Gaussian Process Models

AE 6310: Optimization for the Design of Engineered Systems

Spring 2017

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Lecture Notes Developed By Dr. Brian German

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Primary References

- *Gaussian Processes for Machine Learning* by Rasmussen & Williams
  - Contains nearly everything you could want to know about Gaussian process models
  - It's FREE!!!!
  - Download: http://www.gaussianprocess.org/gpml/

- *Efficient Global Optimization of Expensive Black-box Functions* by Jones et. al.
  - 1998 Journal of Global Optimization

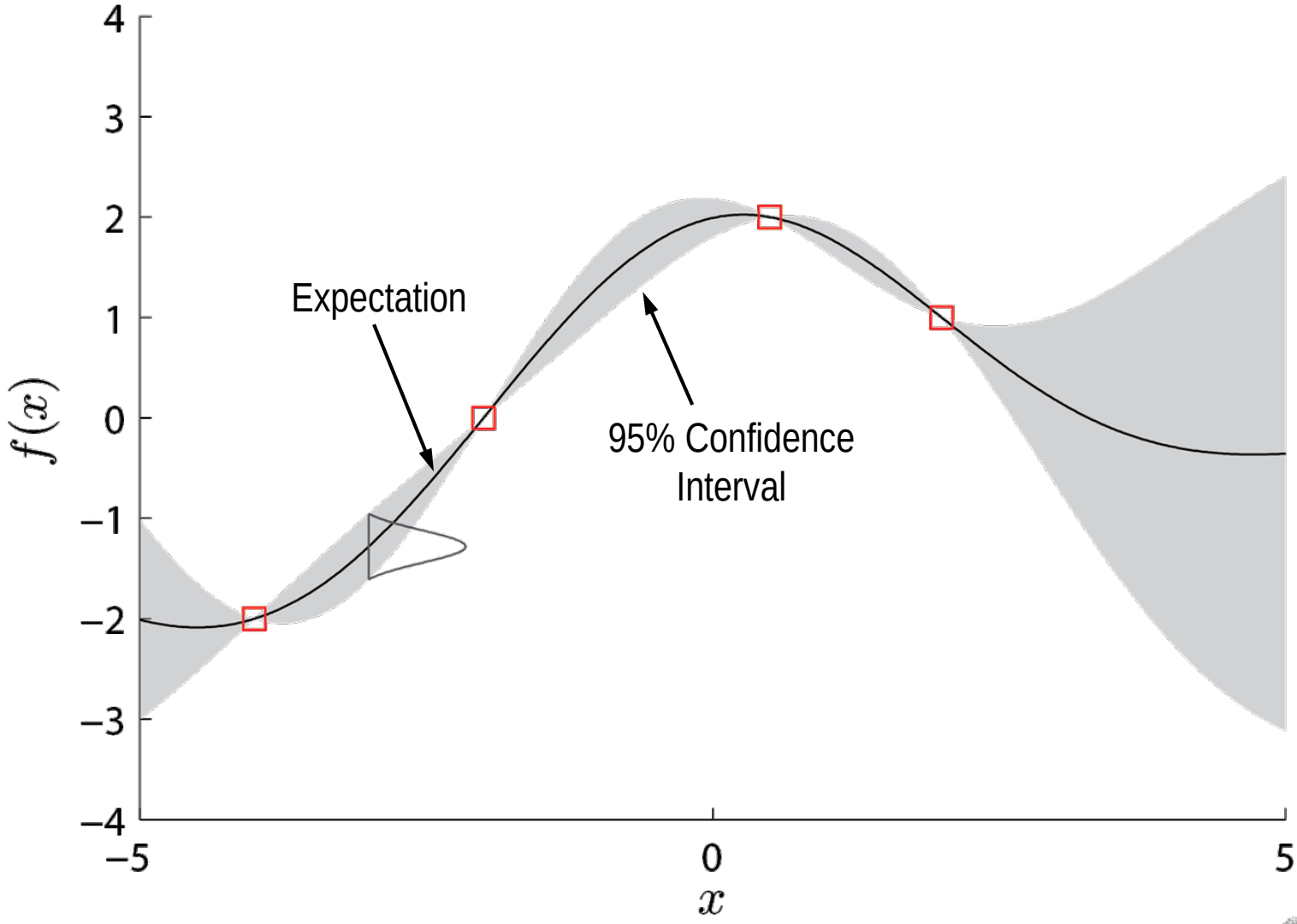
Also Known As…

- Gaussian process models
  - This name is primarily used in the statistical and robotics communities
- Kriging
  - This name is primarily used in the optimization and geostatistics communities
- DACE stochastic process models
  - DACE is an acronym for “Design and Analysis of Computer Experiments”

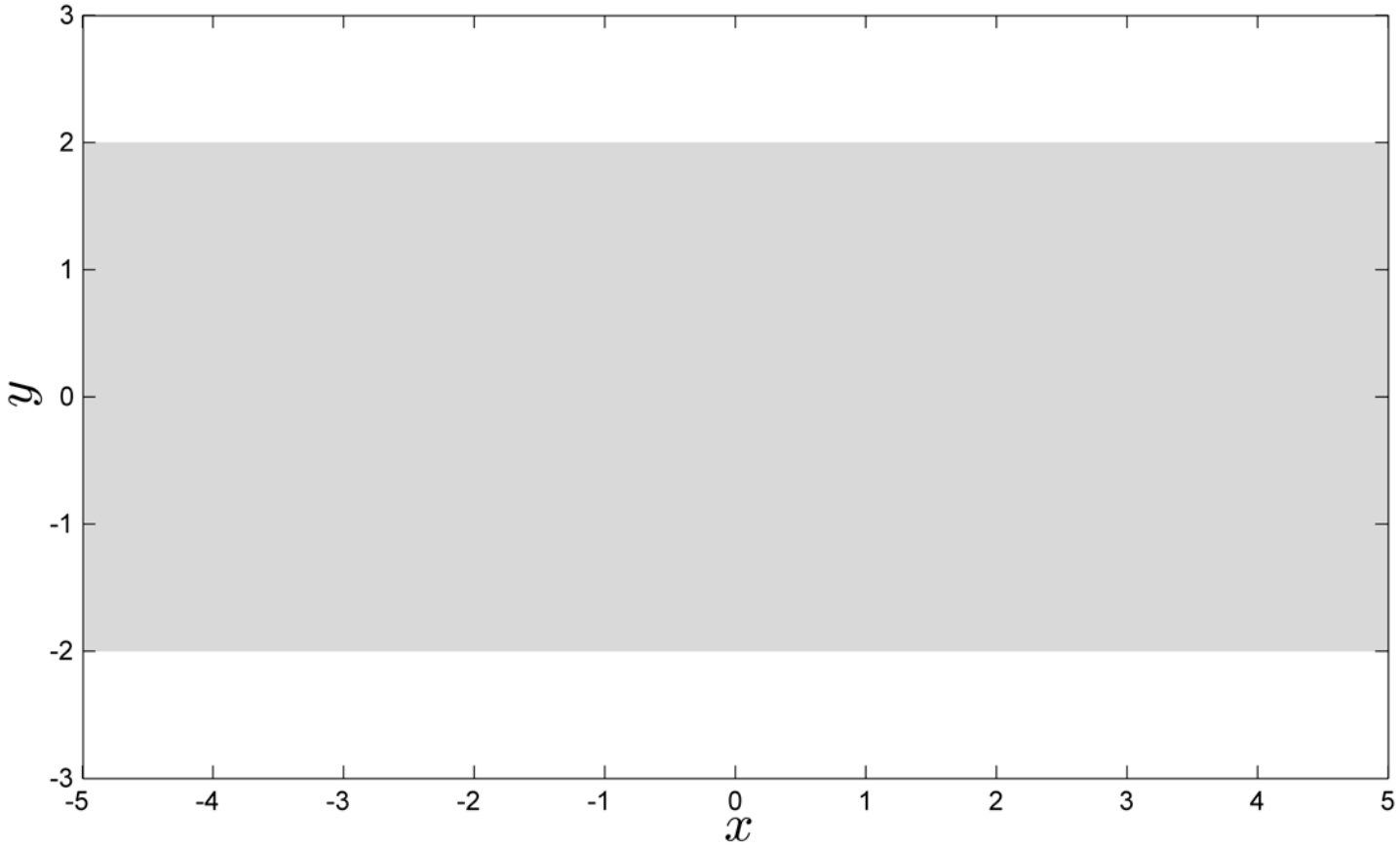
What are Gaussian process models?

- Used for regression
  - Infers the mapping between variables
- Used for classification
  - Is it a car or a truck?
- Supervised learning
  - Uses training data to infer a function
- Non-parametric
  - The model does not assume a functional form
- Stochastic processes
  - Returns a probability distribution for the function value rather than a deterministic value

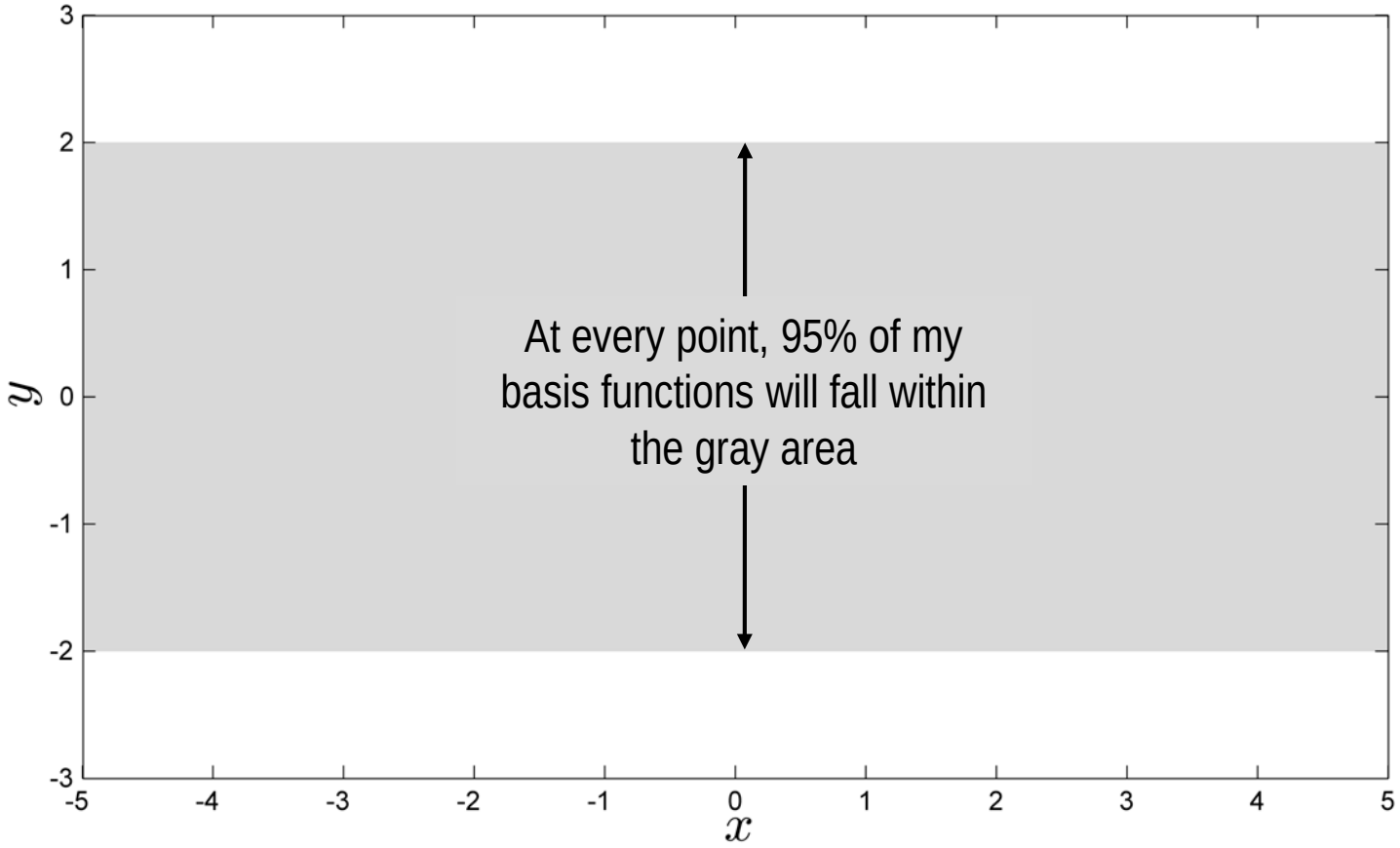
What are Gaussian process models?



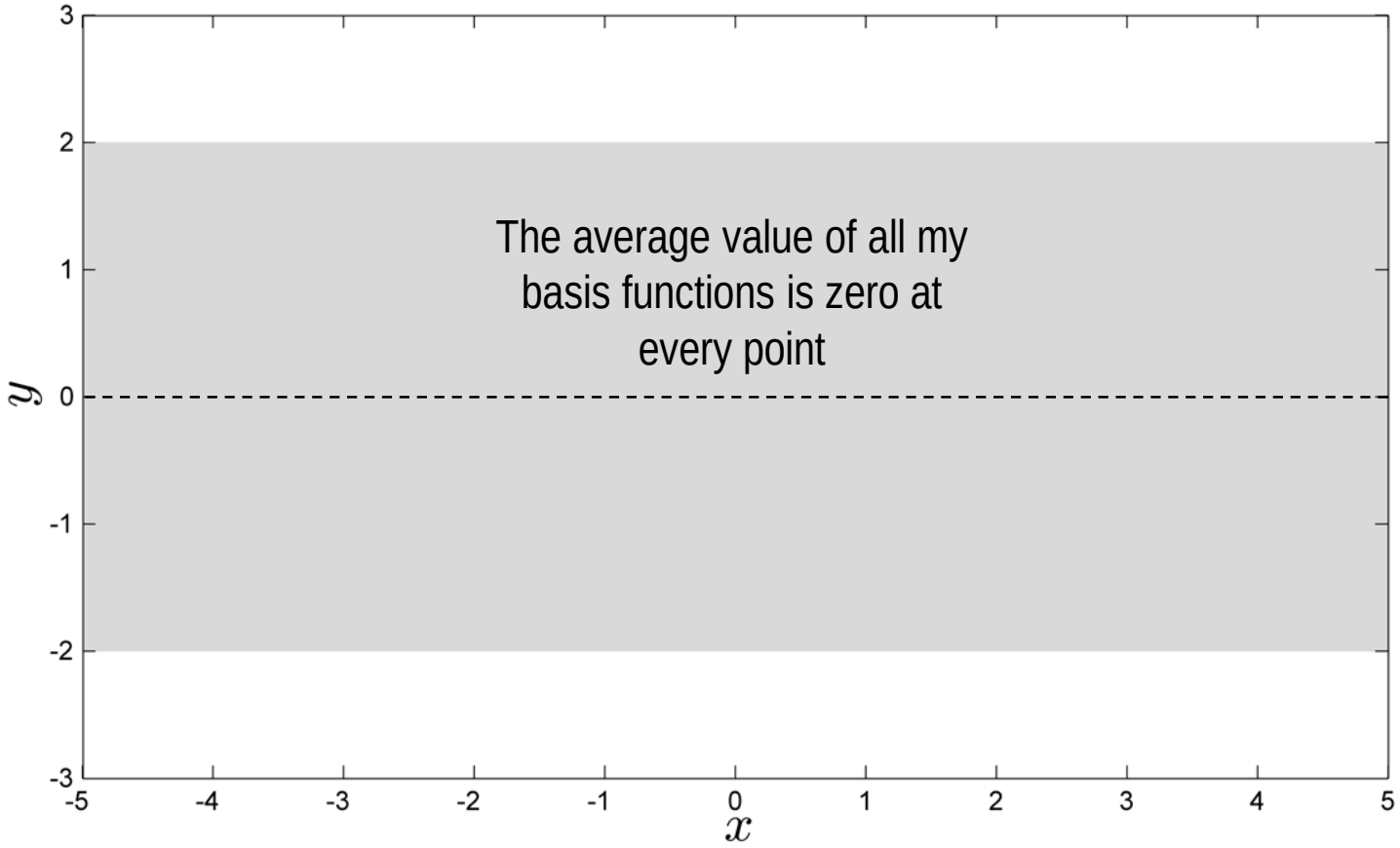
Prior Distribution



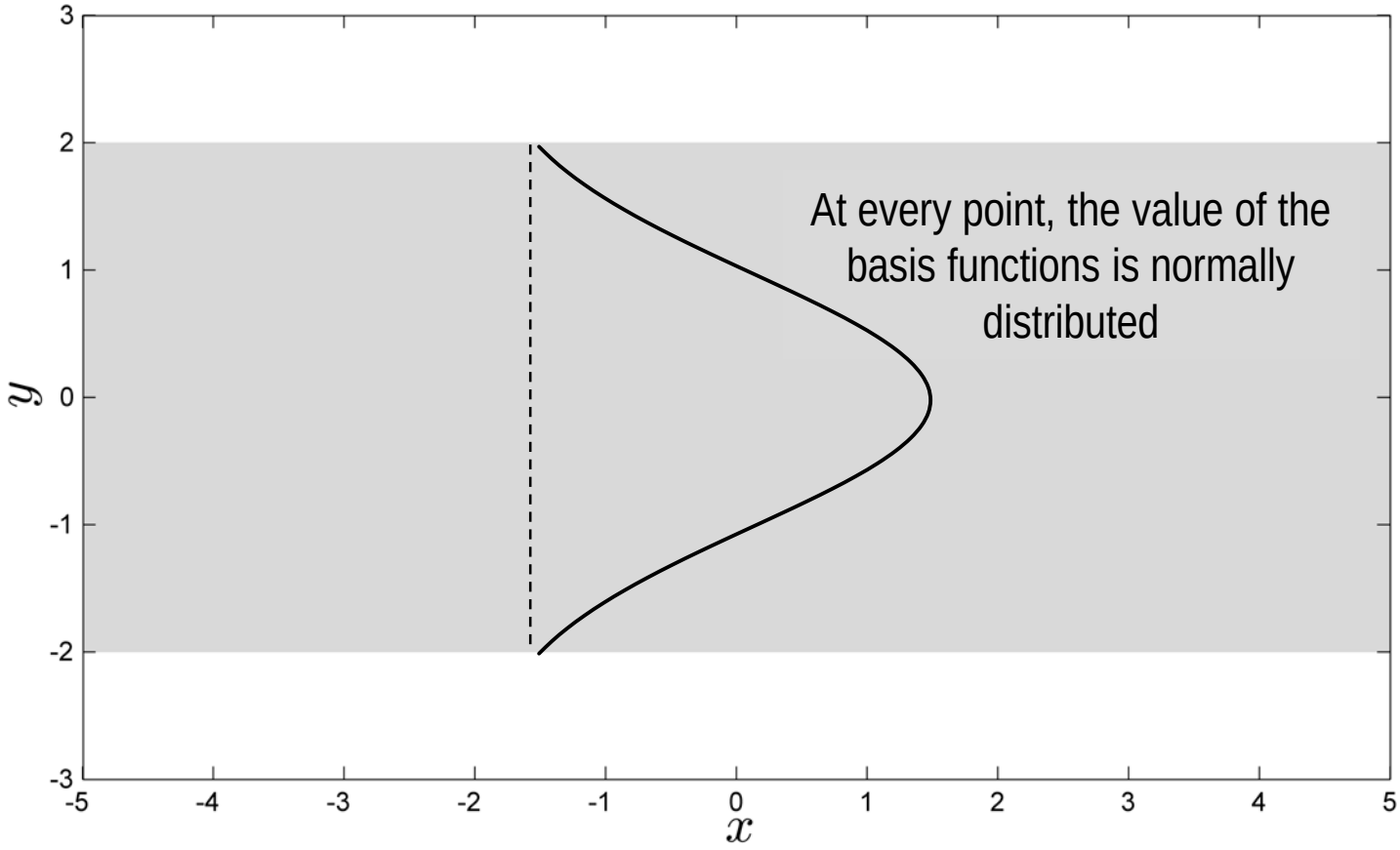
Prior Distribution



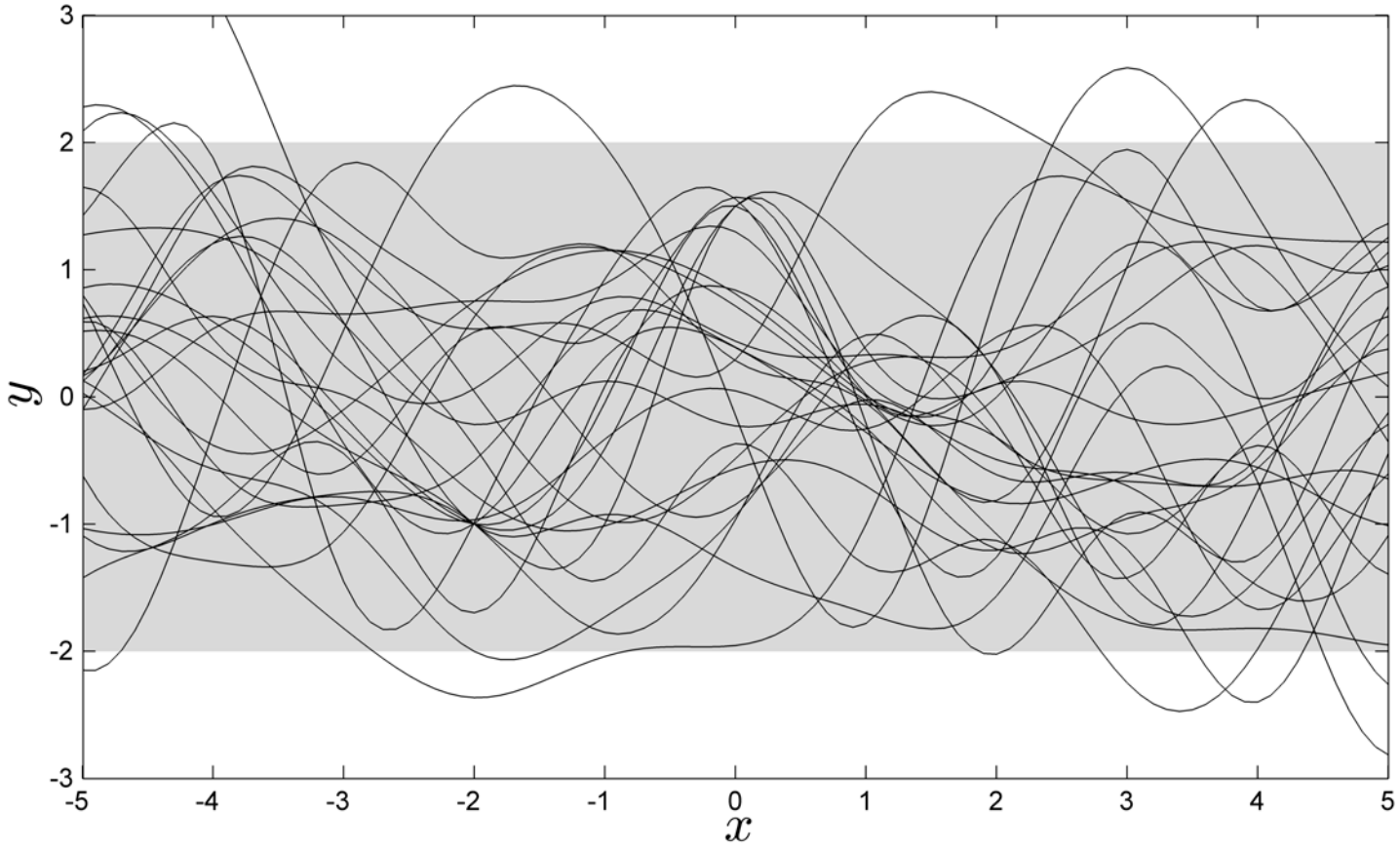
Prior Distribution



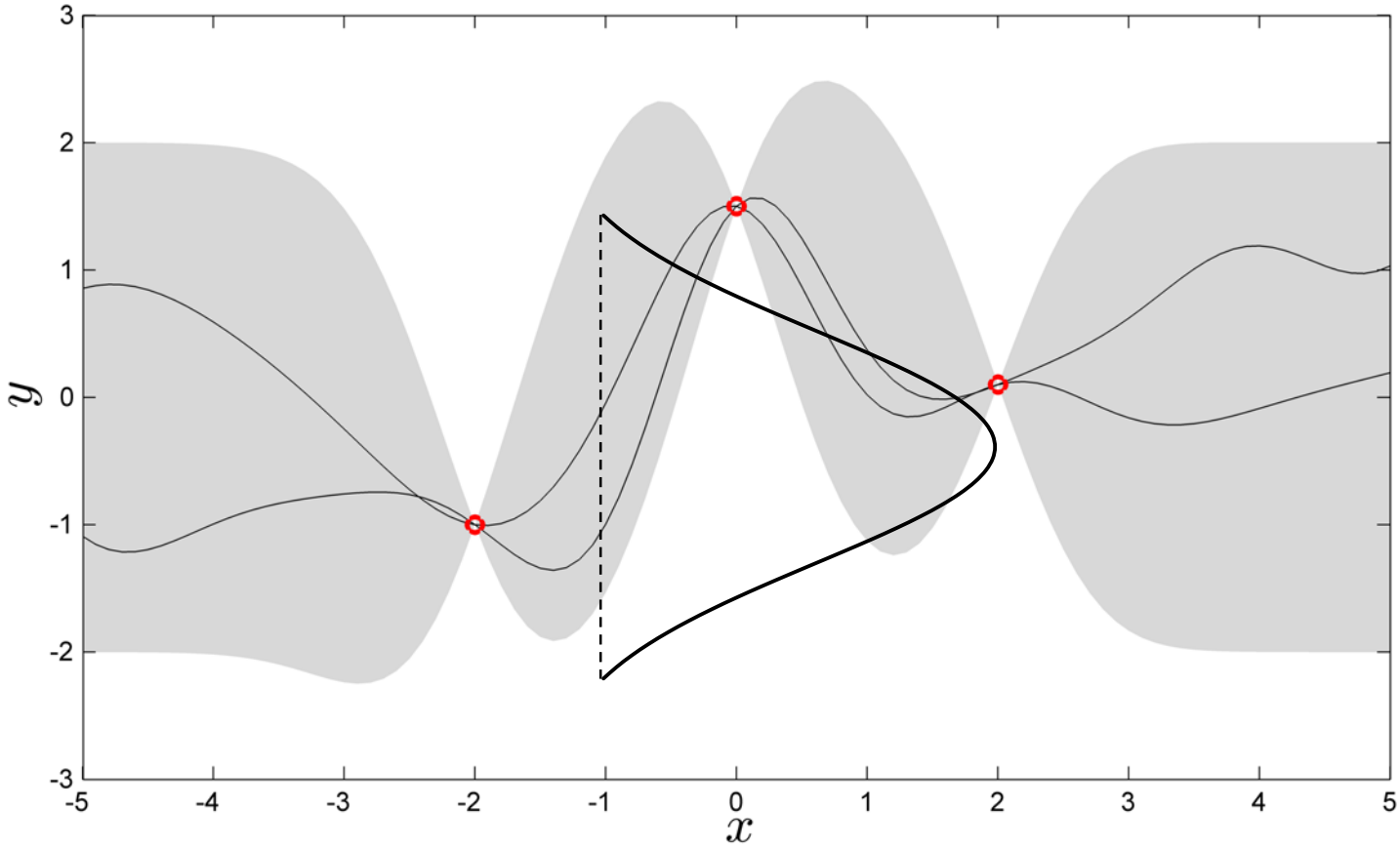
Prior Distribution



Prior Distribution



Posterior Distribution



What's happening?

- The prior distribution is determined entirely by a:
  - Mean function (we will assume this is zero for now)
  - Covariance Function

- Suppose we have n m-dimensional training points and p test points
  - X_{tr} is an m x n matrix of training points
  - Y_{tr} is a row vector of length n
  - X is an m x p matrix of test (prediction) points (we want to know the function value at X)

Covariance Function

❖ Covariance Function:

- Loosely speaking, it describes the relationship between the *function values* of two points based on the *coordinate locations*
- In the earlier example, I used the *squared exponential covariance function:*

$$k(x, x^*) = \sigma^2 \exp\left(-\frac{(x - x^*)^2}{2l^2}\right)$$

- We can create a covariance matrix, *K*, between two sets of points, X and X *
- The (i^{th},j^{th}) term of K equals the covariance of the i^{th} point in X and the j^{th} point X *

Calculating Distributions

- We assume the basis functions are distributed as follows:

$$\begin{bmatrix} Y \\ Y_{tr} \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K(X,X) & K(X,X_{tr}) \\ K(X_{tr},X) & K(X_{tr},X_{tr}) \end{bmatrix}\right)$$

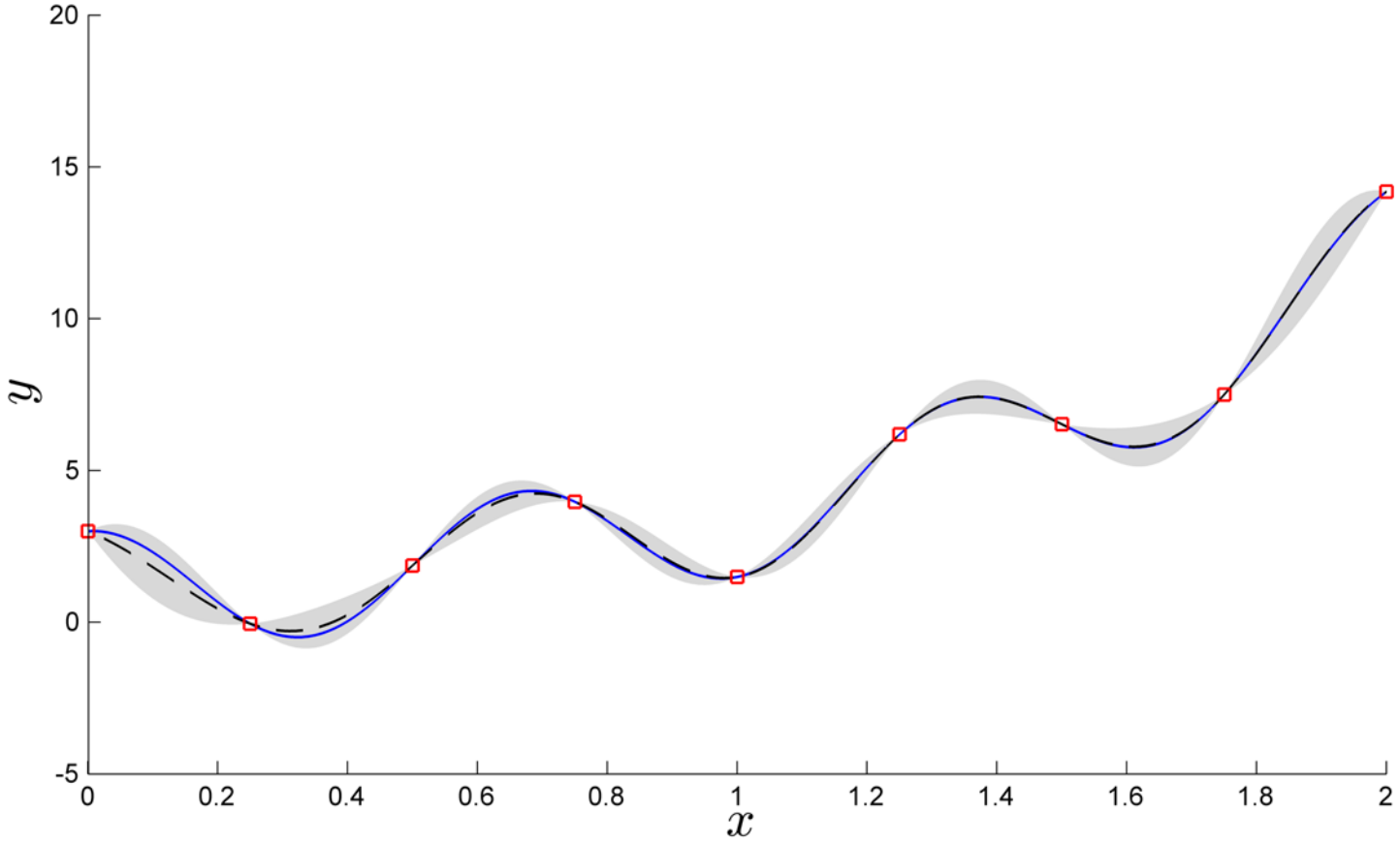
- Using Bayes' Theorem, we can solve for:

$$P(Y|X, X_{tr}, Y_{tr})$$

- The result:

$$Y|X, X_{tr}, Y_{tr} \sim \mathcal{N}\Big(Y_{tr}K(X_{tr},X_{tr})^{-1}K(X_{tr},X), \\ K(X,X) - K(X,X_{tr})K(X_{tr},X_{tr})^{-1}K(X_{tr},X)\Big)$$

Example Gaussian Process



Covariance Functions

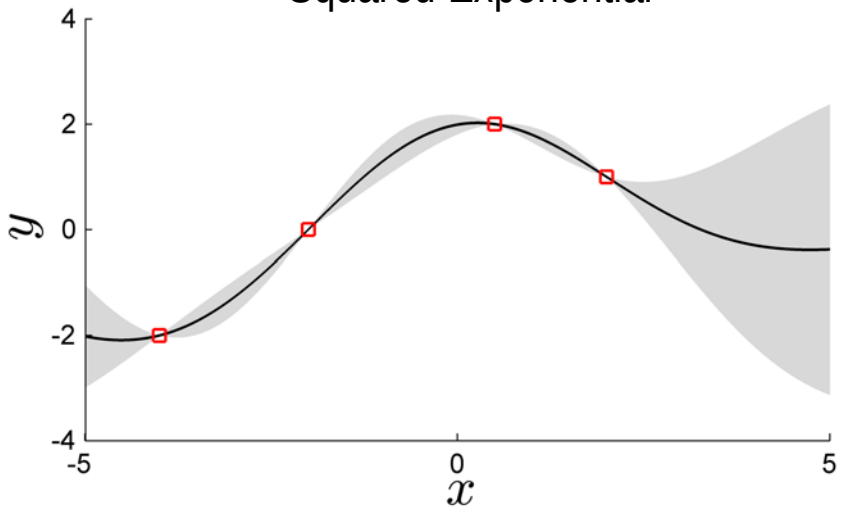
- Squared Exponential

$$k(x, x^*) = \sigma^2 \exp\left(-\frac{(x - x^*)^2}{2l^2}\right)$$

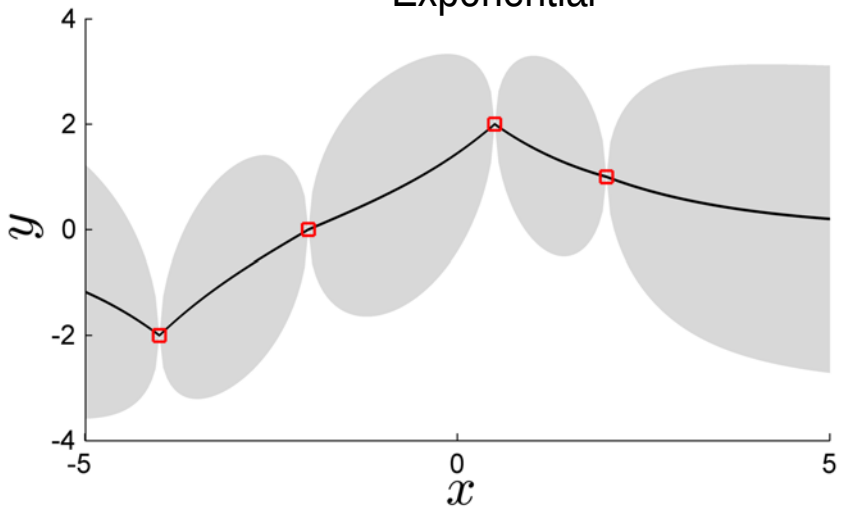
- Assumed Properties:
  - Stationary: function of only the distance between the two points (invariant to translations)
  - Infinitely Differentiable: implies the underlying function is continuous and infinitely differentiable

Other Covariance Functions

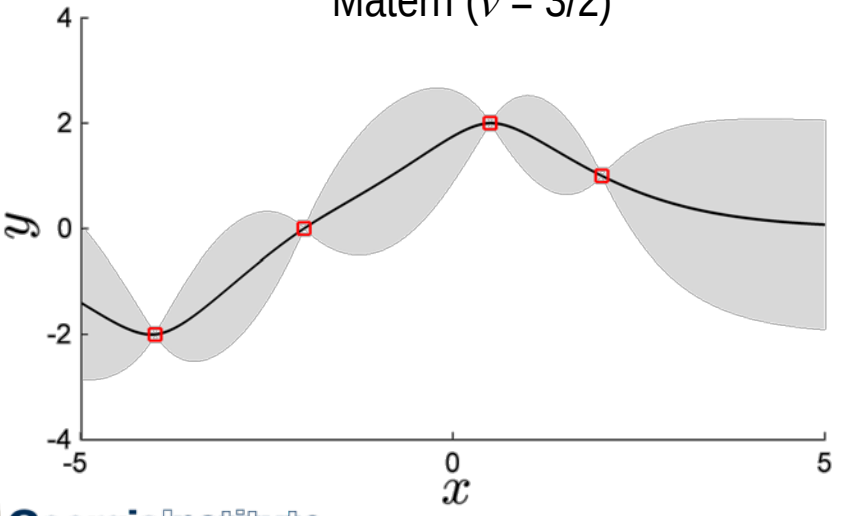
Squared Exponential



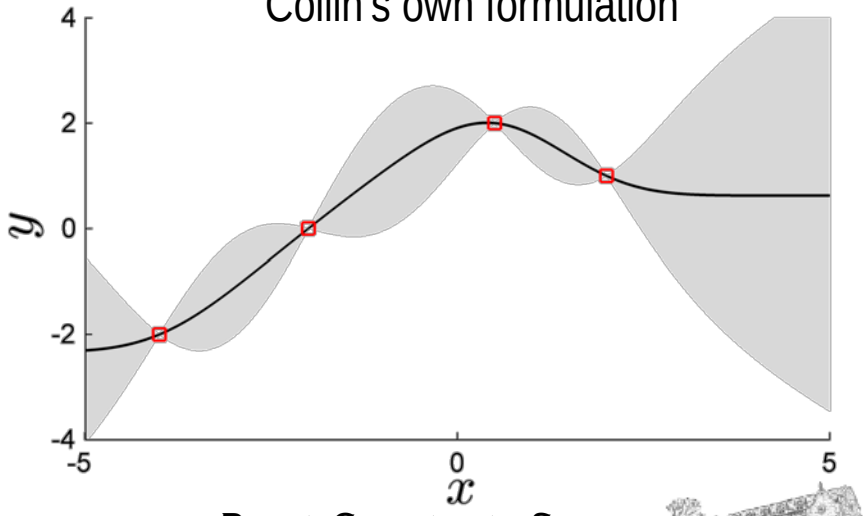
Exponential



Matern (ν = 3/2)



Collin's own formulation

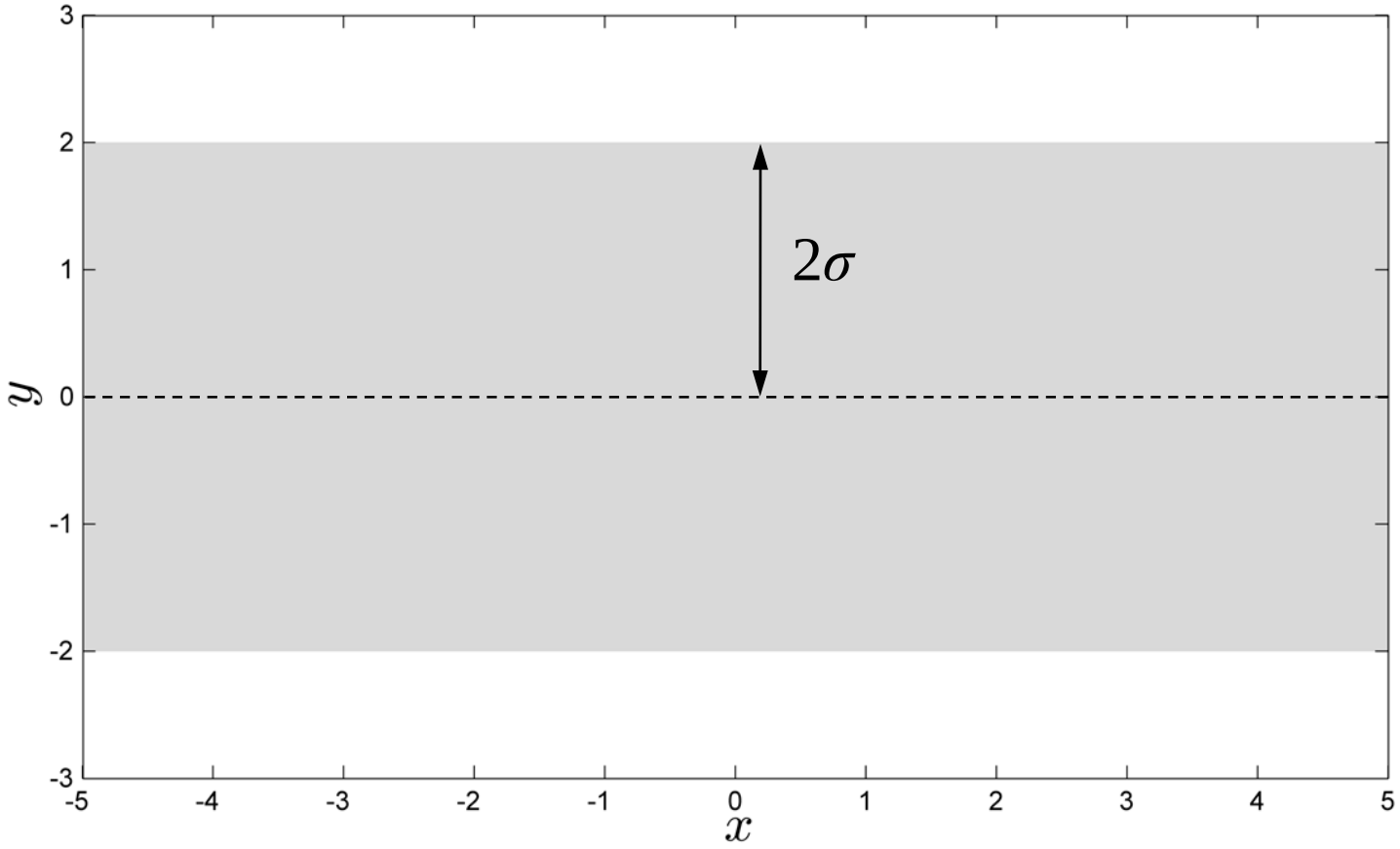


Hyperparameters

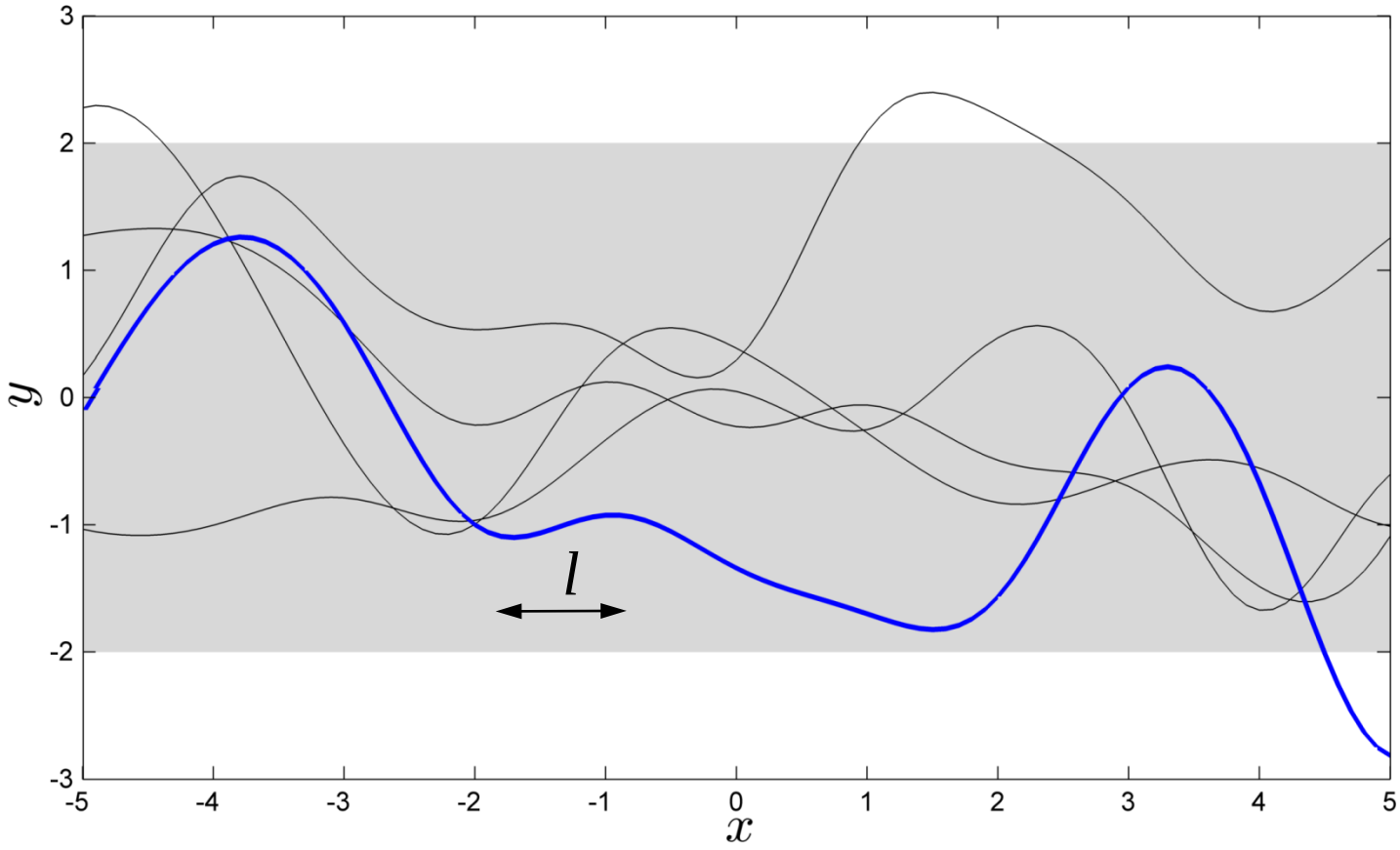
$$k(x, x^*) = \sigma^2 \exp\left(-\frac{(x - x^*)^2}{2l^2}\right)$$

- What are σ and l?
  - Hyperparameters: they affect the shape of the Gaussian process model

Hyperparameters



Hyperparameters



Hyperparameters

$$k(x, x^*) = \sigma^2 \exp\left(-\frac{(x - x^*)^2}{2l^2}\right)$$

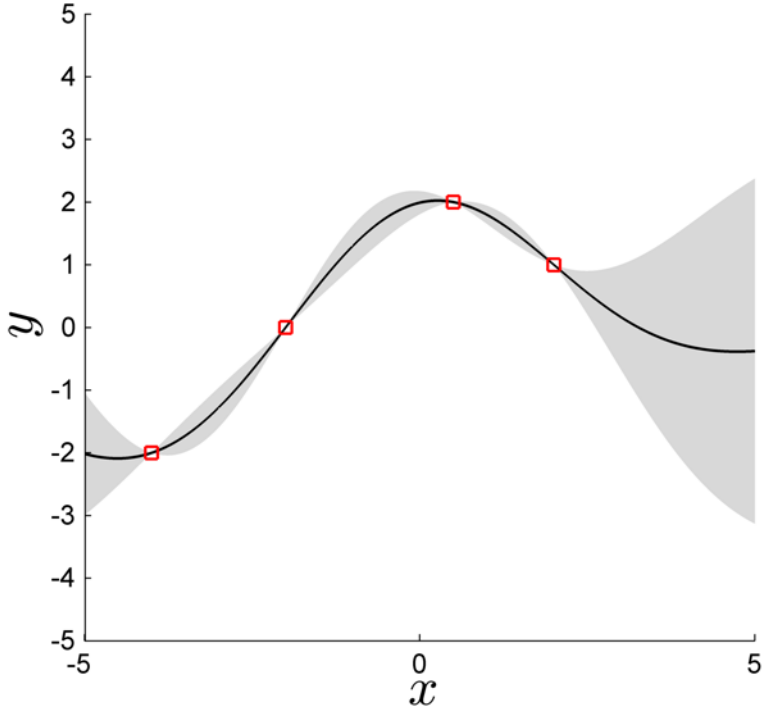
- What are σ and l?
  - Hyperparameters: they affect the shape of the Gaussian process model
- How do we determine their values?
  - Maximize ***marginal likelihood*** : $p(Y_{tr}|X_{tr}, \Theta)$
  - Most people minimize the negative log transform:

Hyperparameters

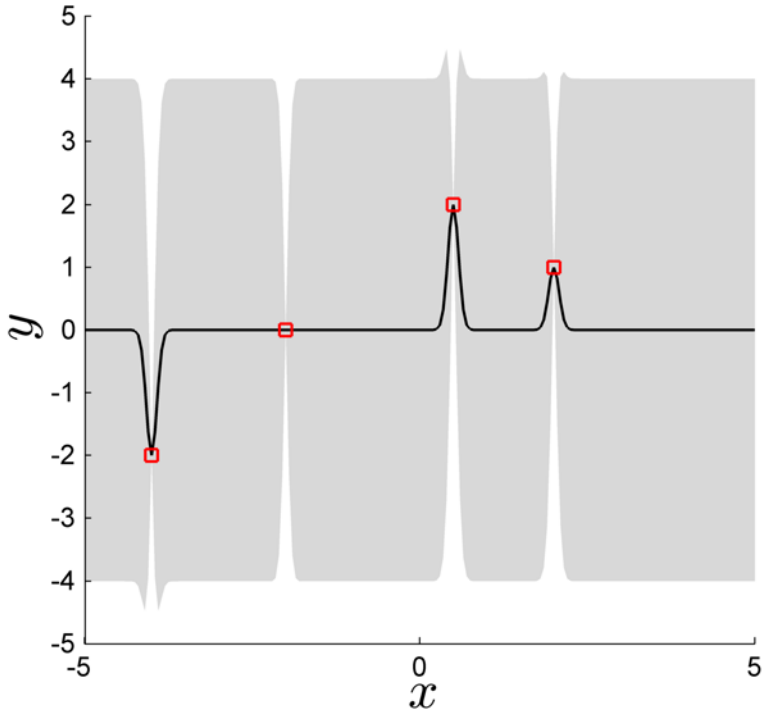
$$-\log p(Y_{tr}|X_{tr}, \Theta) = \frac{1}{2}\log(\det(K(X_{tr}, X_{tr}))) - \frac{1}{2}Y_{tr}K(X_{tr}, X_{tr})^{-1}Y_{tr}^T - \frac{n}{2}\log 2\pi$$

Hyperparameters

Good Hyperparameters



Bad Hyperparameters



What about the mean?

- If $\mu = 0$ is a bad assumption, there are other options:
  - Simple Kriging
    - Mean is zero
  - Ordinary Kriging
    - Mean is stationary but unknown
    - Maximum likelihood estimator is often used
  - Universal Kriging
    - Mean is assumed to be a polynomial
  - Many other methods exist…

Gaussian Processes in Optimization

- Efficient Global Optimization (EGO):
  - "Warm start:" DOE is performed on the design space to obtain training points
  - Gaussian process model is fit to the training data
  - The next sample point is chosen by maximizing ***expected improvement***
  - After each iteration, we refit the Gaussian process model
  - Branch-and-bound methods exist that guarantee finding the global maximum of expected improvement
  - Intuitively balances *exploration* and *exploitation*

Expected Improvement

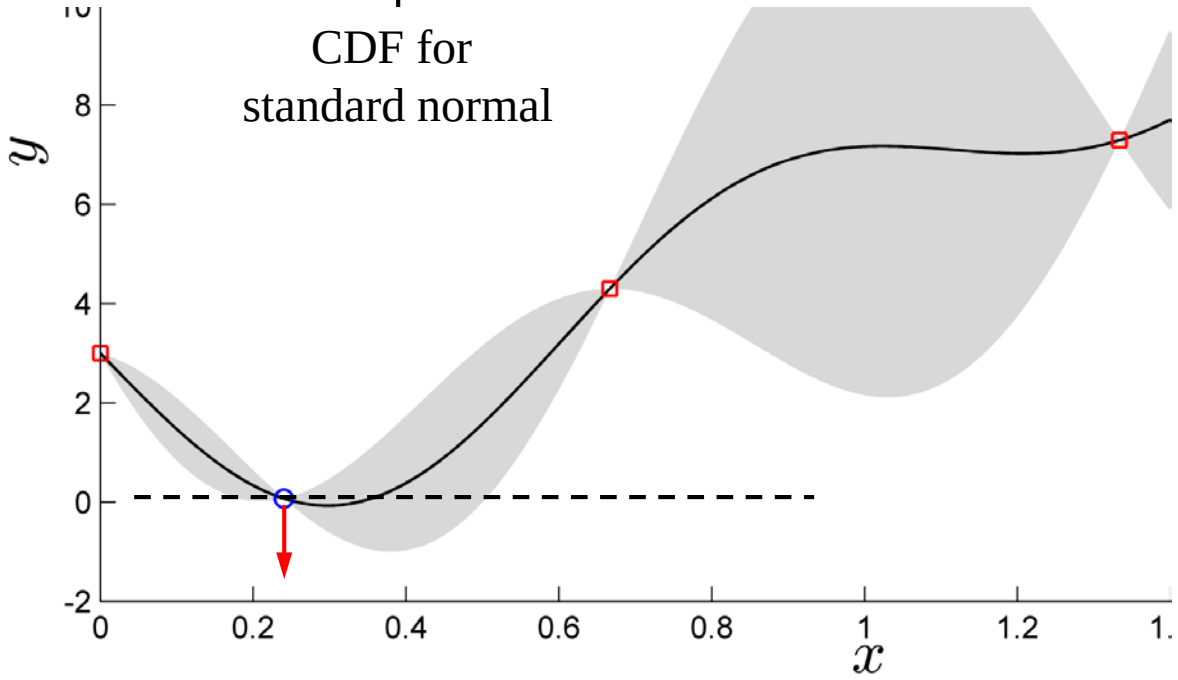
- Expected improvement:

PDF for standard normal

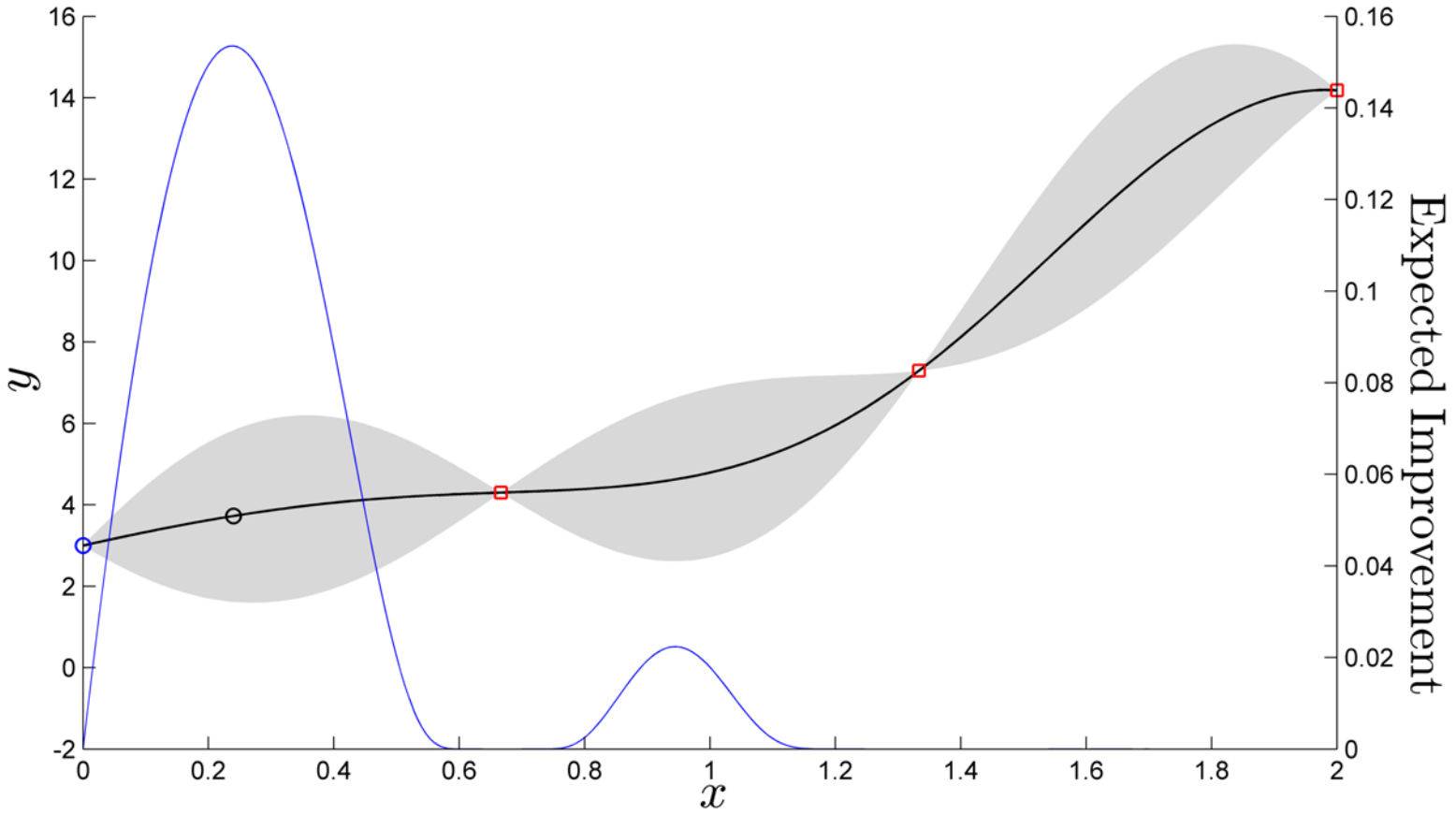
$$\mathrm{E}[I(x)] = \mathrm{E}[\max(f_{\min} - Y, 0)]$$

$$= (f_{\min} - \mu)\Phi\left(\frac{f_{\min} - \mu}{\sigma}\right) + \sigma\phi\left(\frac{f_{\min} - \mu}{\sigma}\right)$$

CDF for standard normal



EGO Example


16
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y
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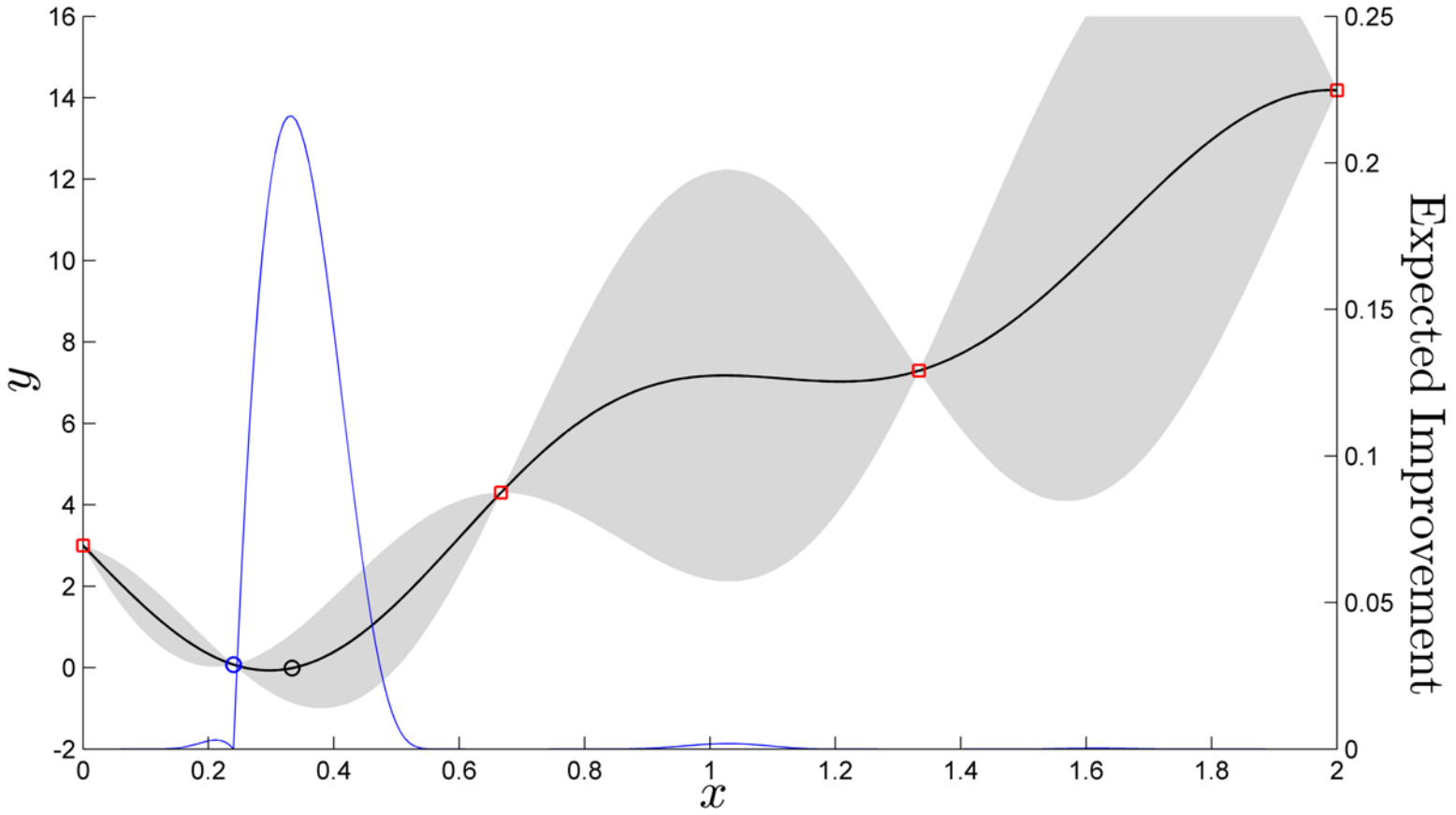
Expected Improvement

EGO Example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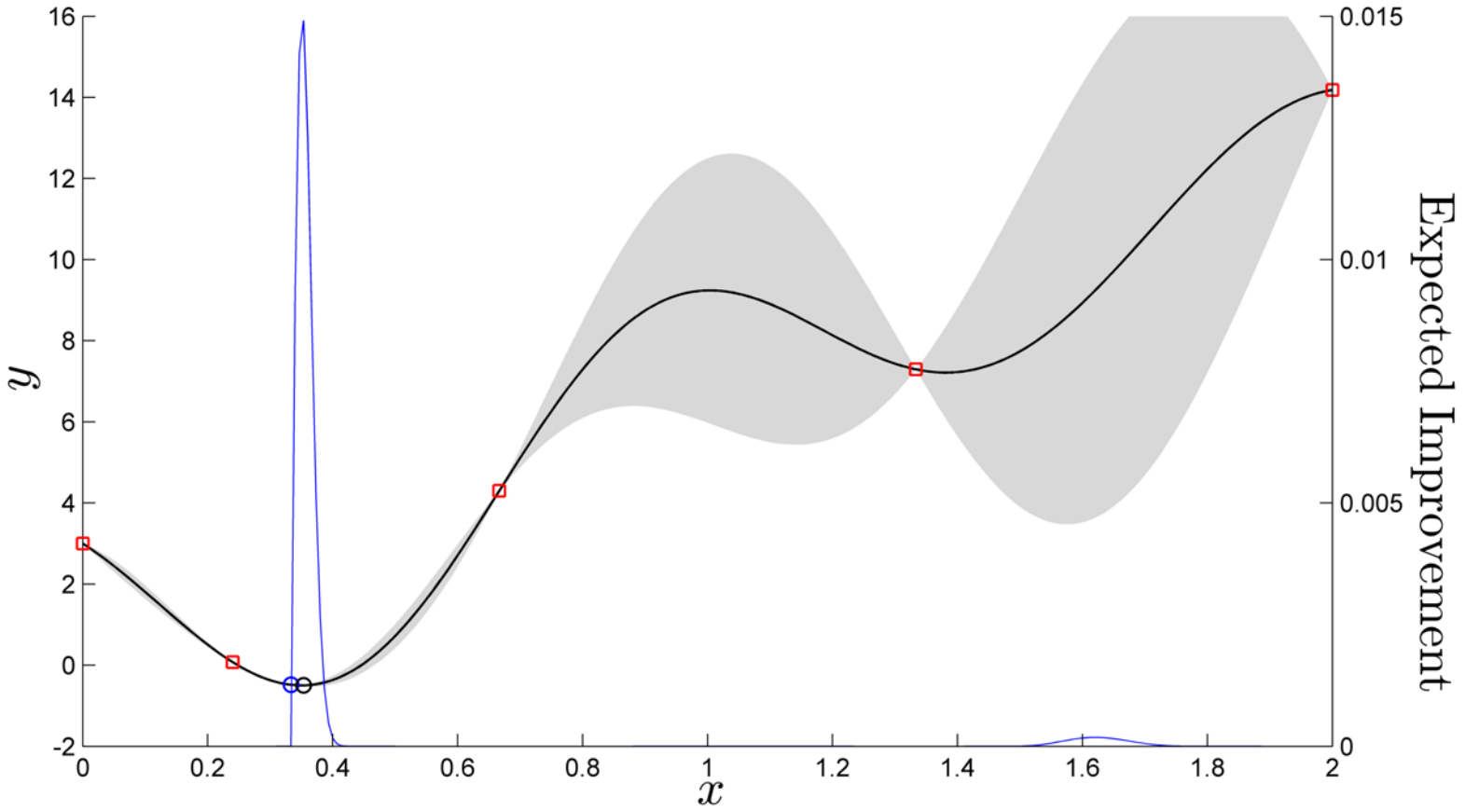
Expected Improvement

EGO Example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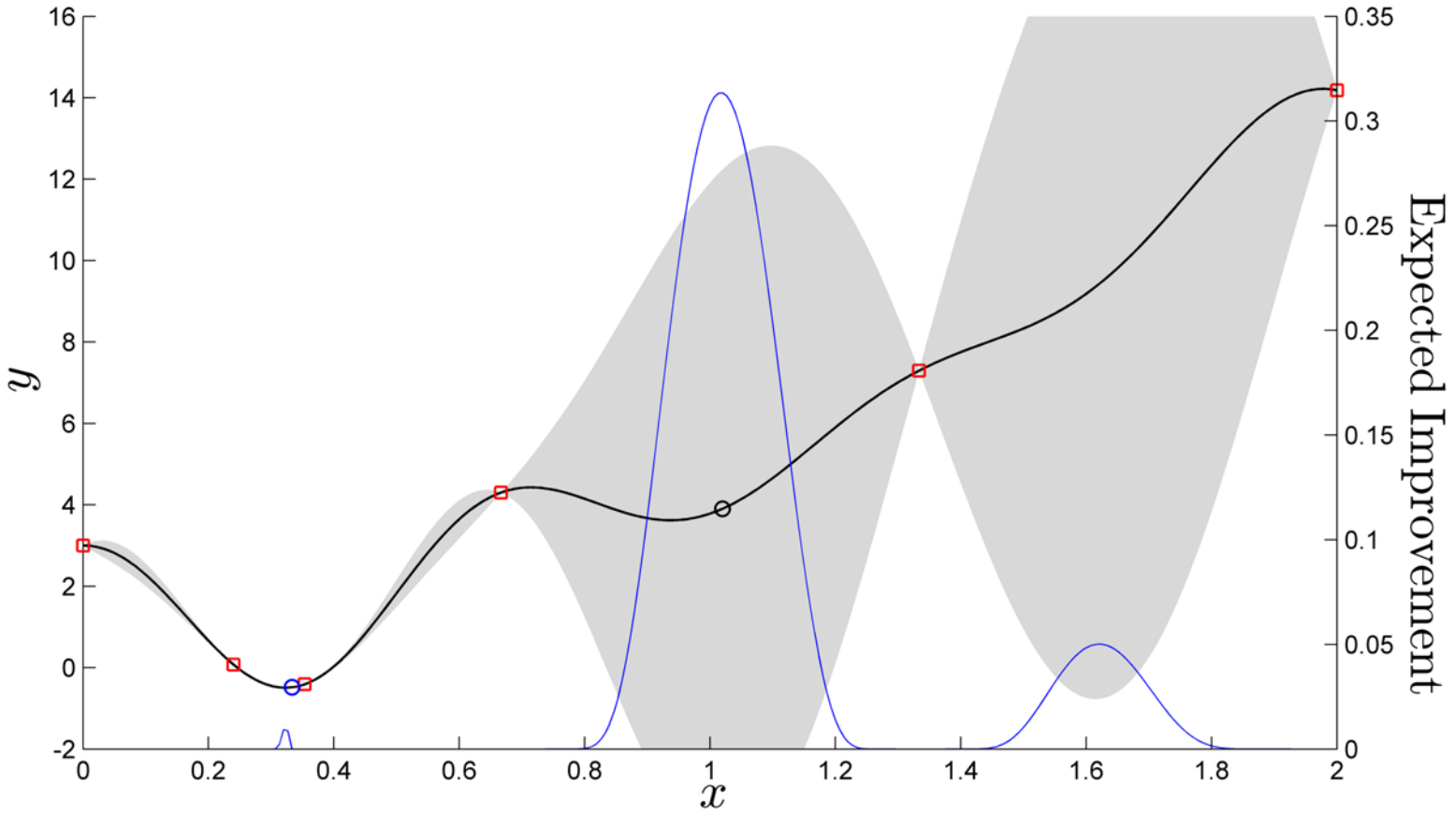
Expected Improvement

EGO Example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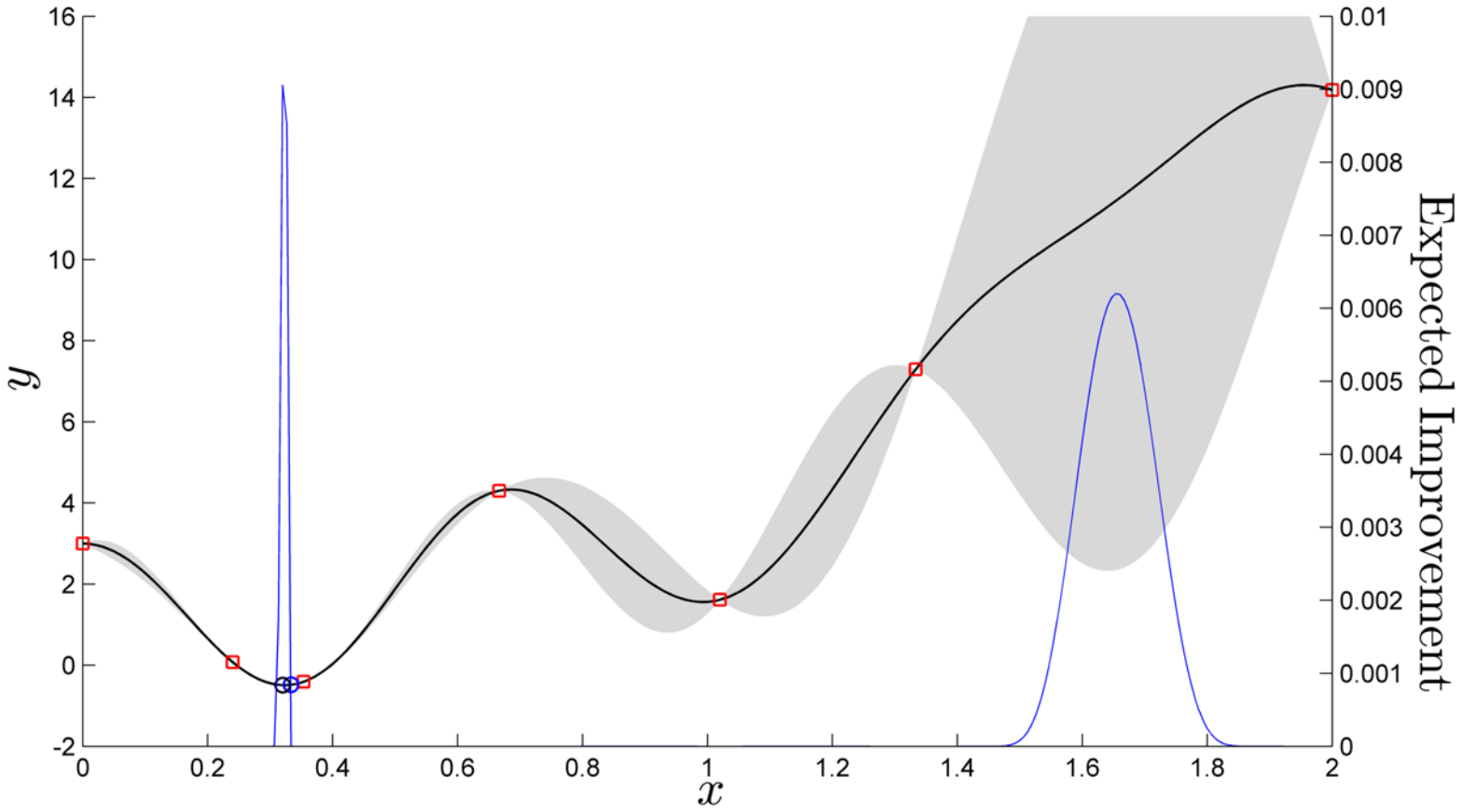
Expected Improvement

EGO Example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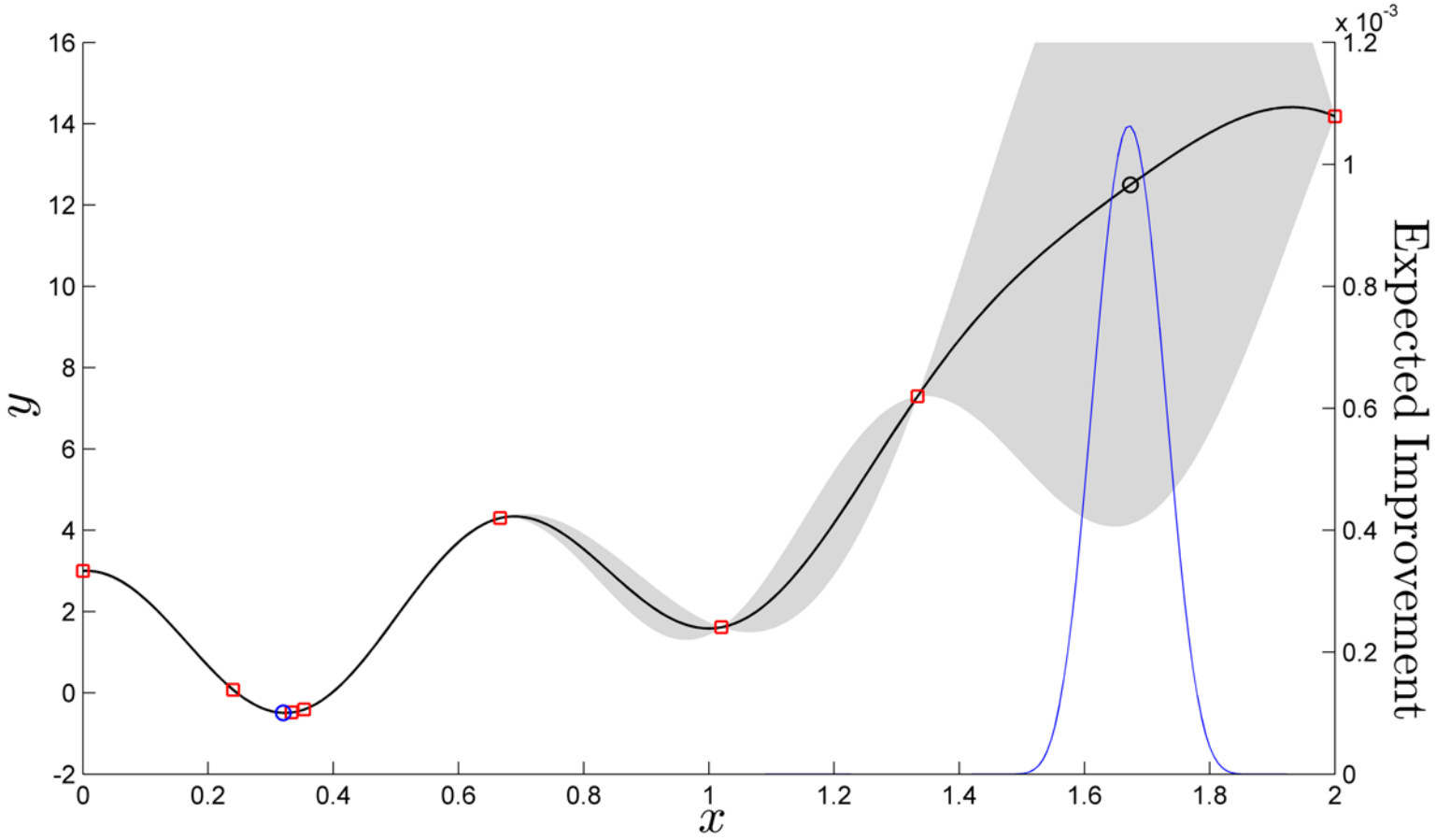
Expected Improvement

EGO Example


x 10^-3
1.2
1
0.8
0.6
0.4
0.2
0
Expected Improvement
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y
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1.2
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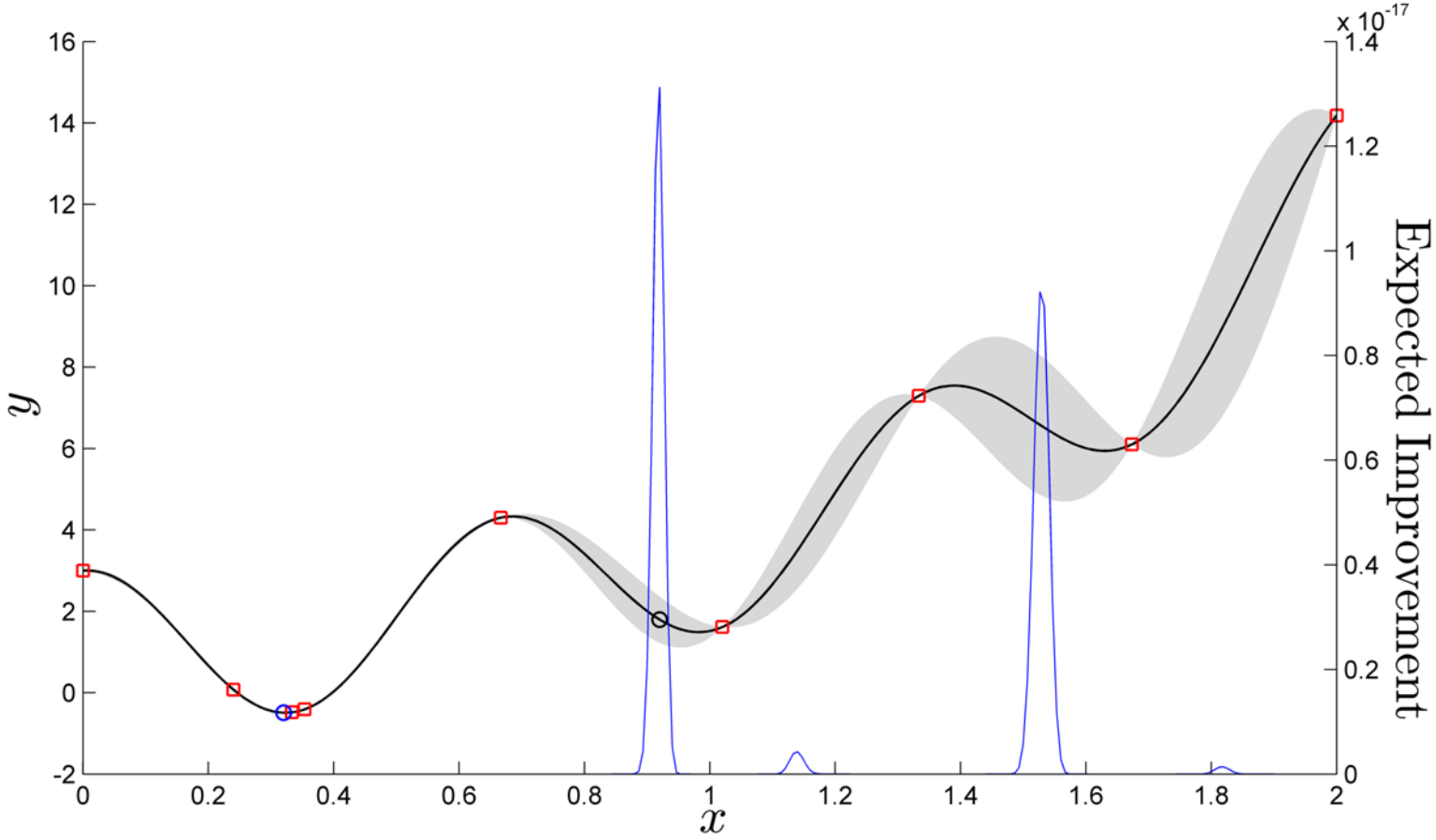
x

EGO Example


x 10^-17
Expected Improvement
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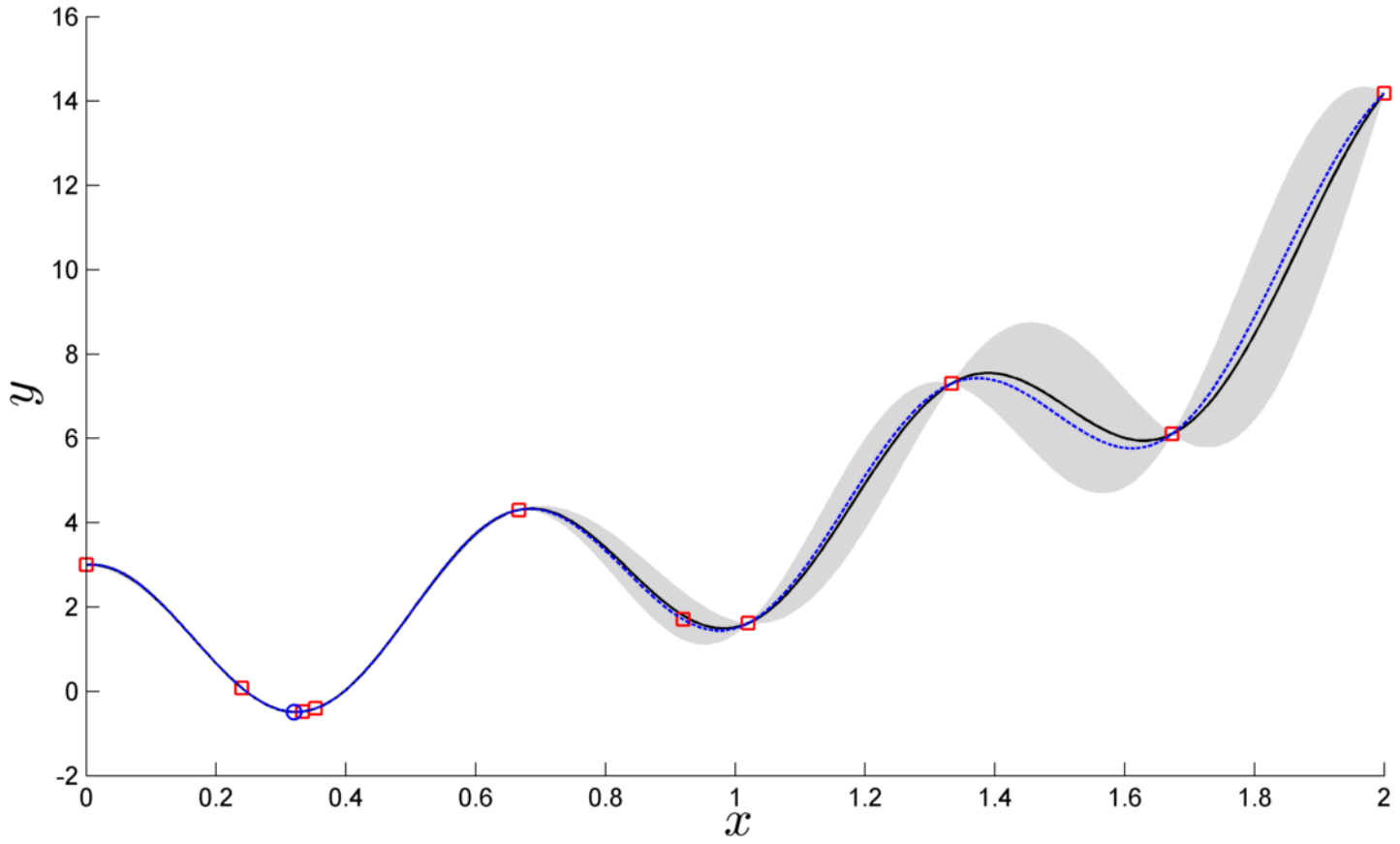
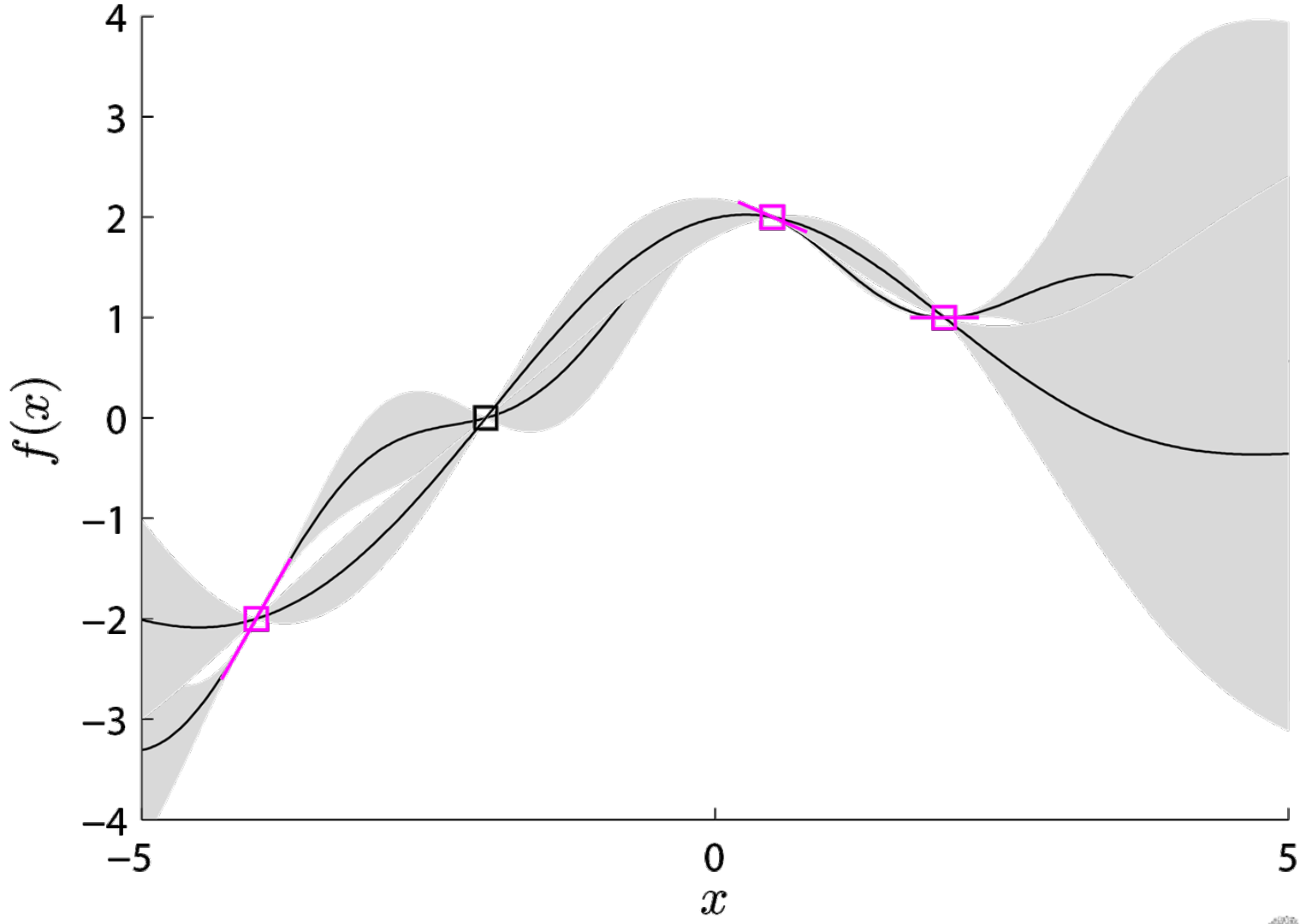
EGO Example



Other Features

- Gradient Information
  - Requires only a simple modification of the covariance function
  - Slovak et al “Derivative observations in Gaussian process models of dynamic systems” in *Conference on Neural Information Processing Systems* 2003

Gradient Information



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- Gradient Information
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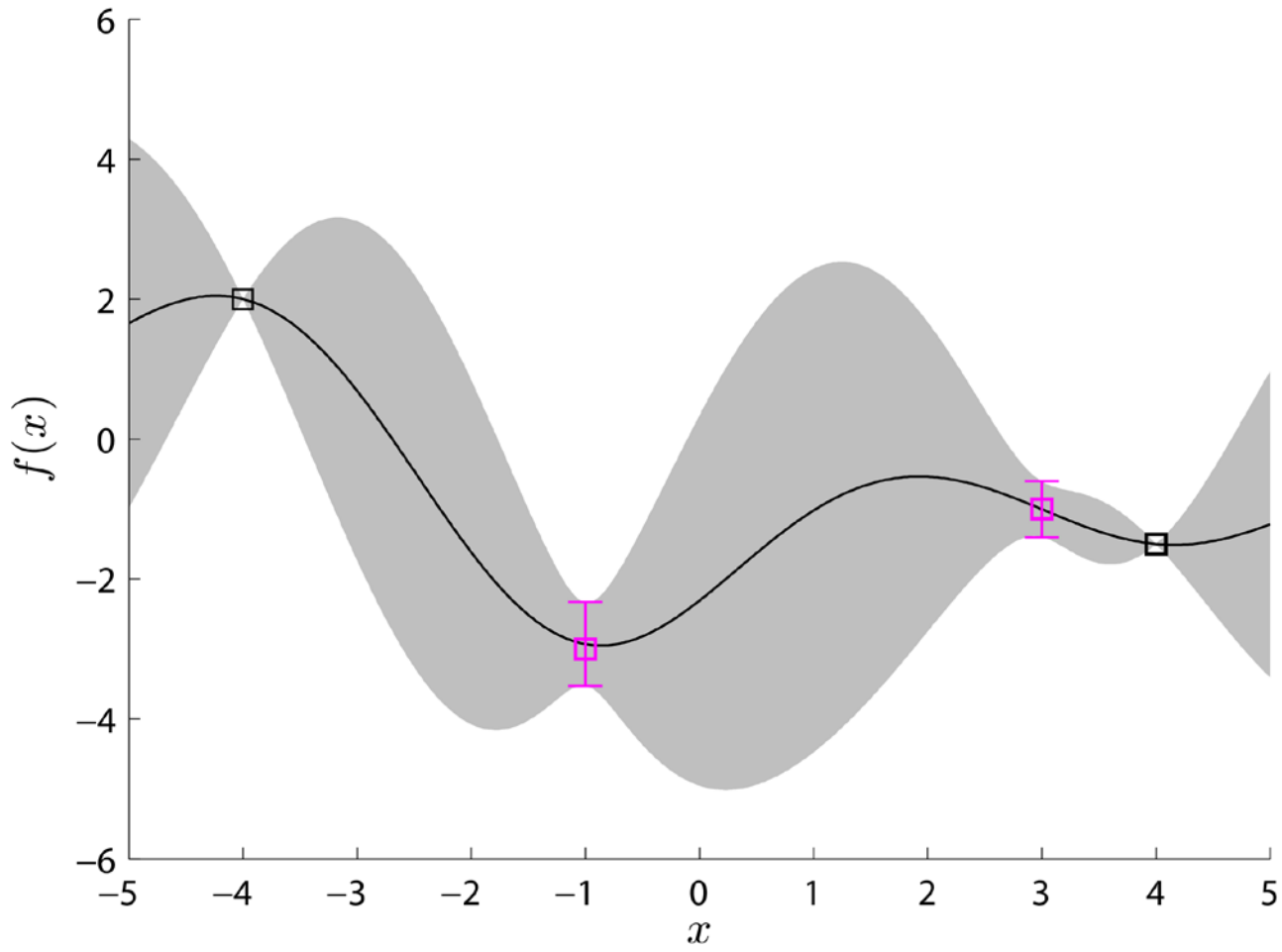
- Training Data with Noise
  - Allows for the inclusion of uncertainty

Gaussian Process with Noise



Other Features

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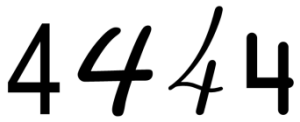
- Training Data with Noise
  - Allows for the inclusion of uncertainty
- Classification Problems
  - Map inputs into discrete outputs
  - Example: Text recognition software



Keep in mind…

- A model is only as good as the assumptions behind it
  - Be careful when choosing a covariance function
  - Stationary and differentiable may not be good assumptions for your model
- Gaussian process models are useful for applications other than surrogate modeling and optimization
  - Geostatistics
  - Robotics
  - Meteorology
  - Artificial Intelligence
  - Many more…