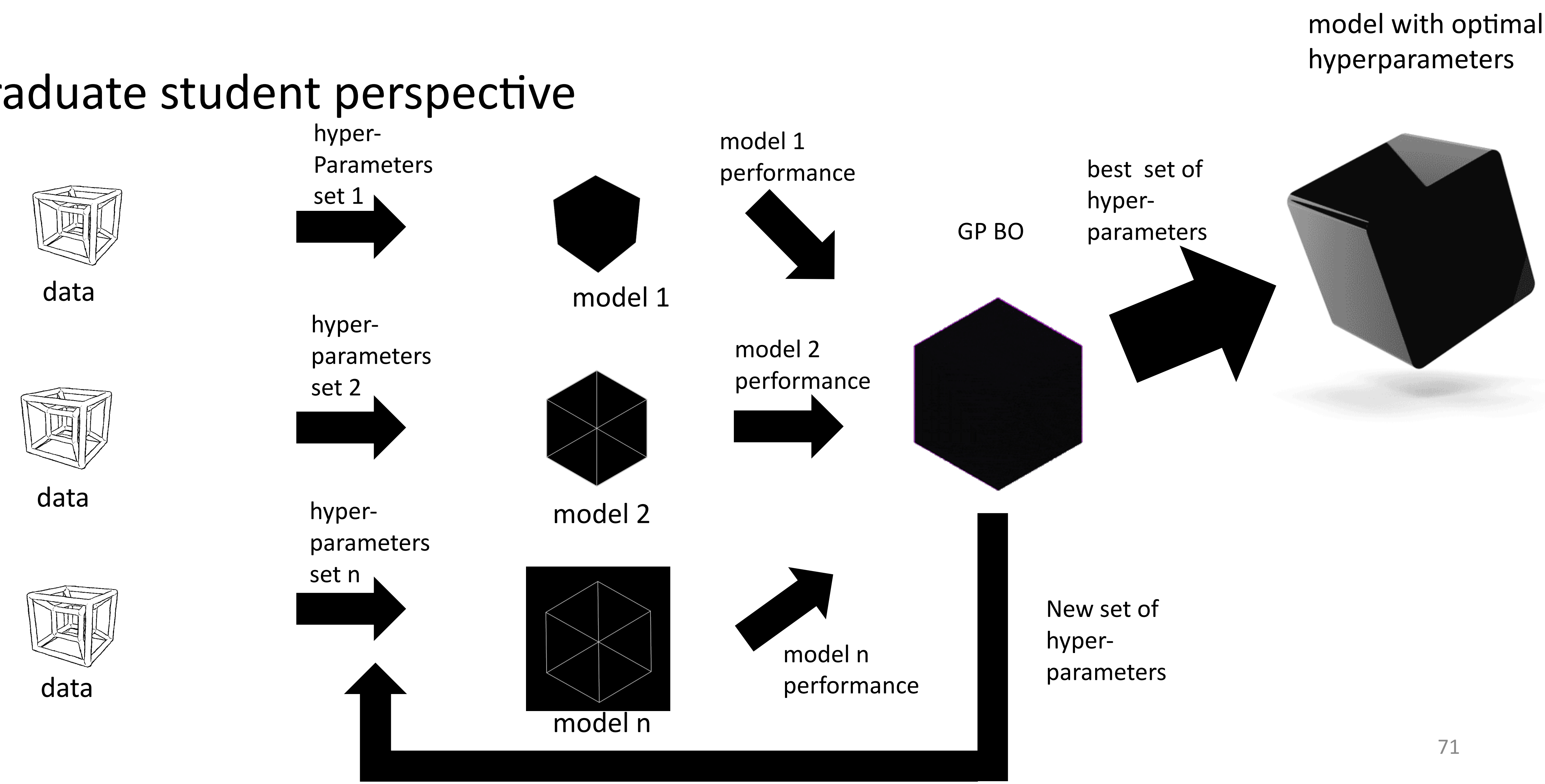

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