Lecture 10
Priors on Function Spaces: Gaussian Processes

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Objectives

- Express prior knowledge/beliefs about model outputs using Gaussian process (GP)
- Sample functions from the probability measure defined by GP
- Describe a GP with a finite number of variables: The Karhunen-Loeve expansion

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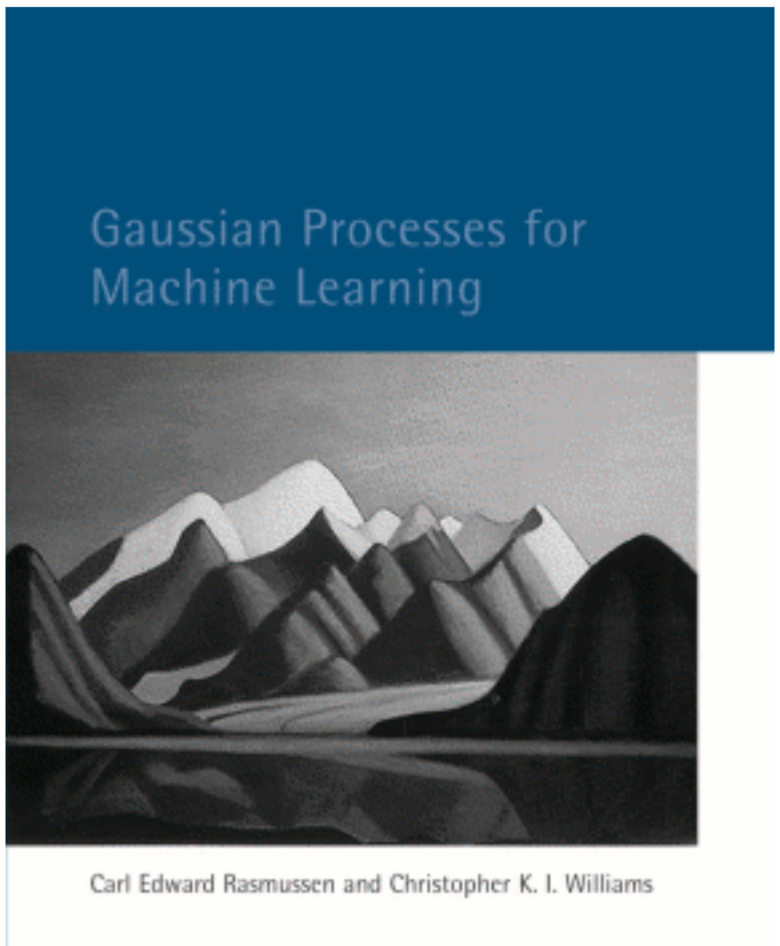
The Best Book on the Subject



Gaussian Processes for Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams
The MIT Press, 2006. ISBN 0-262-18253-X.

Free online at www.gaussianprocess.org.
With Matlab code.

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The Best Code on the Subject

GPy (in Python) from the group of N. Lawrence @ University of Sheffield
https://github.com/SheffieldML/GPy

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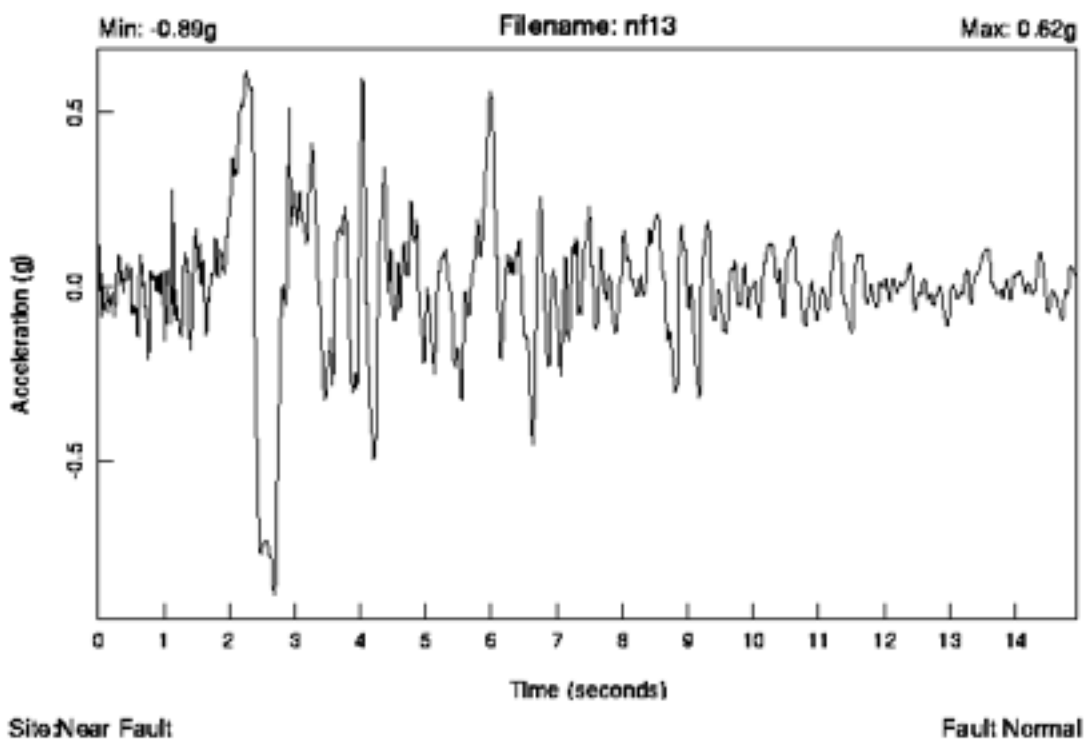
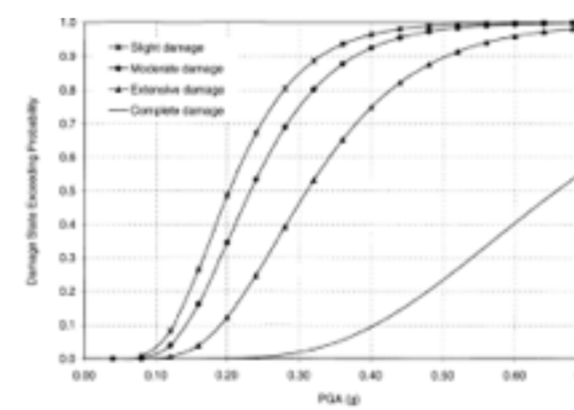
Why do we need probability measures on functions?



Uncertainty in external forcing

Simulation



Fragility Curve

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Why do we need probability measures on functions?

Portfolio Risk

Uncertainty in external forcing

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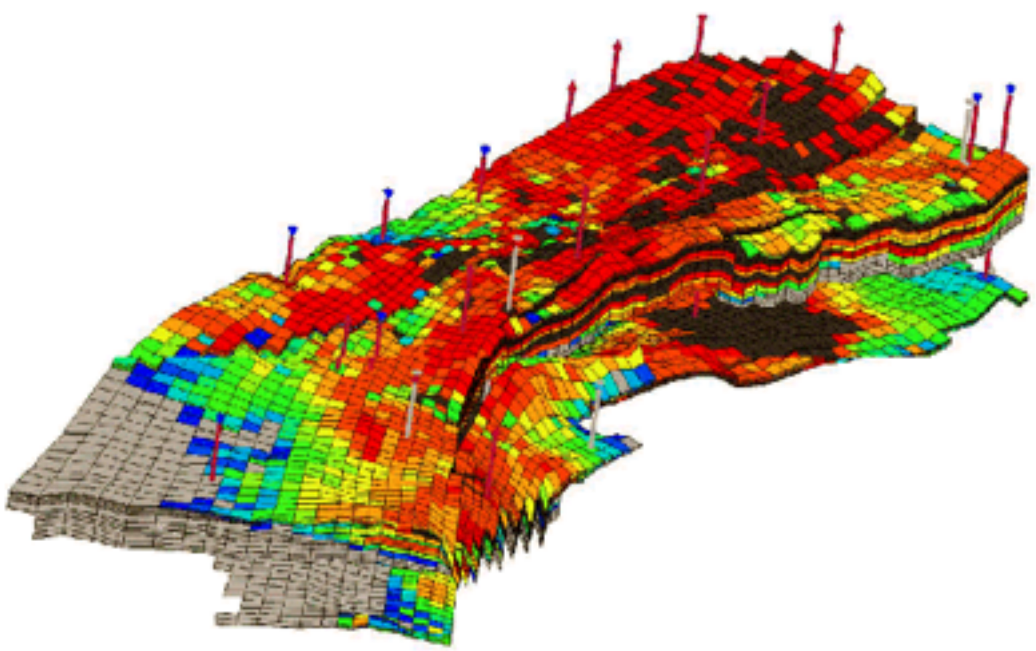
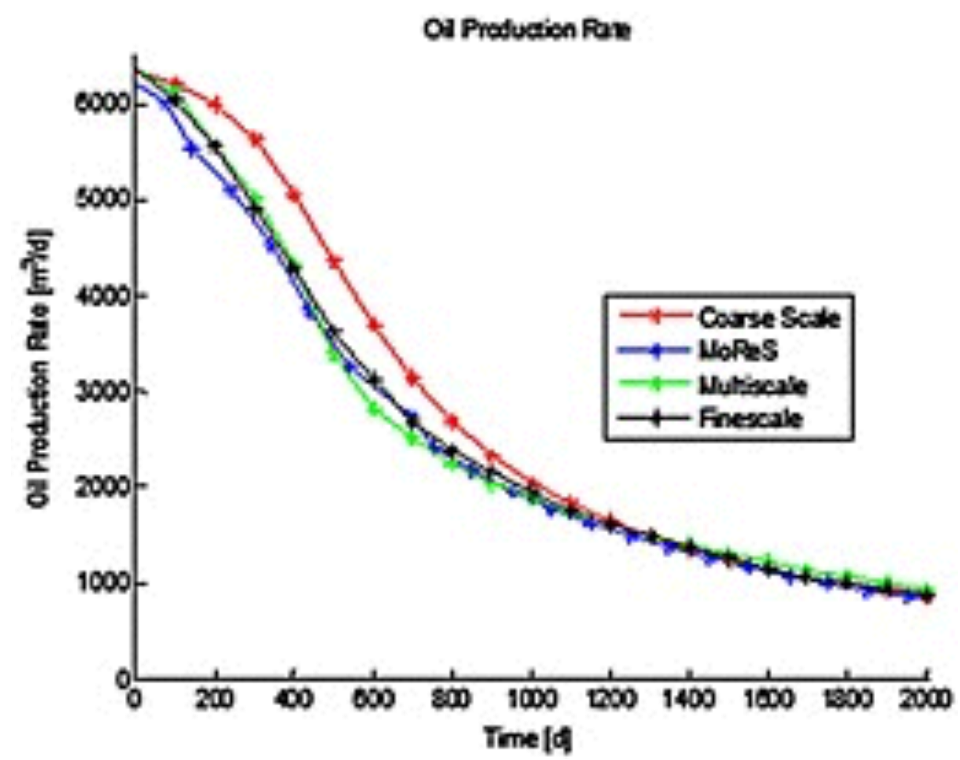
Why do we need probability measures on functions?



Simulation



Oil produced over time

Uncertainty in field parameters

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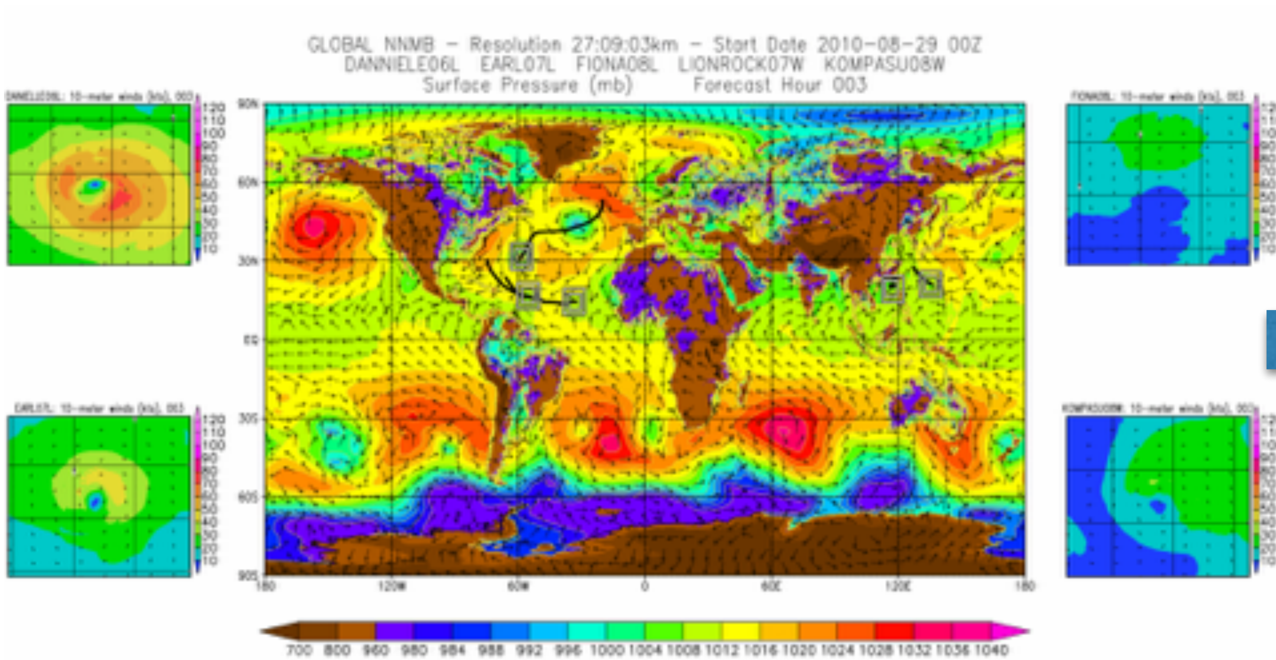
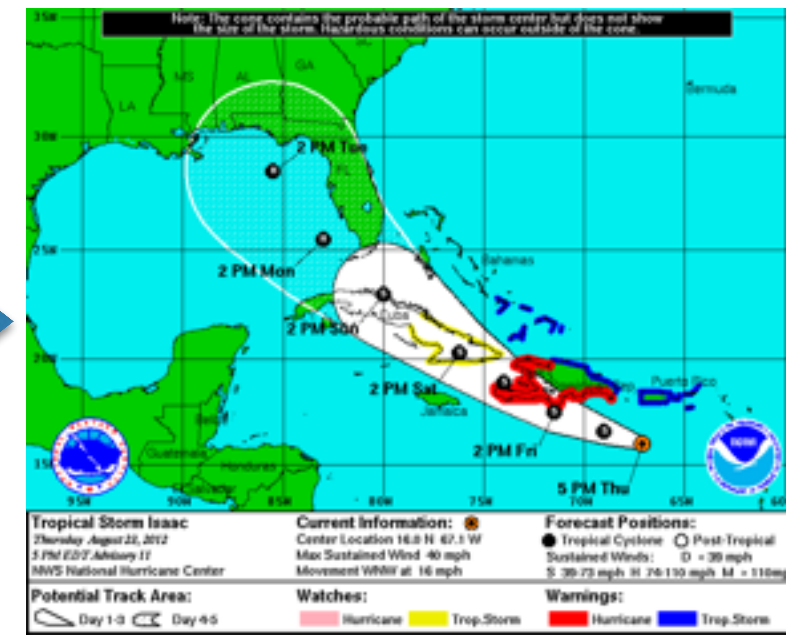
Why do we need probability measures on functions?





Hurricane path

Uncertainty in initial conditions

http://hwrf.aoml.noaa.gov/

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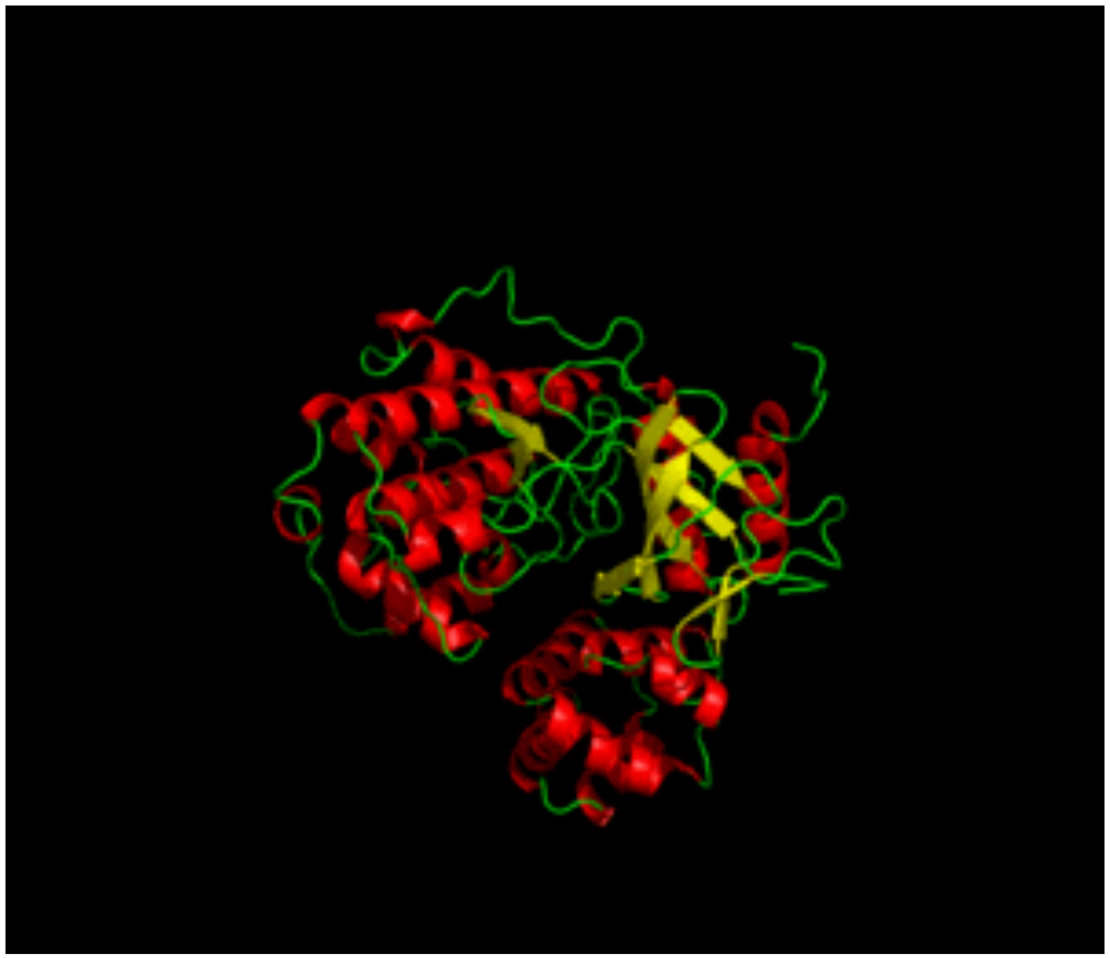
Why do we need probability measures on functions?



Simulation of the interaction of two biomolecules

Statistical mechanics:

$$p(\mathbf{q}) \propto \exp\left\{-\frac{V(\mathbf{q})}{k_B T}\right\}$$

Temperature

Positions of all atoms

Boltzmann constant

Empirical potential. We are not exactly sure about its form…

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For quantifying uncertainties in:

- External forcing
- Field parameters
- Initial conditions in PDEs
- Boundary conditions in PDEs
- Physical laws (e.g., constitutive relations, empirical force fields, etc.)
- …

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Probability measures on function spaces

- Simplest of all: Gaussian random field or Gaussian process.
- As usual, first we assign a prior, then we update with some data (next lecture).
- It turns out that you can also do regression with this (next lecture).

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Definition of a Gaussian process

~~*A Gaussian process is a collection of "random" variables, any finite number of which have a joint Gaussian distribution.*~~

Let's just explain in plain English what it is…

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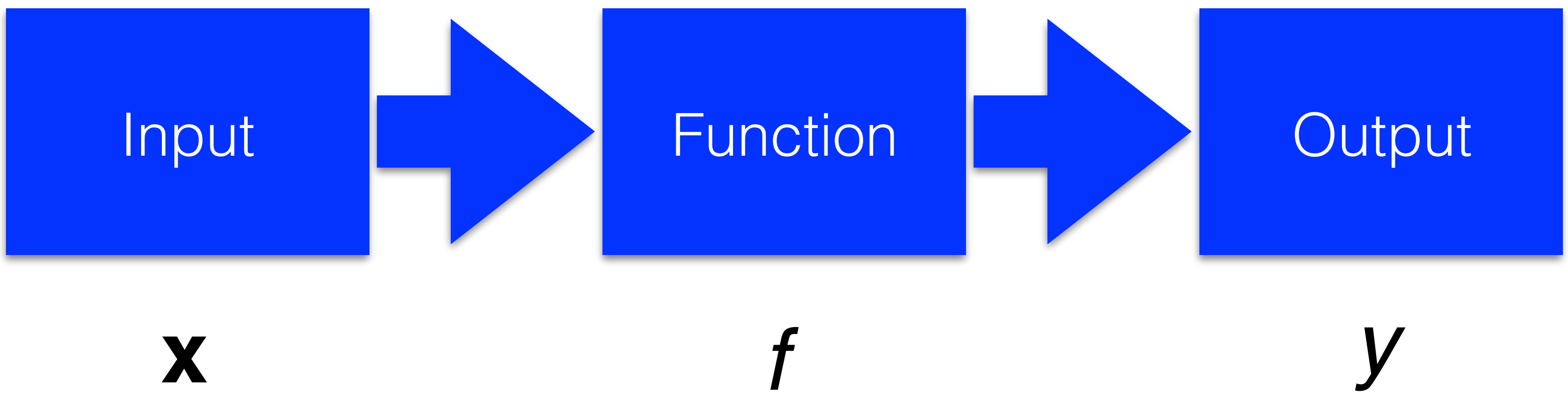
Definition of a Gaussian process



- Treat f as unknown
- Unknown = uncertain = “random”, i.e., described with probabilities
- Let us denote our beliefs about f as follows:

$$f(\cdot) \sim p(f(\cdot))$$

Definition of a Gaussian process

A Gaussian process needs two ingredients:

- a mean function
- a covariance function

It uses them to define a probability measure on the space of functions.

We write: $$f(\cdot) \sim p(f(\cdot)) = \mathrm{GP}\left(f(\cdot) \mid m(\cdot), k(\cdot,\cdot)\right)$$

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The mean function

- What do you think *f(x)* could be?

- Define the *mean function* by:

$$m(x) = \mathbb{E}[f(x)]$$

- It models your *expectation* about *f(x).*

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The covariance function

- How sure are you about this prediction?
- Consider the *variance*:

$$k(x,x) = \mathbb{E}\left[\left(f(x) - m(x)\right)^2\right]$$

- It models your *uncertainty* about *f(x).*

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The covariance function

- Now, consider two inputs *x* and *x'*. How close do you think the corresponding outputs are?

- Consider the *covariance function*:

$$k(\mathbf{x},\mathbf{x}') = \mathbb{E}\left[\left(f(\mathbf{x}) - m(\mathbf{x})\right)\left(f(\mathbf{x}') - m(\mathbf{x}')\right)\right]$$

- It models yours beliefs about the similarity of *f(x)* and *f(x').*

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To wrap it up

- We write:

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

- and we interpret:
  - $m(x)$: What do I think $f(x)$ could be?
  - $k(x, x)$: How sure am I about my expectation of $f(x)$?
  - $k(x, x')$: How similar are $f(x)$ and $f(x')$?

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The most common covariance function: Squared Exponential (SE)

- Also known as radial basis function (RBF).

$$k(\mathbf{x},\mathbf{x}') = v \exp\left\{-\frac{1}{2}\sum_{i=1}^{d}\frac{(x_i - x_i')^2}{\ell_i^2}\right\}.$$

Variance
models uncertainty
about *f(x)*

Length-scale
models similarity
of specific input dimensions

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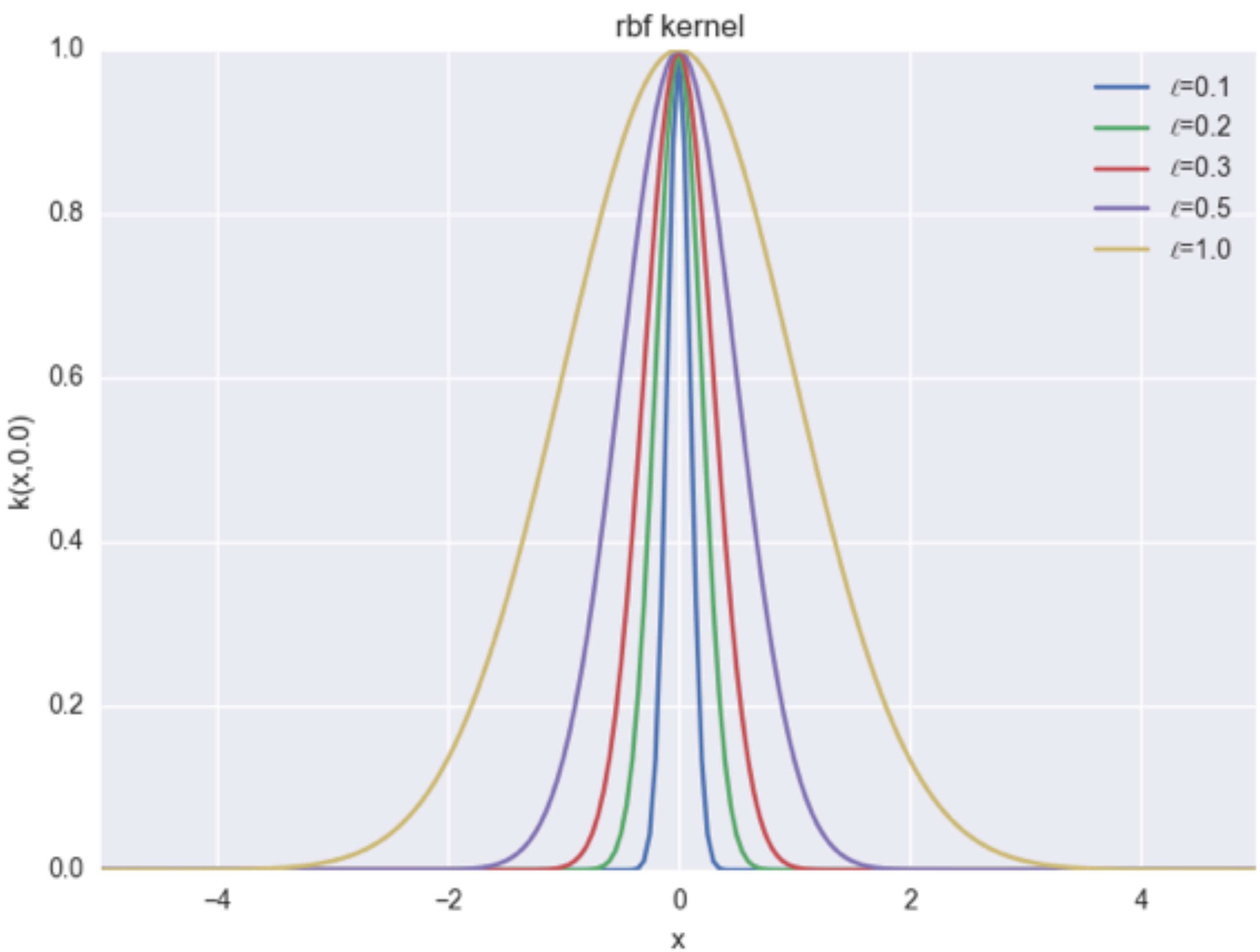
Example 1.1: Drawing covariance functions



You have 10 minutes

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The covariance matrix

- Consider an arbitrary selection of input points and their corresponding outputs:

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \rightarrow \mathbf{f} = \{f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)\}$$

- The *covariance matrix* is defined to be:

$$\mathbb{E}\left[(\mathbf{f}-\mathbf{m})(\mathbf{f}-\mathbf{m})^T\right] := \mathbf{K} := \begin{pmatrix} k(\mathbf{x}_1,\mathbf{x}_1) & \dots & k(\mathbf{x}_1,\mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n,\mathbf{x}_1) & \dots & k(\mathbf{x}_n,\mathbf{x}_n) \end{pmatrix}$$

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Restrictions on the covariance functions

- The covariance function has to be *positive definite*.
- That is, for any finite collection of inputs, the covariance matrix must be *positive definite*:

$$\mathbf{K} := \begin{pmatrix} k(\mathbf{x}_1,\mathbf{x}_1) & \dots & k(\mathbf{x}_1,\mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n,\mathbf{x}_1) & \dots & k(\mathbf{x}_n,\mathbf{x}_n) \end{pmatrix}$$

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Covariance function factory

- The sum of two covariance functions is a covariance function.

$$k(\mathbf{x},\mathbf{x}') = k_1(\mathbf{x},\mathbf{x}') + k_2(\mathbf{x},\mathbf{x}')$$

- What does this model?

- The belief that the response comes from two sources:

$$f(\mathbf{x}) = f_1(\mathbf{x}) + f_2(\mathbf{x})$$

$$f_i(\cdot) \sim \mathrm{GP}\left(f_i(\cdot) \mid m_i(\cdot), k_i(\cdot,\cdot)\right), i = 1,2$$

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Covariance function factory

- The product of two covariance functions is a covariance function.

$$k(\mathbf{x},\mathbf{x}') = k_1(\mathbf{x},\mathbf{x}')k_2(\mathbf{x},\mathbf{x}')$$

- What does this model?

- The belief that the response comes from two sources:

$$f(\mathbf{x}) = f_1(\mathbf{x})f_2(\mathbf{x})$$

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The covariance matrix

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Example 2: The covariance matrix and some properties of covariance functions

You have 10 minutes

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Sampling a Gaussian process

- A Gaussian process defines a probability measure over a function space:

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

- How can we sample functions from it?

- Sample *f* at a finite, albeit large, set of inputs.

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Sampling a Gaussian process

- Take a *finite* number of inputs:

$$\mathbf{x}_{1:n} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \rightarrow \mathbf{f} = \{f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)\}$$

- and consider the model output on them:

$$\mathbf{f} = \{f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)\}$$

- We *believe* that they are distributed according to:

$$\mathbf{f} \sim \mathcal{N}\left(\mathbf{f} \mid \mathbf{m}, \mathbf{K}\right)$$

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Sampling a Gaussian process

- Ok, so we need to be able to sample from this:

$$\mathbf{f} \sim \mathcal{N}\left(\mathbf{f} \mid \mathbf{m}, \mathbf{K}\right)$$

- with

$$\mathbf{m} = \begin{pmatrix} m(\mathbf{x}_1) \\ \vdots \\ m(\mathbf{x}_n) \end{pmatrix}, \mathbf{K} := \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \dots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \dots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix}.$$

Sampling a Gaussian process

- To sample from:

$$\mathbf{f} \sim \mathcal{N}\left(\mathbf{f} \mid \mathbf{m}, \mathbf{K}\right)$$

- Take the lower Cholesky decomposition **L** of **K**:

$$\mathbf{K} = \mathbf{L}\mathbf{L}^{\mathrm{T}}$$

- Sample a standard normal:

$$\mathbf{z} \sim \mathcal{N}\left(\mathbf{z} \mid \mathbf{0}_n, \mathbf{I}_n\right)$$

- and set:

$$\mathbf{f} = \mathbf{m} + \mathbf{L}\mathbf{z}$$

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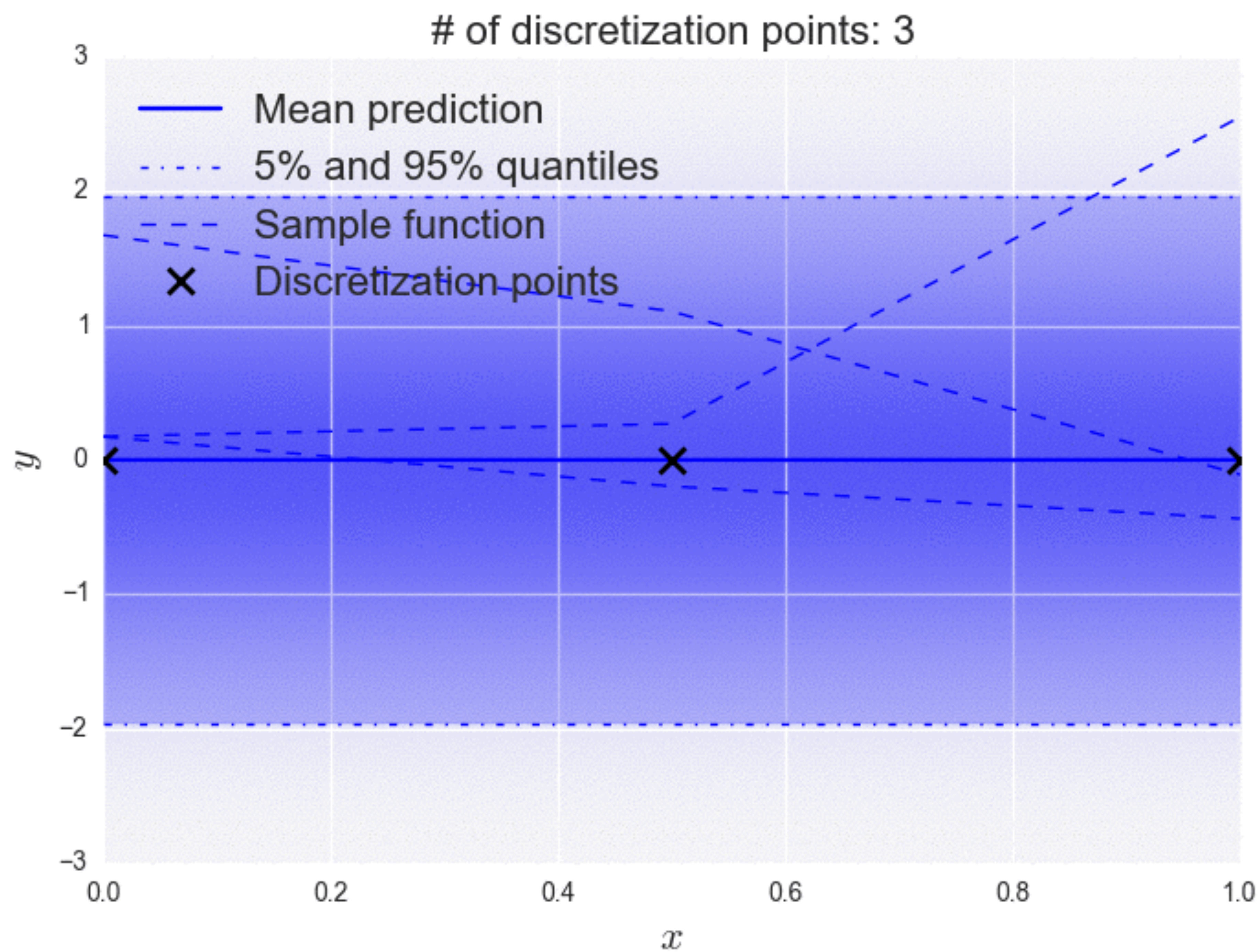
Sampling from a Gaussian



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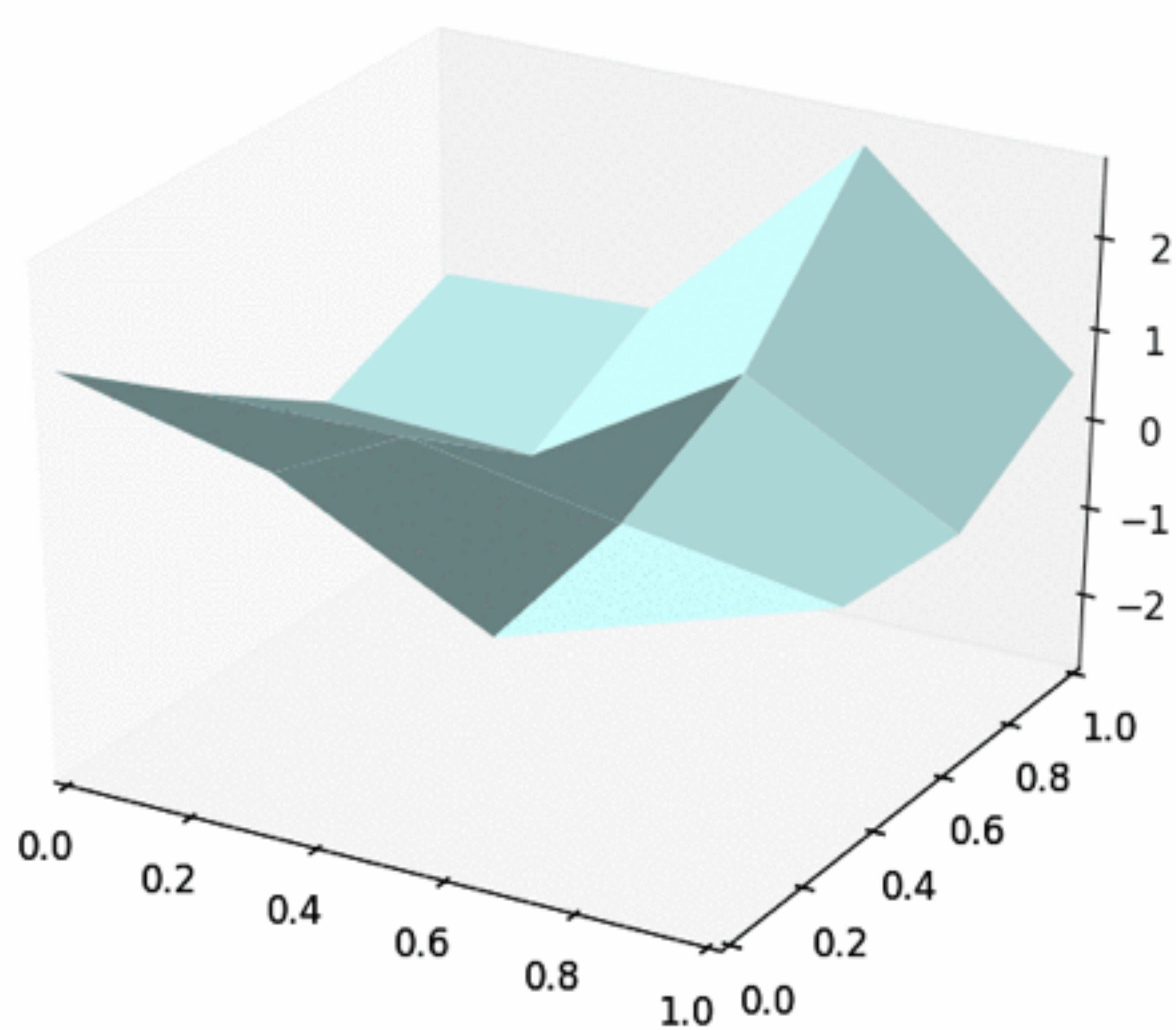
Sampling from a Gaussian process



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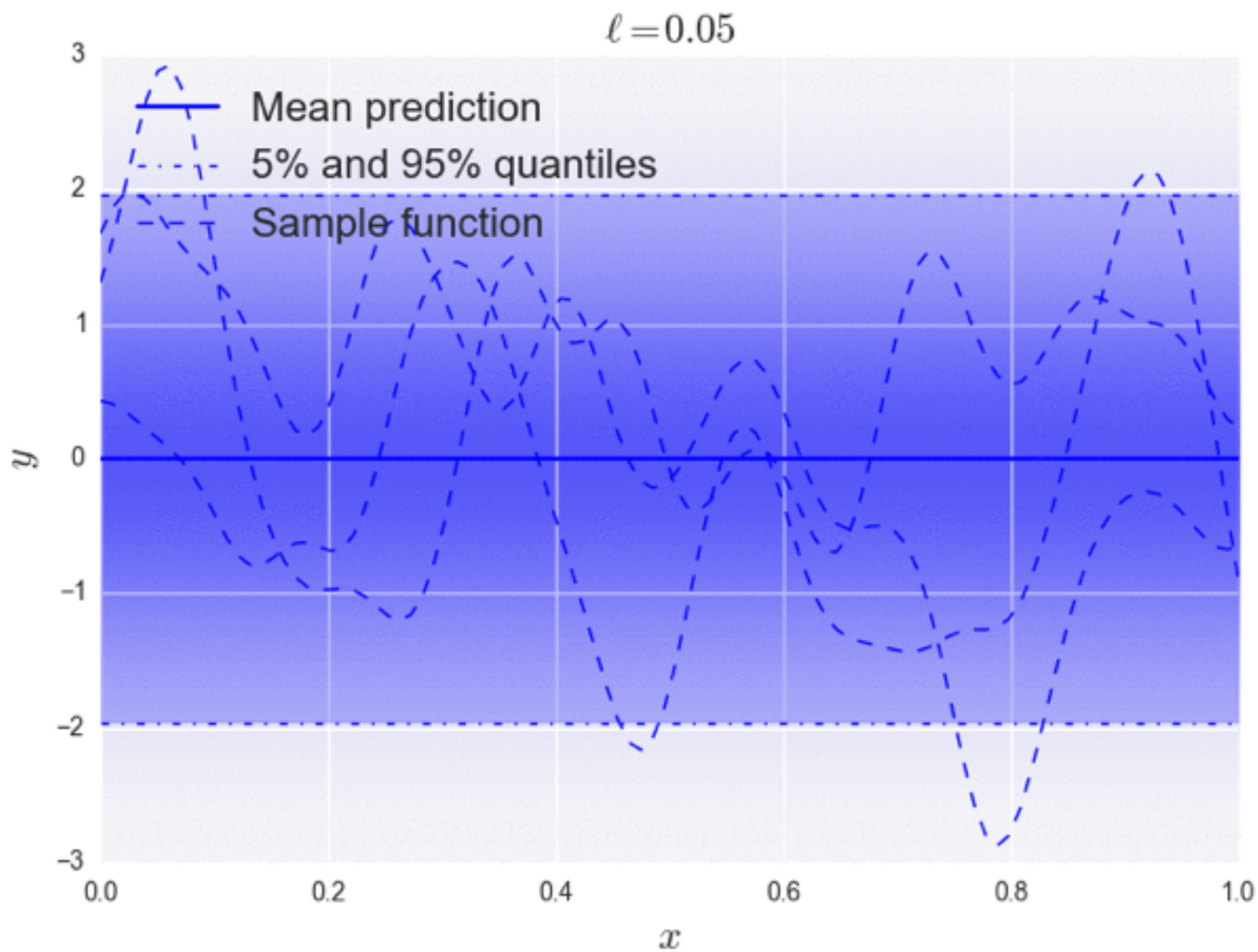
Changing the length scale



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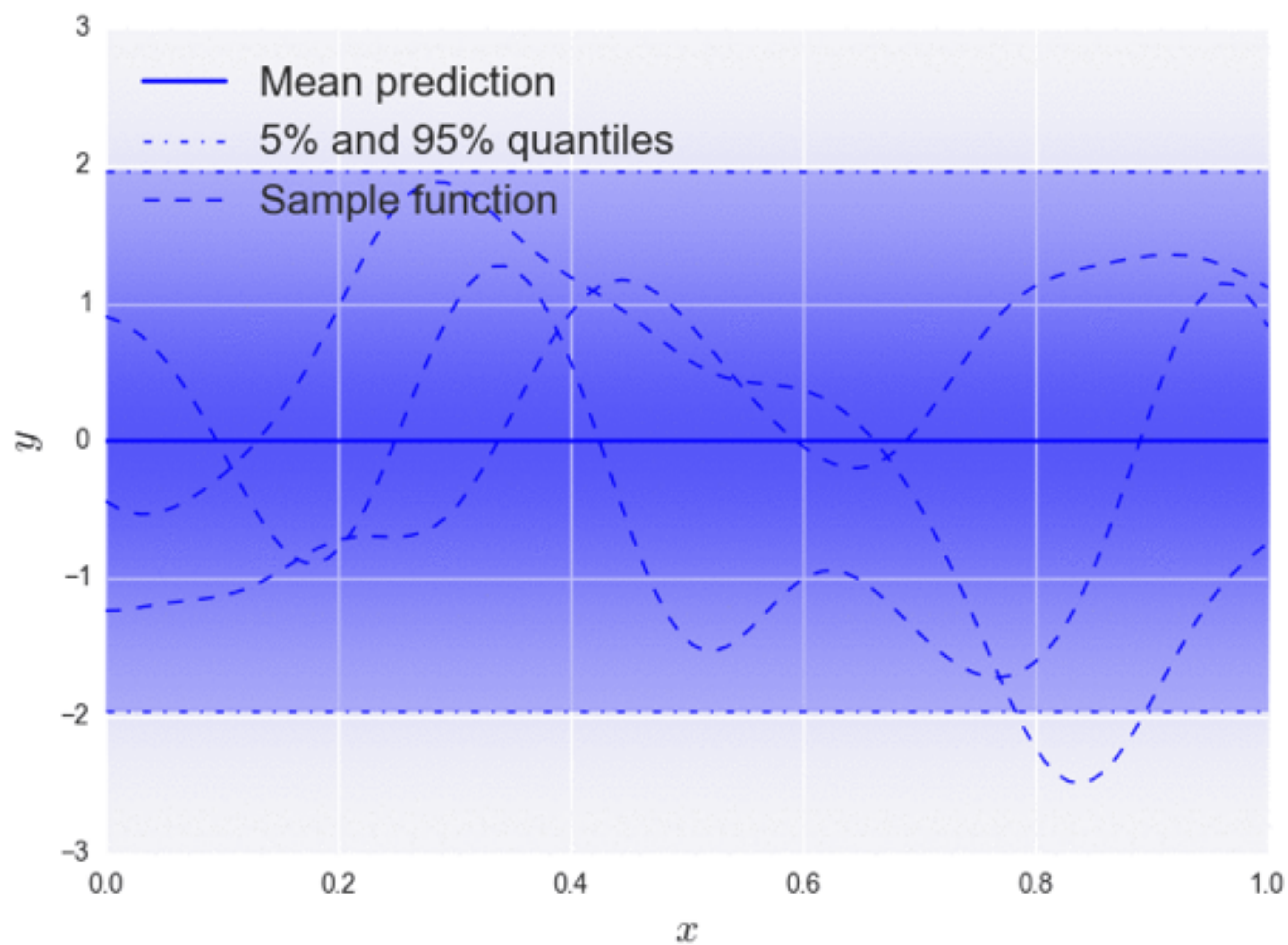
The samples are as smooth as the covariance

Infinitely smooth SE covariance



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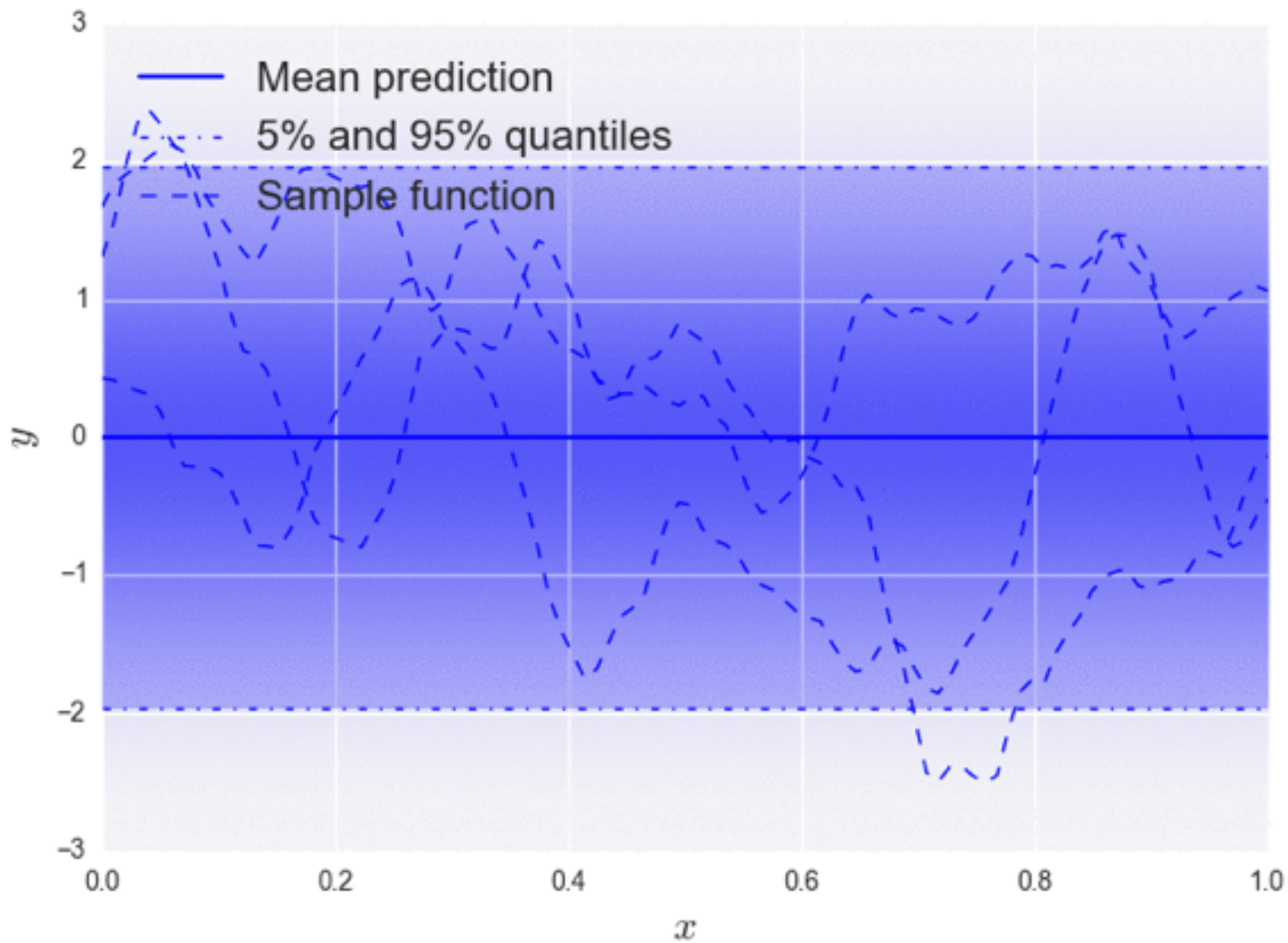
The samples are as smooth as the covariance

Matern 2-3, 2 times differentiable



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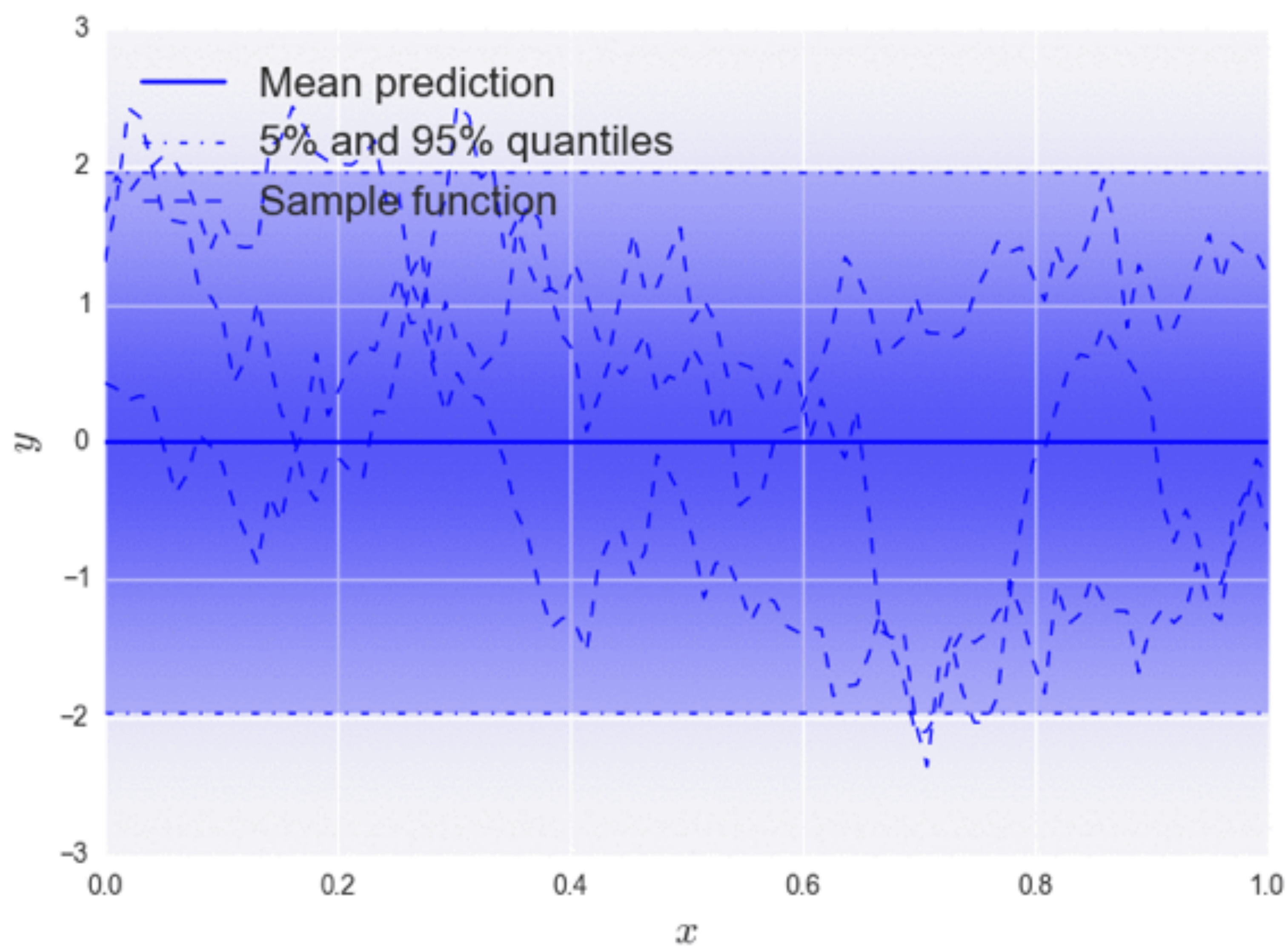
The samples are as smooth as the covariance

Exponential, continuous, nowhere differentiable



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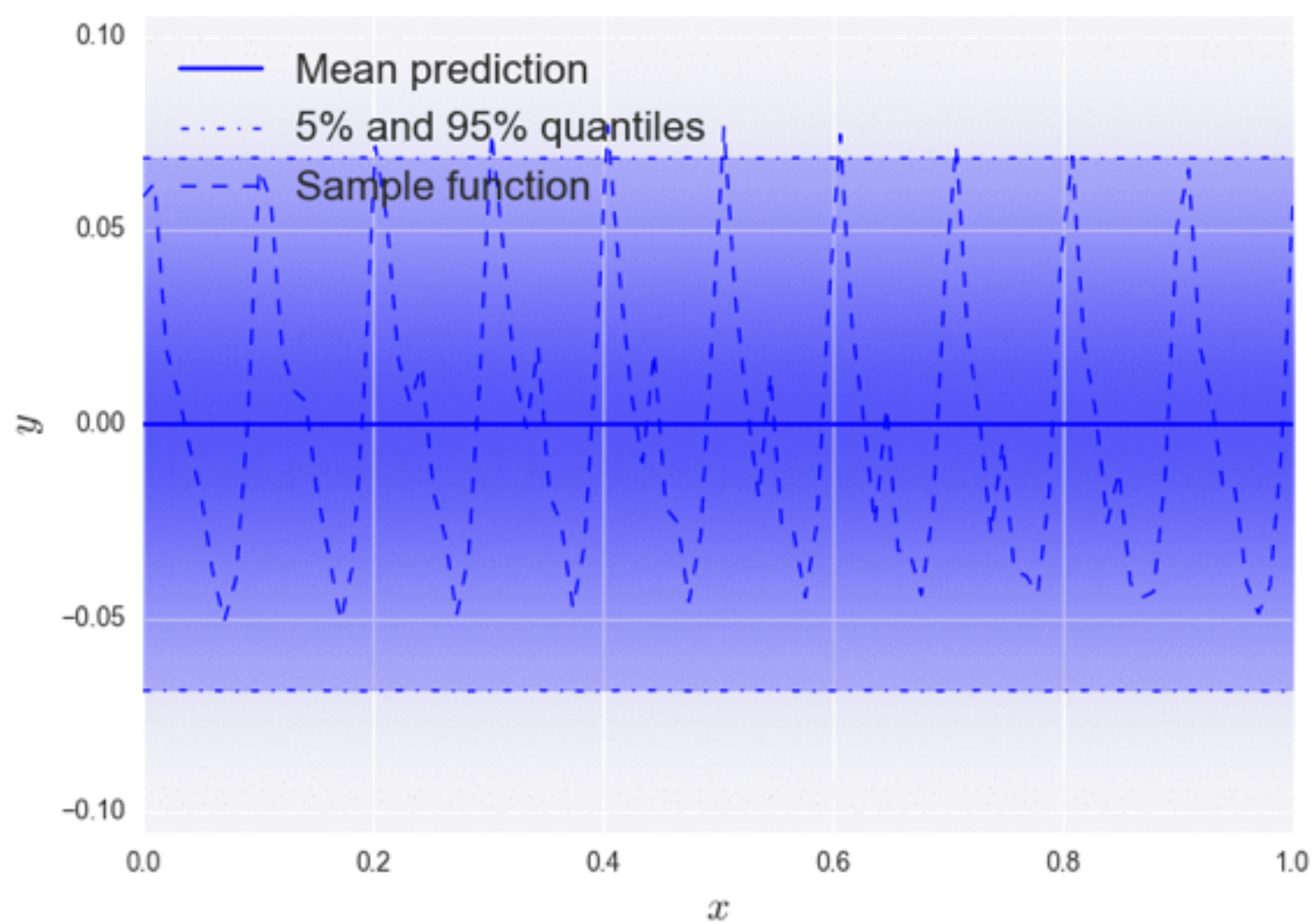
Invariances may be built-into covariance functions

Periodic Exponential, period = 0.1



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Example 3: Drawing Samples from a Gaussian Process

You have until the end of class

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