SageMaker Automatic Model Tuning

Part 1: Theory

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Many hyperparameters for training

Model:

- Number of layers: 1, 2, 3, …
- Activation functions: Sigmoid, tanh, RELU, …

Optimization:

- Method: SGD, Adam, AdaGrad, …
- Learning Rate: 0.01 to 2

Data:

- Batch Size: 8, 16, 32 …
- Augmentation: Resize, Normalize, Color Jitter, …

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Choose function to optimize

Optimize model-params: λ

$$\min_{\lambda} f(\lambda|\theta)$$

Optimize hyper-params: θ

$$\min_{\theta} h(\theta)$$

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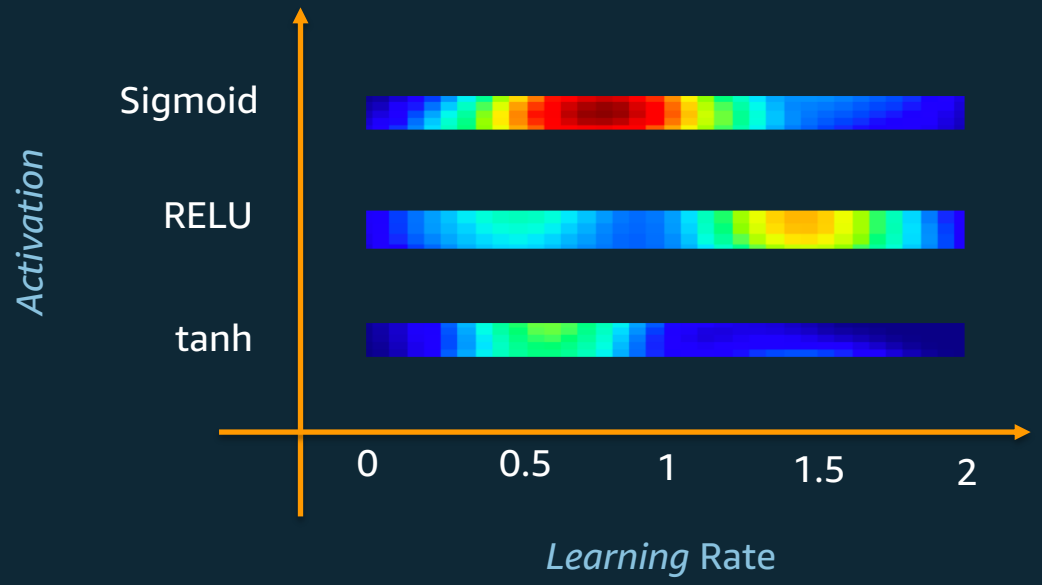
Grid Search



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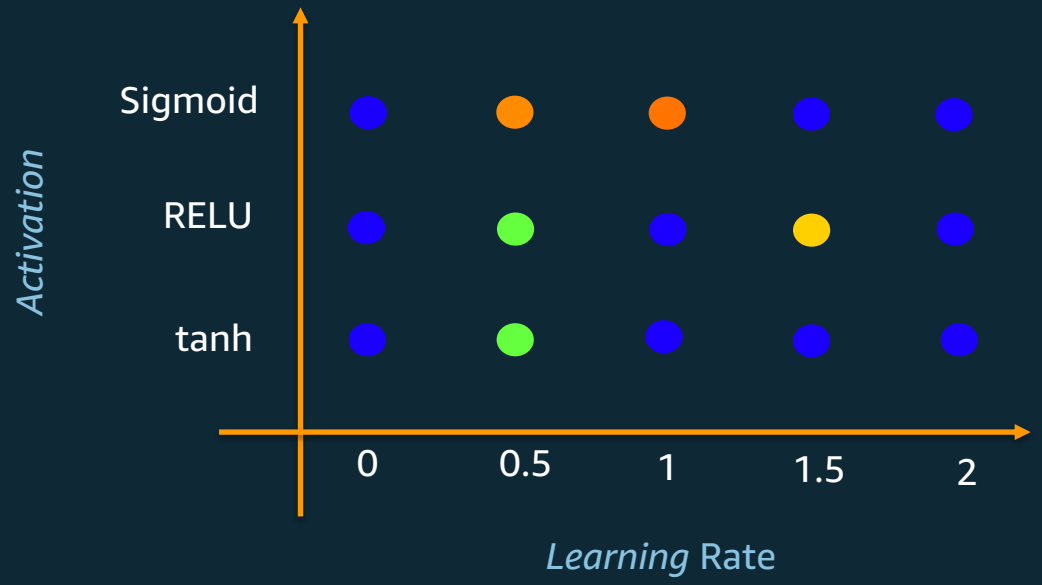
Grid Search



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Grid Search

Assume each hyper-param has 5 options
e.g. Learning Rate: 0, 0.5, 1, 1.5, 2

1 HP = 5 combinations
2 HPs = 5*5 = 25 combinations
3 HPs = 5*5*5 = 125 combinations
…
10 HPs = 5^10 = 9,765,625 combinations

N HPs = 5^N combinations

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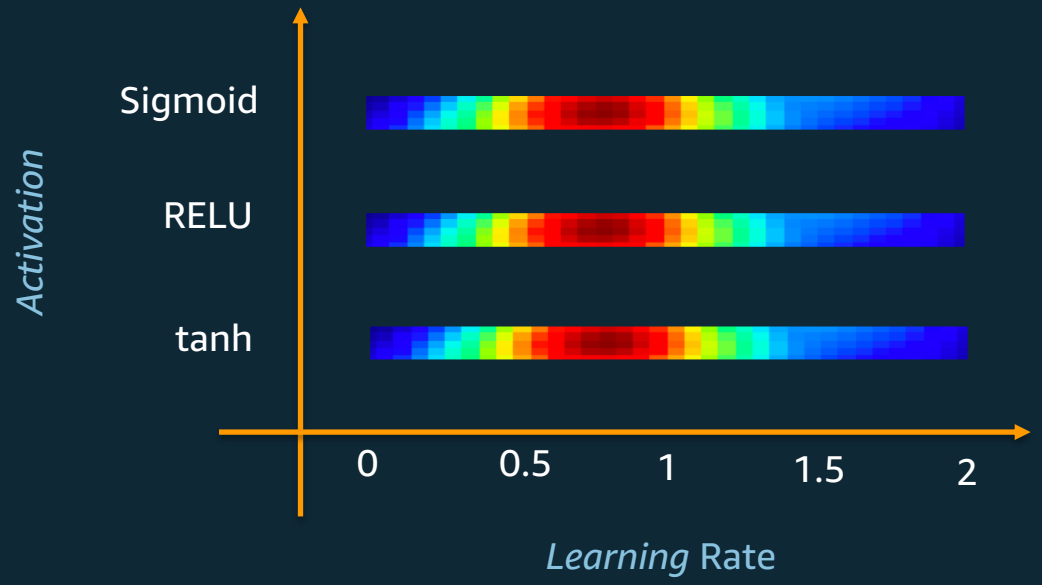
Grid Search



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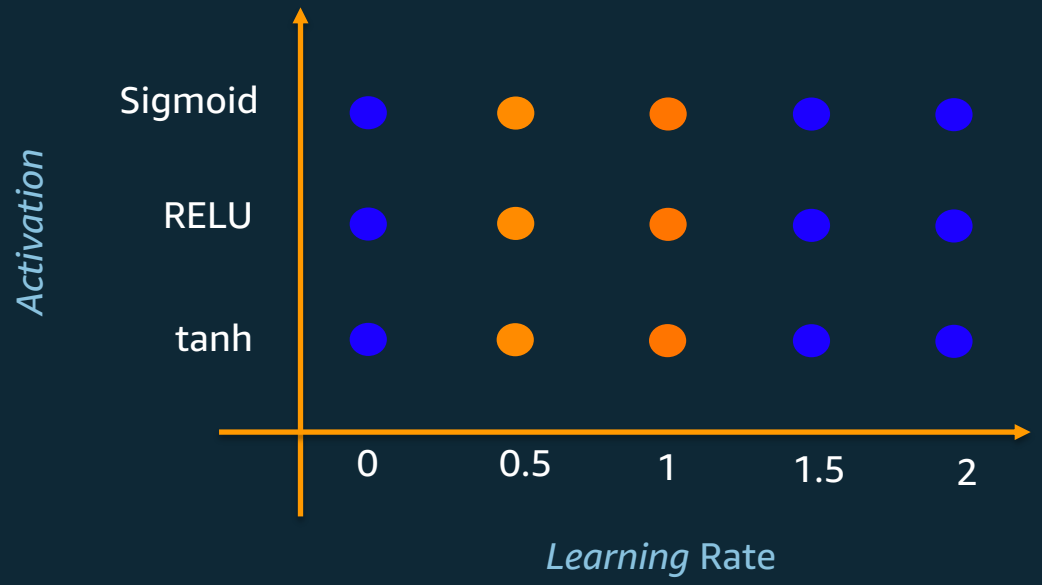
Grid Search



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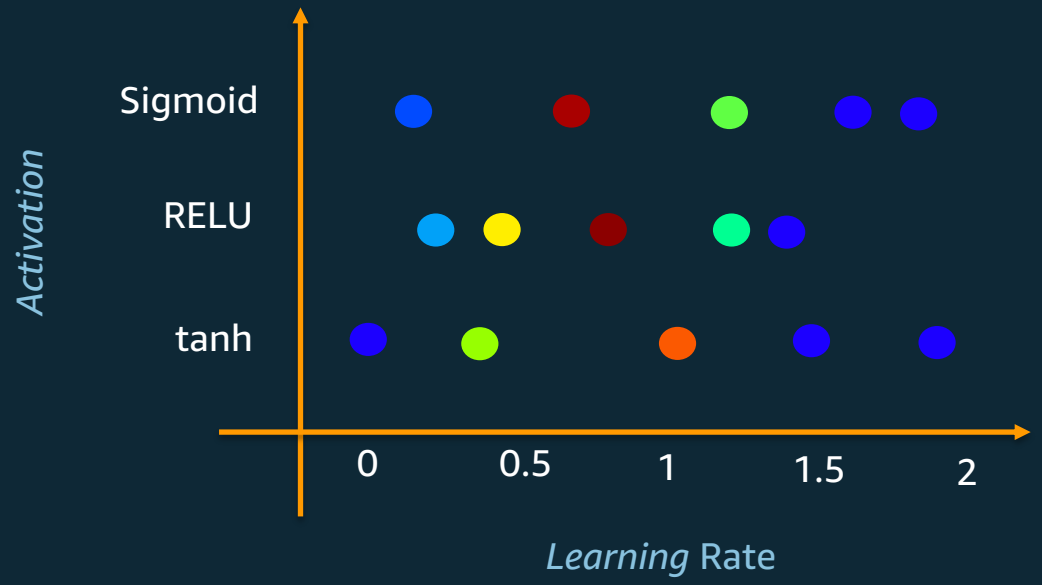
Random Grid Search



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Create model of model loss

Approximate expensive $h(\theta)$

$$h(\theta) \approx h'(\theta)$$

Use previous evaluations: D

$$h'(\theta|D)$$

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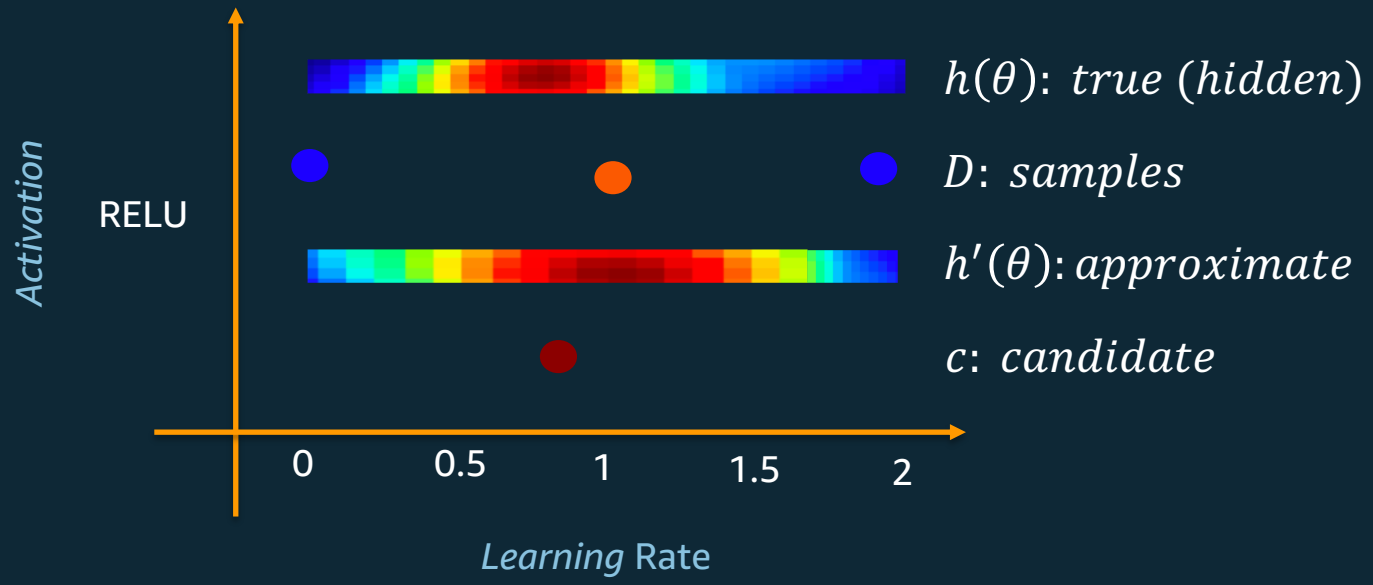
Use model of model loss



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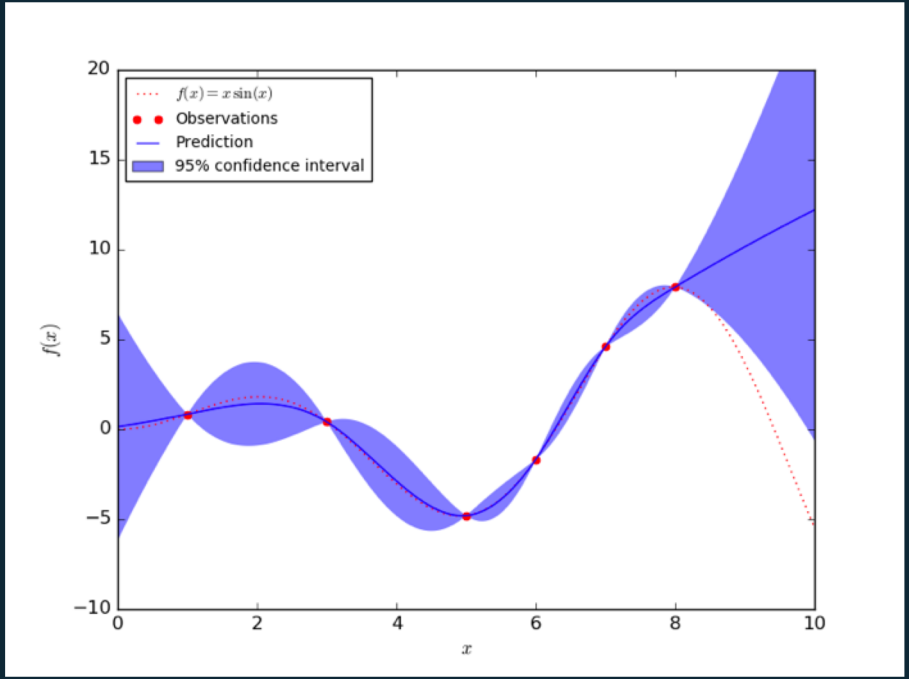
Gaussian Process for model of model loss



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Gaussian Process

$$f(X_{t_1}), f(X_{t_2}), \ldots, f(X_{t_n}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

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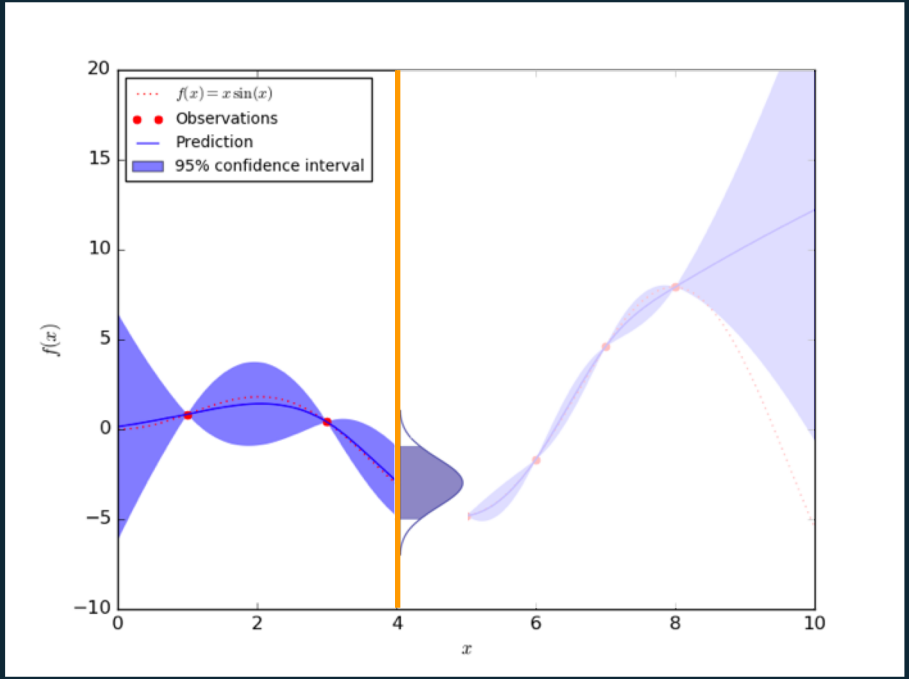
Gaussian Process for model of model loss



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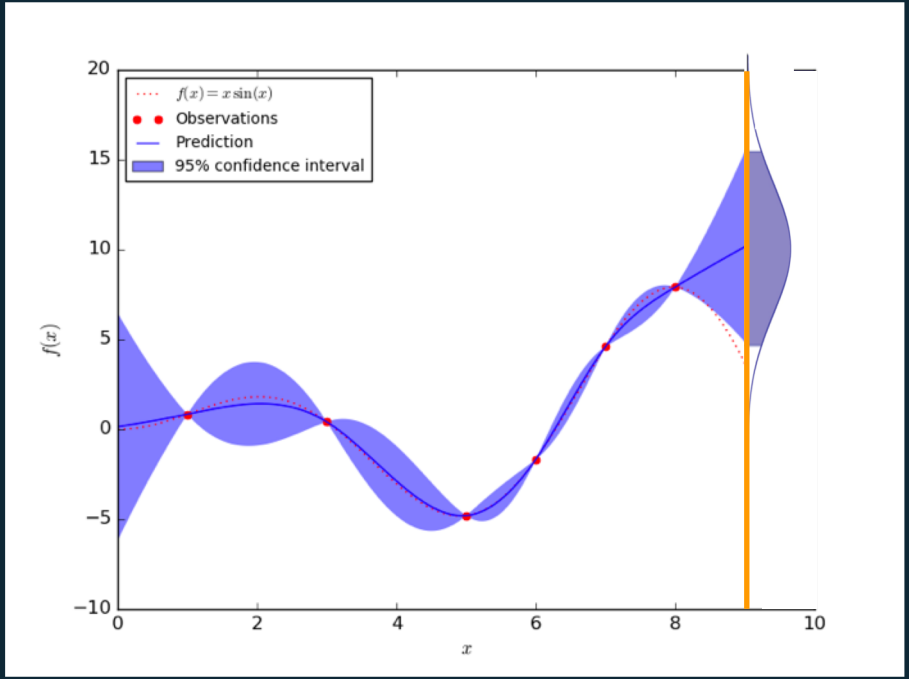
Gaussian Process for model of model loss



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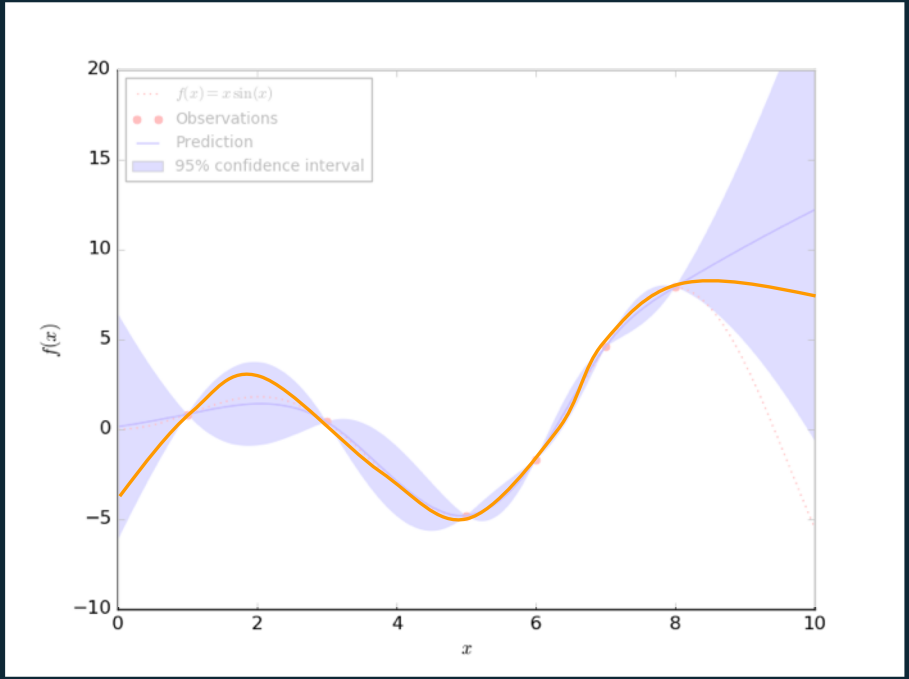
Gaussian Process for model of model loss



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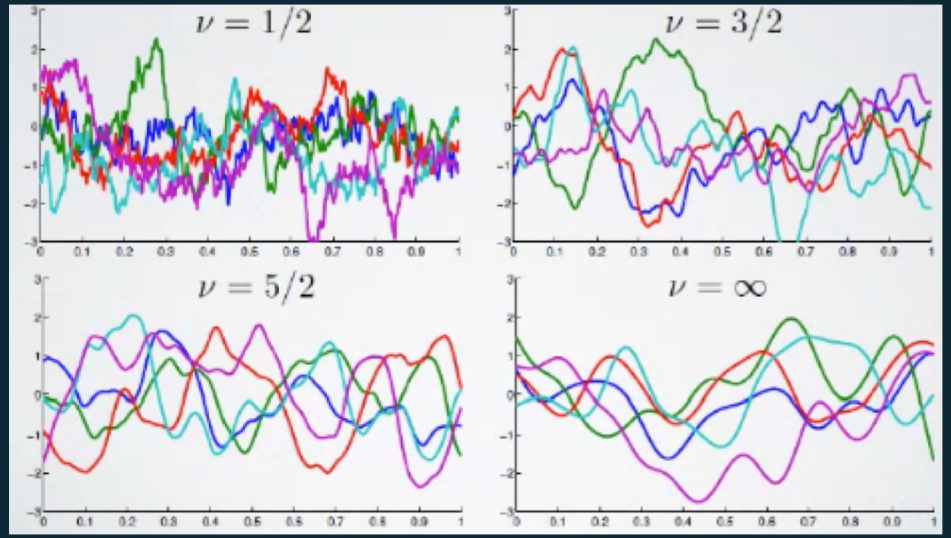
Covariance Matrix

Similarity between 2 points: controls ‘smoothness’.

SageMaker uses Matérn kernel with $\upsilon = 5/2$



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Closed form expressions

- For any two vectors $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$:

$$K_\theta(\mathbf{x}, \mathbf{x}') \triangleq \theta_0 \cdot \left[1 + \sqrt{5} r(\mathbf{x}, \mathbf{x}') + \frac{5}{3} r^2(\mathbf{x}, \mathbf{x}')\right] \cdot e^{-\sqrt{5} r(\mathbf{x}, \mathbf{x}')}$$

with

$$r^2(\mathbf{x}, \mathbf{x}') \triangleq \sum_{j=1}^{d} \frac{(\mathbf{x}_j - \mathbf{x}'_j)^2}{\theta_j^2}.$$

$$\begin{aligned}
\mu_\theta(f(\mathbf{x}) | \{\mathbf{x}^c, y^c\}_{c \in \mathcal{C}}) &\triangleq \mathbf{k}_\mathcal{C}(\mathbf{x})^\top [\mathbf{K}_\mathcal{C} + \theta_\sigma^2 \mathbf{I}]^{-1} \mathbf{y}_\mathcal{C} \\
\Sigma_\theta(f(\mathbf{x}) | \{\mathbf{x}^c, y^c\}_{c \in \mathcal{C}}) &\triangleq K(\mathbf{x}, \mathbf{x}) - \mathbf{k}_\mathcal{C}(\mathbf{x})^\top [\mathbf{K}_\mathcal{C} + \theta_\sigma^2 \mathbf{I}]^{-1} \mathbf{k}_\mathcal{C}(\mathbf{x})
\end{aligned}$$

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Acquisition Function

Given posterior distribution of functions…

Used as criteria for selecting next candidate hyperparams for evaluation.

Often depends on the best hyperparams seen so far in search.

Controls exploration vs exploitation in search.

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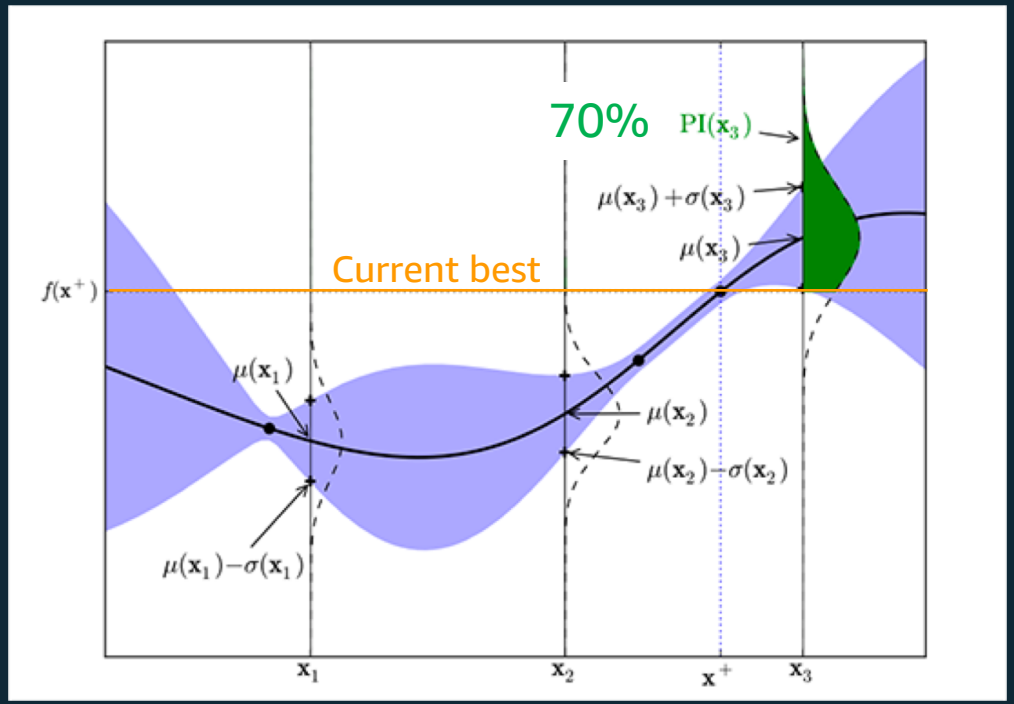
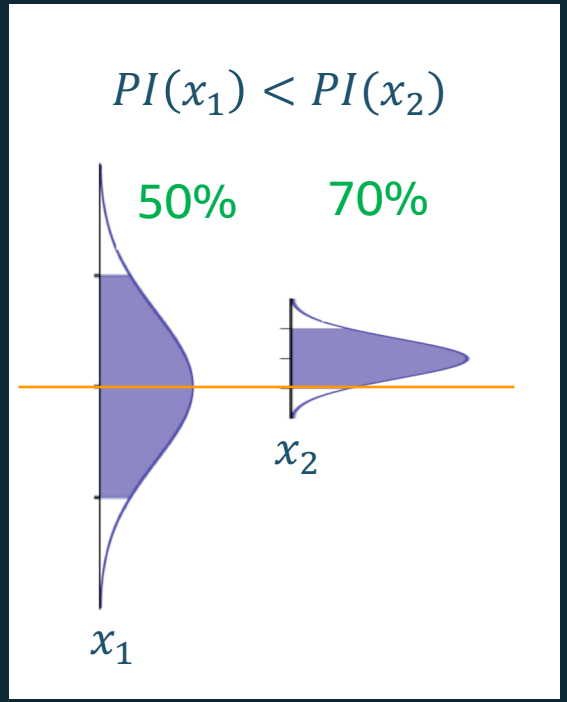
Acquisition Function: Probability of Improvement





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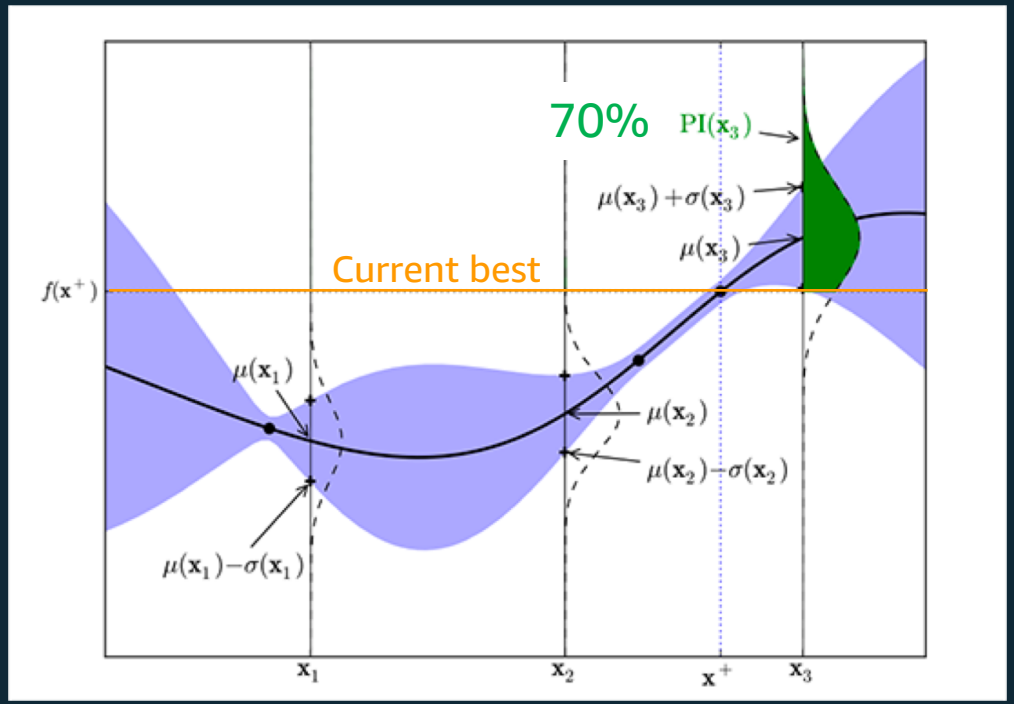
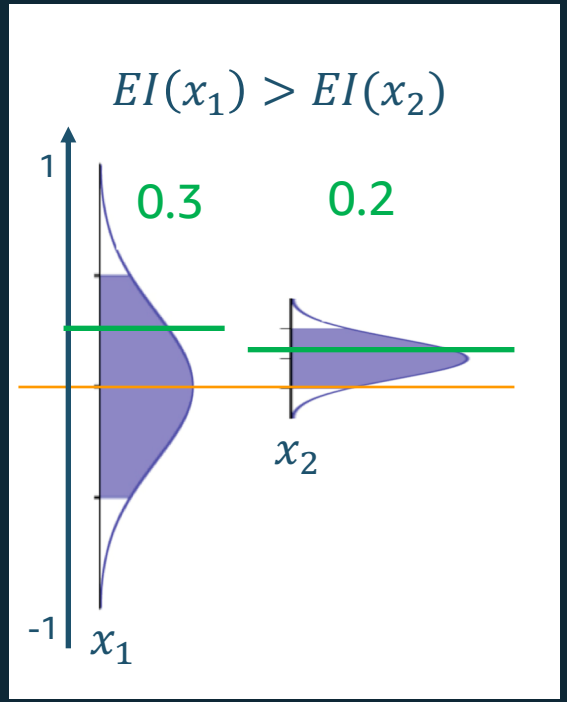
Acquisition Function: Expected Improvement





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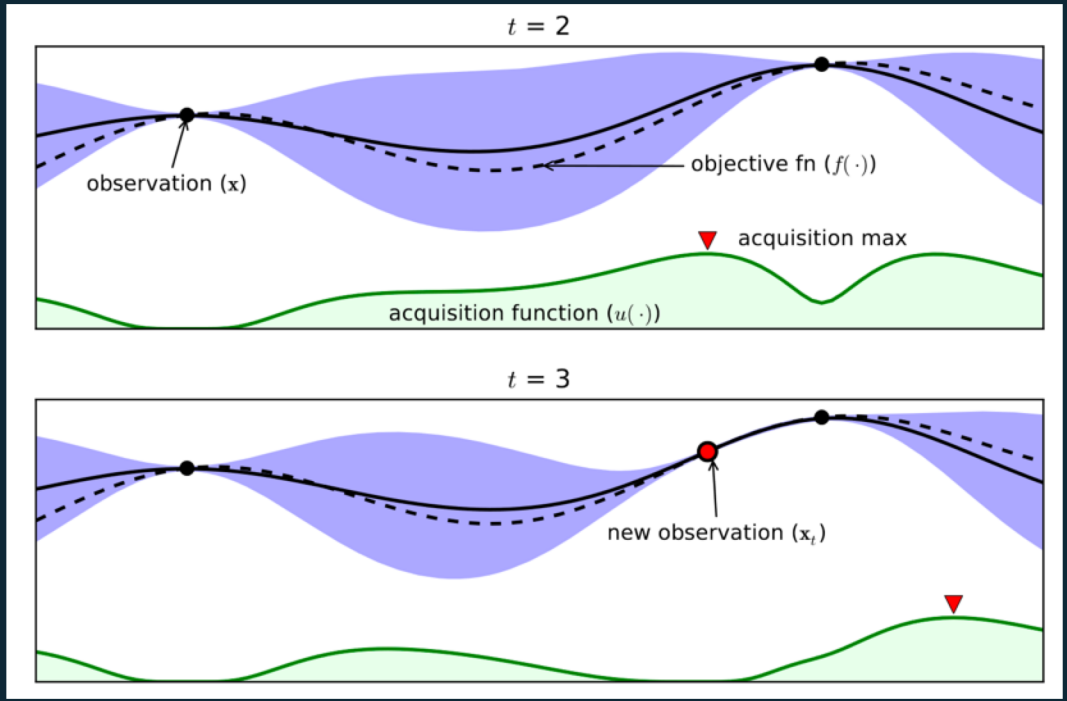
Using Acquisition Functions



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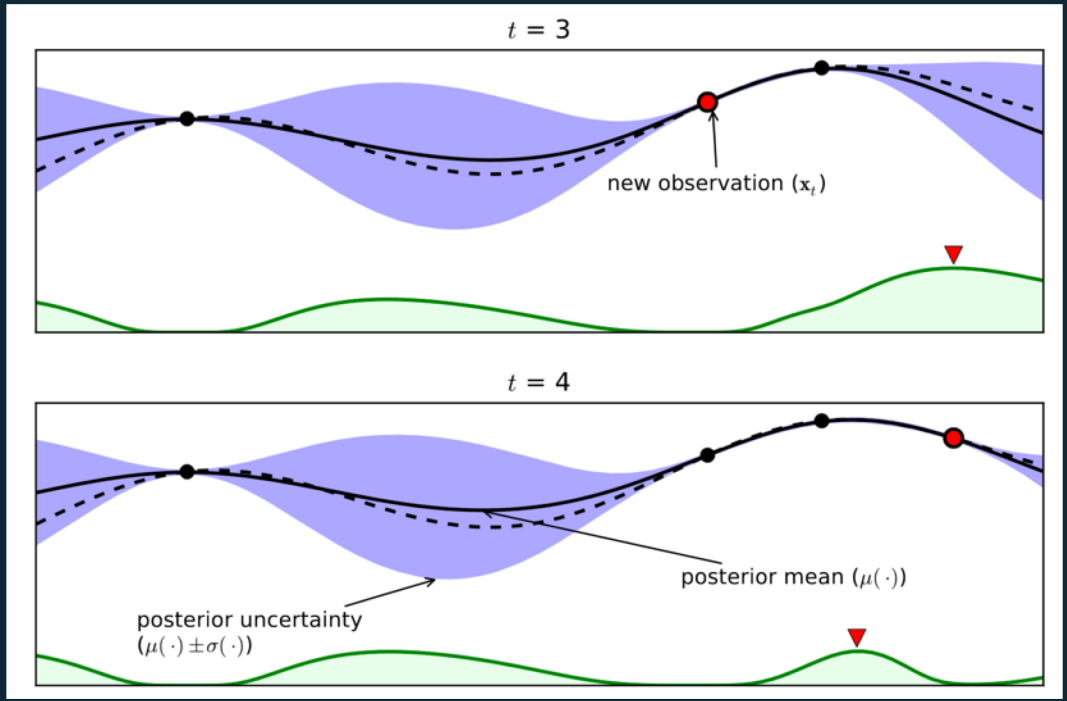
Using Acquisition Functions



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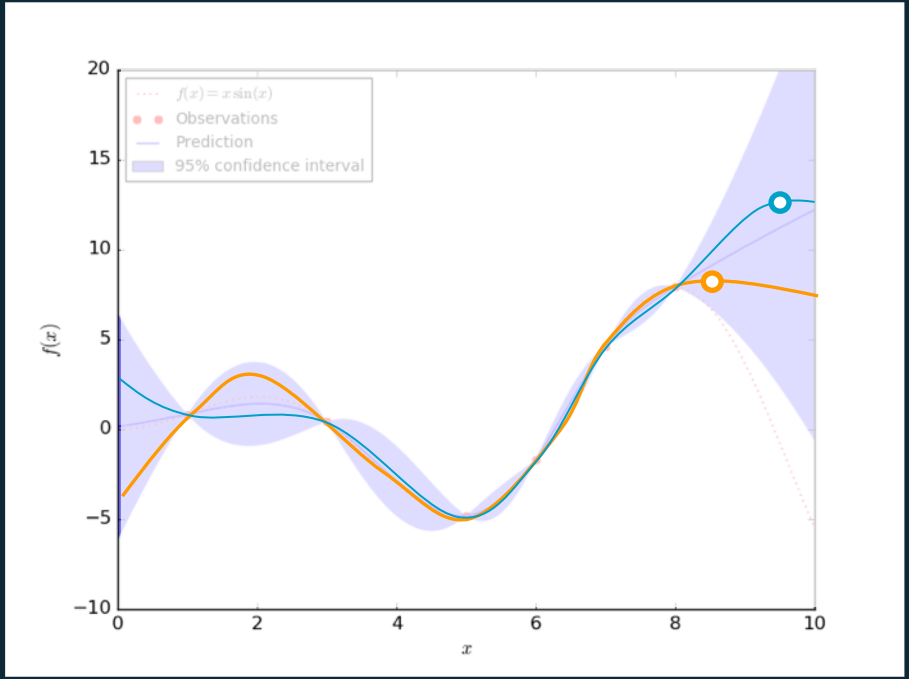
Add parallelism with Thompson Sampling



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Input Mapping

Create a ***unit hypercube*** from all input hyperparameters

Continuous – e.g. learning rate

$$[0,2] \rightarrow [0,1]$$

Integral – e.g. number of epochs

$$\{1,2,\ldots,50\} \rightarrow [0,1]$$

Categorical – e.g. type of activation

$$\{Sigmoid, RELU, tanh\} \rightarrow [0,1]^3$$

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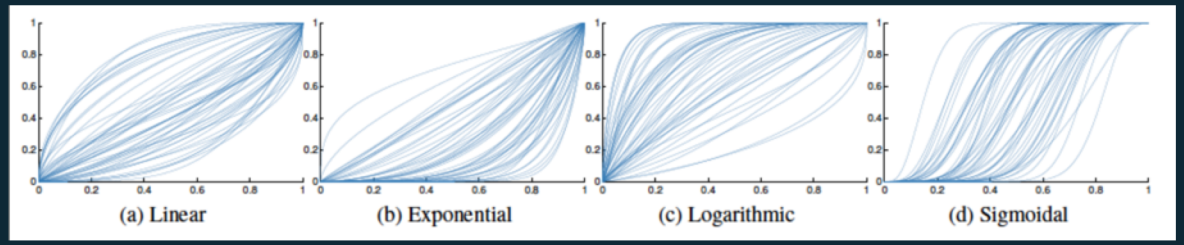
Input Warping

Apply transformation of variables within the hypercube.

Automatic selection of transform per variable from Beta CDF:



e.g. for learning rate

{0.3, 0.6, 0.9} less effective search space than

{0.01, 0.1, 1} (i.e. log transform)

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Part 2: Practical

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