M5MS10
Machine Learning

Spring 2018

Lecture 6

Dr Ben Calderhead

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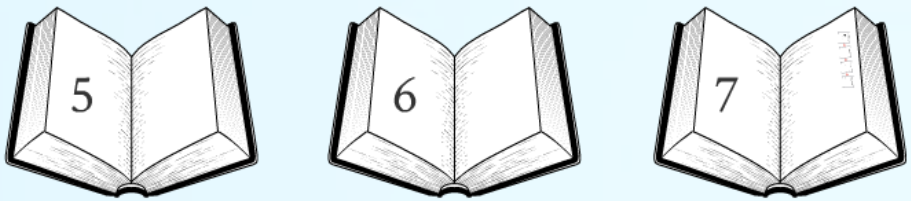
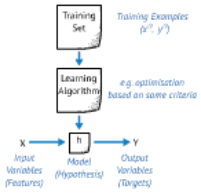
Non-parametric Methods



Introduction to Gaussian Processes

Nonparametric Regression



We'll consider continuous output variables, i.e. *regression*.

Gaussian Processes

A Gaussian process is an infinite collection of random variables, any *finite* number of which have a (consistent) multivariate Gaussian distribution.

We can think of this as a generalisation of a multivariate Gaussian to *infinite* dimensions.

A Gaussian process defines a distribution over functions.

- We can consider a function to approximately be an infinitely long vector.

Gaussian Process versus Gaussian Distribution

Gaussian distribution: $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$

Gaussian process: $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$

Gaussian Process versus Gaussian Distribution

A Gaussian distribution is a distribution over a variable of a given dimension.

- It is fully specified by a mean vector and a covariance matrix: $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$.
- For each index i denoting each dimension of $\mathbf{x}$, the mean and variance is defined directly.

A GP is a distribution over functions and so the index set is of infinite dimension.

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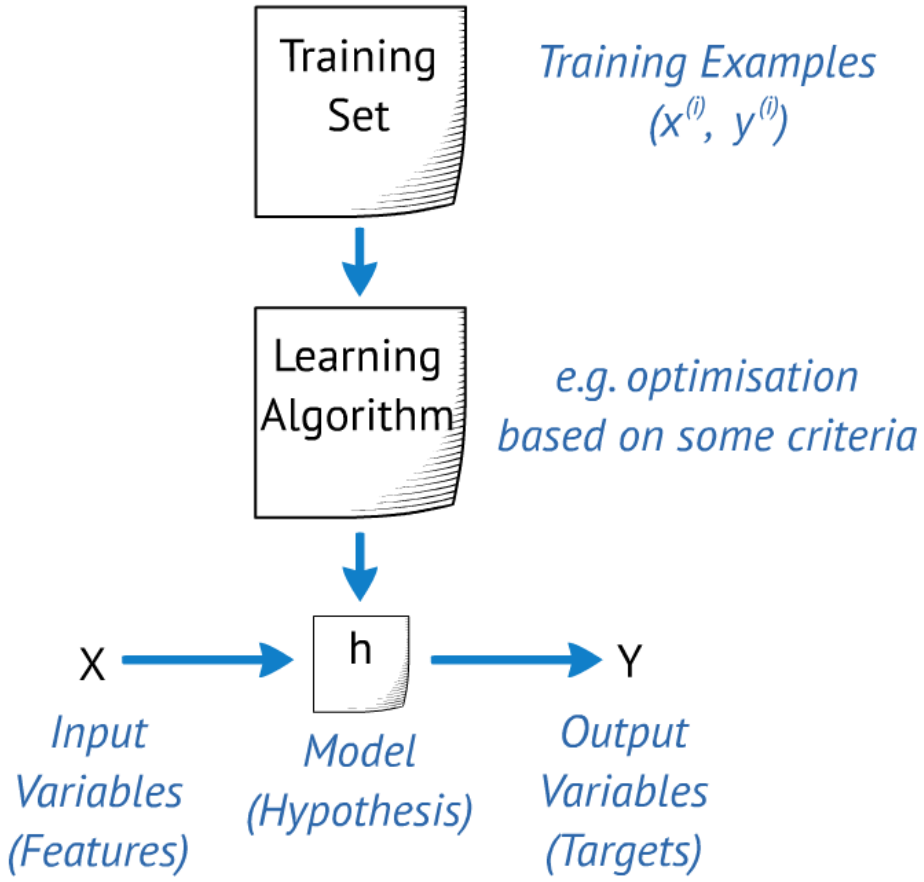

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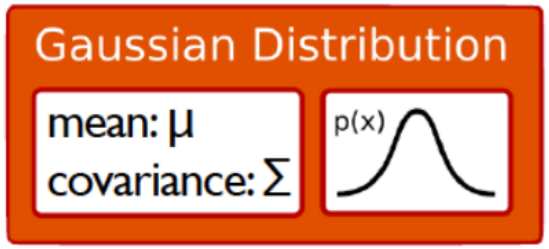

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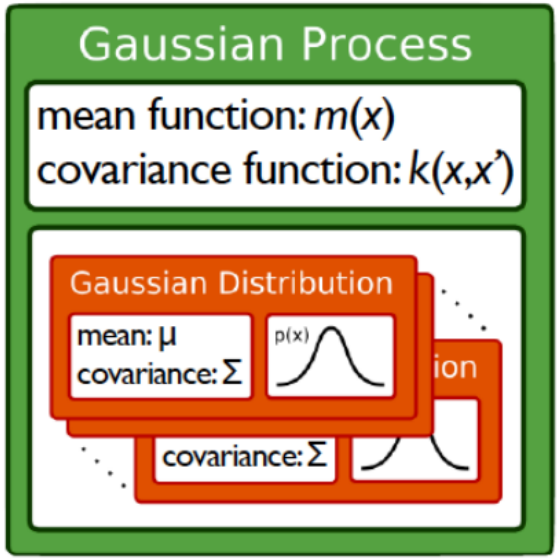

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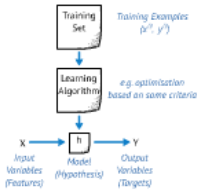

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Multivariate Gaussian Distributions

Multivariate Gaussian

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Multivariate Gaussian

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8.1.8 Product of gaussian densities

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$$\mathcal{N}_x(\mathbf{m}_1, \boldsymbol{\Sigma}_1) \cdot \mathcal{N}_x(\mathbf{m}_2, \boldsymbol{\Sigma}_2) = c_c \mathcal{N}_x(\mathbf{m}_c, \boldsymbol{\Sigma}_c) \tag{371}$$

$$\begin{aligned} c_c &= \mathcal{N}_{\mathbf{m}_2}(\mathbf{m}_2, (\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2)) \\ &= \frac{1}{\sqrt{\det(2\pi(\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2))}} \exp\left[-\frac{1}{2}(\mathbf{m}_1 - \mathbf{m}_2)^T(\boldsymbol{\Sigma}_1 + \boldsymbol{\Sigma}_2)^{-1}(\mathbf{m}_1 - \mathbf{m}_2)\right] \\ \mathbf{m}_c &= (\boldsymbol{\Sigma}_1^{-1} + \boldsymbol{\Sigma}_2^{-1})^{-1}(\boldsymbol{\Sigma}_1^{-1}\mathbf{m}_1 + \boldsymbol{\Sigma}_2^{-1}\mathbf{m}_2) \\ \boldsymbol{\Sigma}_c &= (\boldsymbol{\Sigma}_1^{-1} + \boldsymbol{\Sigma}_2^{-1})^{-1} \end{aligned}$$

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Matrix Cookbook...

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The marginal densities

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Gaussian Process Priors

Gaussian Process Prior

We have quite a lot of freedom when choosing the mean and covariance functions that will define our prior over functions.

Usually the mean is set to be the zero function.

The covariance function is much more interesting however, since it defines how the points in our function covary with one another.

The only requirement of a covariance function is that it is positive semi-definite.

Covariance Functions

If k, k_1 and k_2 are positive semi-definite, then we can create new valid covariance functions according the to following functions, which are also positive semi-definite.

1. $ak(\mathbf{x}, \mathbf{x}')R$, for $a \geq 0$
2. $k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}')$
3. $k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}')$
4. $P(k(\mathbf{x}, \mathbf{x}'))$, where $P()$ is some polynomial function with positive coefficients
5. $exp(k(\mathbf{x}, \mathbf{x}'))$
6. $f(\mathbf{x})k(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')$
7. $k(\phi(\mathbf{x}), \phi(\mathbf{x}'))$

Squared Exponential Covariance Function

The squared exponential covariance function is a common choice,

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

Intuitively, we see that function variables close to each other in the input space are highly correlated, whereas those far from each other are uncorrelated.

There are hyperparameters that change the output of the covariance function: σ controls the amplitude, λ controls the lengthscale.

The squared exponential produces very smooth functions, since it is *infinitely differentiable*.

Matern Covariance Function

The Matern exponential covariance function is another common choice,

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

where K_ν is a modified Bessel function.

There are hyperparameters that change the output of the covariance function: ν controls the roughness of the sample functions, λ controls the lengthscale.

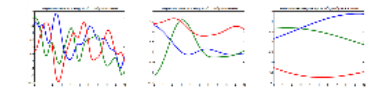
With $\nu = \infty$ we recover the squared exponential covariance, with $\nu = \frac{1}{2}$ we obtain an Ornstein-Uhlenbeck process.

Periodic Covariance Function

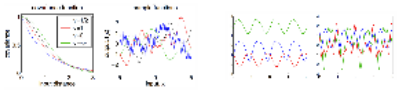
We can even model periodic functions,

$$k(x, x') = \exp\left(\frac{-2\sin^2(x - x')}{\lambda^2}\right)$$

Covariance Function Comparison



Squared Exponential



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6. $f(\mathbf{x})k(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')$
7. $k(\phi(\mathbf{x}), \phi(\mathbf{x}'))$

Squared Exponential Covariance Function

The squared exponential covariance function is a common choice,

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

Intuitively, we see that function variables close to each other in the input space are highly correlated, whereas those far from each other are uncorrelated.

There are hyperparameters that change the output of the covariance function: σ controls the amplitude, λ controls the lengthscale.

The squared exponential produces very smooth functions, since it is *infinitely differentiable*.

Matern Covariance Function

The Matern exponential covariance function is another common choice,

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

where K_{ν} is a modified Bessel function.

There are hyperparameters that change the output of the covariance function: ν controls the roughness of the sample functions, λ controls the lengthscale.

With $\nu = \infty$ we recover the squared exponential covariance, with $\nu = \frac{1}{2}$ we obtain an Ornstein-Uhlenbeck process.

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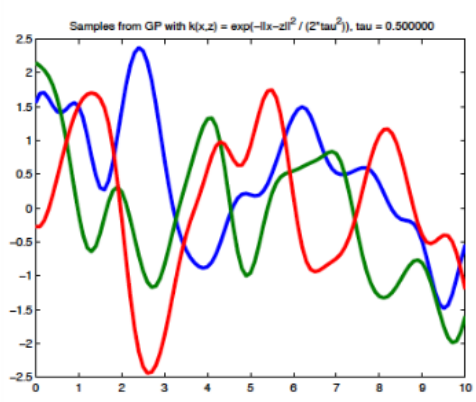

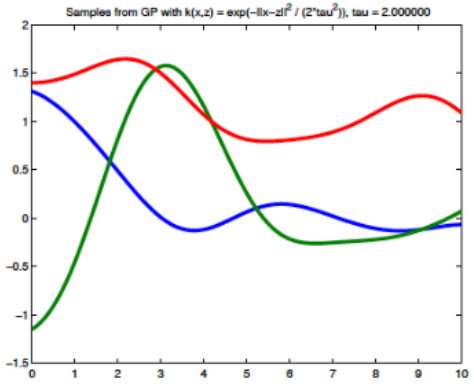

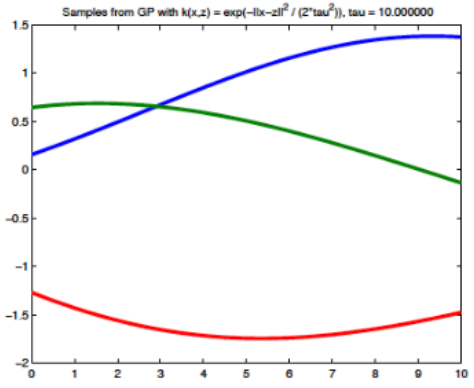

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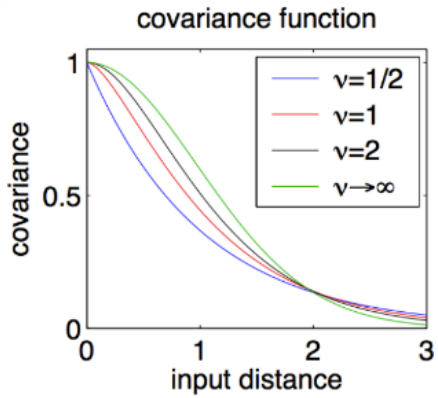

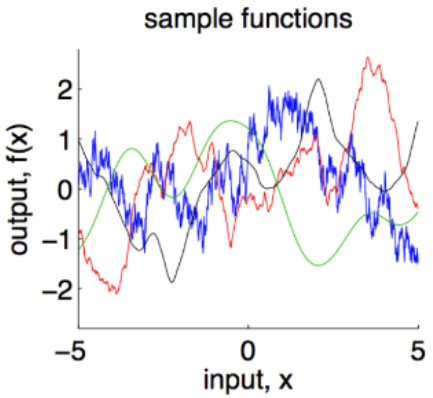

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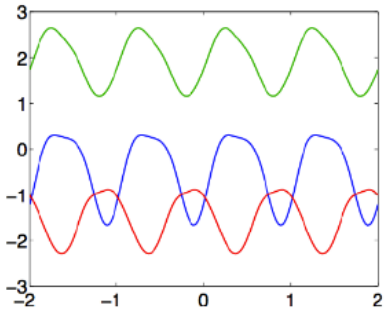

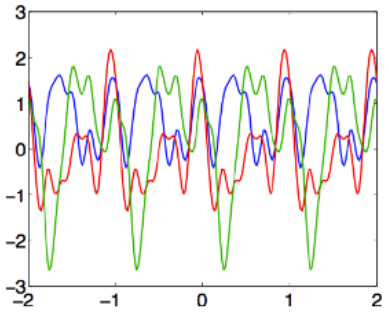

Periodic

Gaussian Process Priors

Gaussian Process Prior

We have quite a lot of freedom when choosing the mean and covariance functions that will define our prior over functions.

Usually the mean is set to be the zero function.

The covariance function is much more interesting however, since it defines how the points in our function covary with one another.

The only requirement of a covariance function is that it is positive semi-definite.

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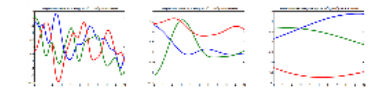

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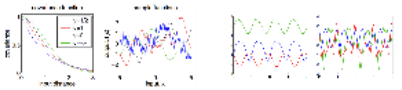

Matern

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Gaussian Process Regression

We can therefore model each datapoint as some function of the inputs plus noise, such that

$$y_i = f(x_i) + \epsilon_i$$

where we can define our prior over functions as a Gaussian process,

$$\mathbf{f}(\mathbf{x}) \sim \mathcal{GP}(m = \mathbf{0}, k)$$

and we can assume Gaussian noise for the likelihood,

$$p(\mathbf{y}|\mathbf{f}) \sim \mathcal{N}(\mathbf{f}, \sigma^2)$$

Conveniently, because everything is Gaussian, we can integrate over all the functions to obtain the marginal likelihood,

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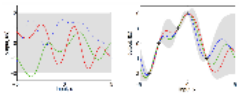

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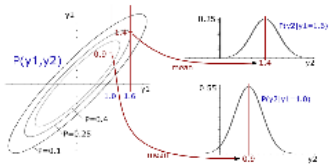

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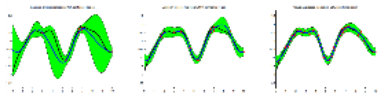

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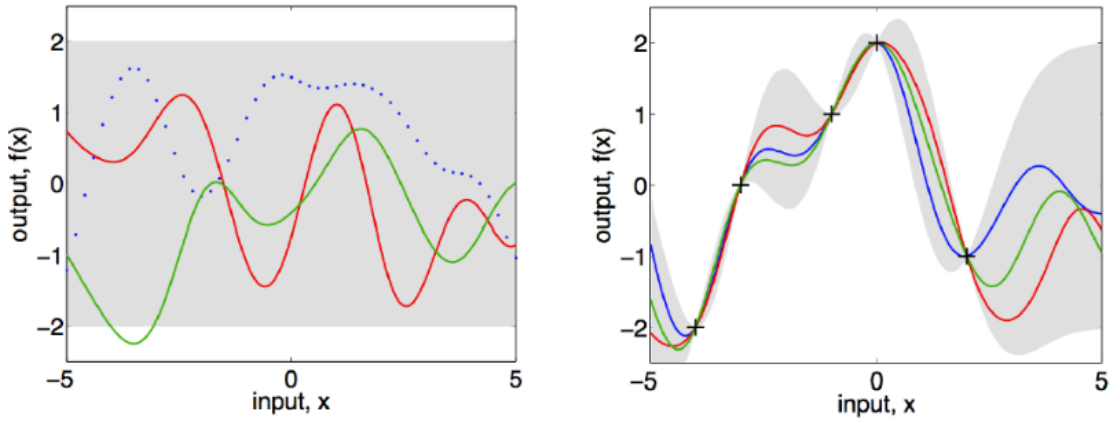

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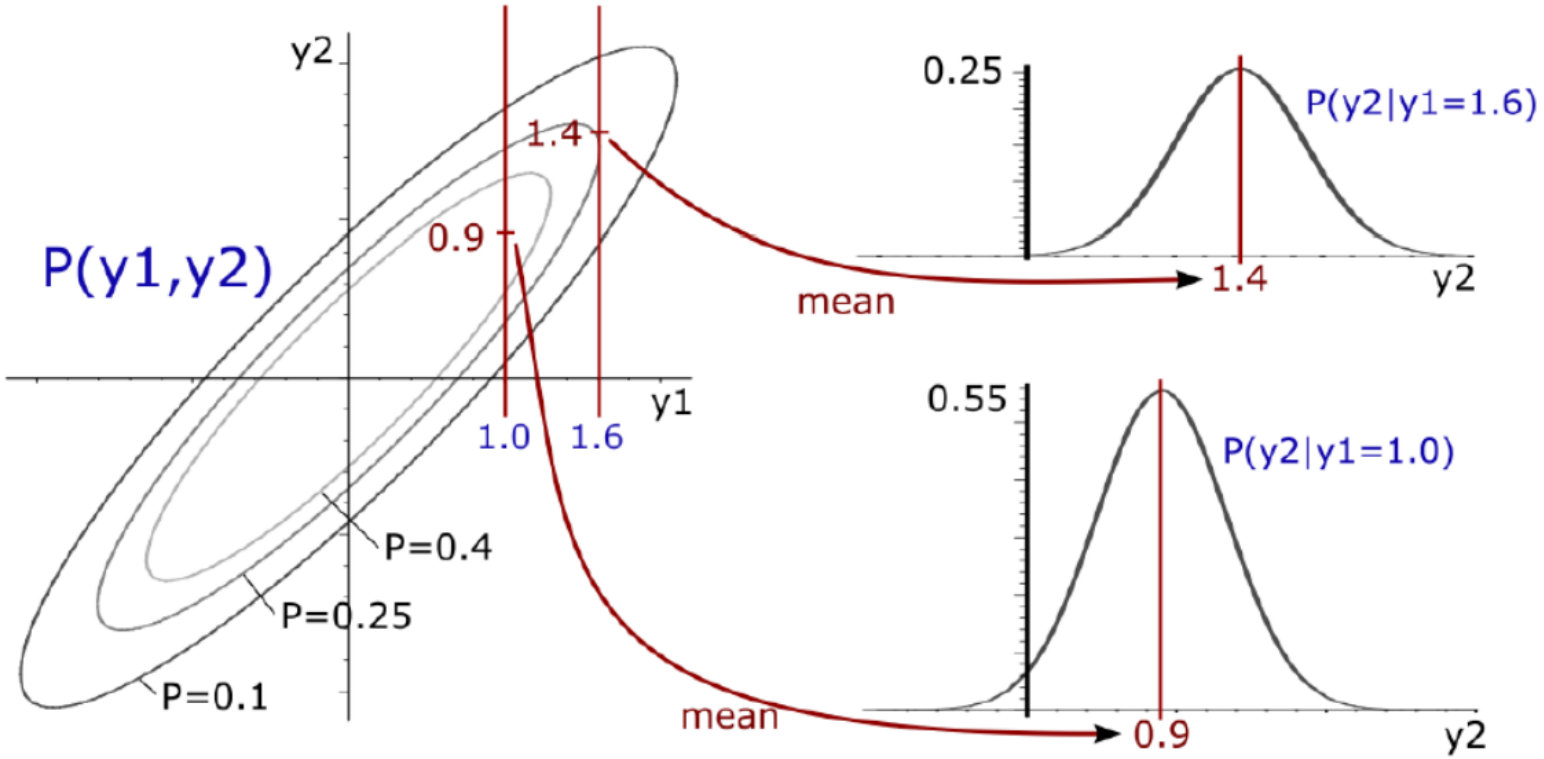

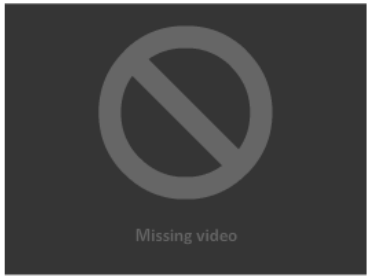

Missing video

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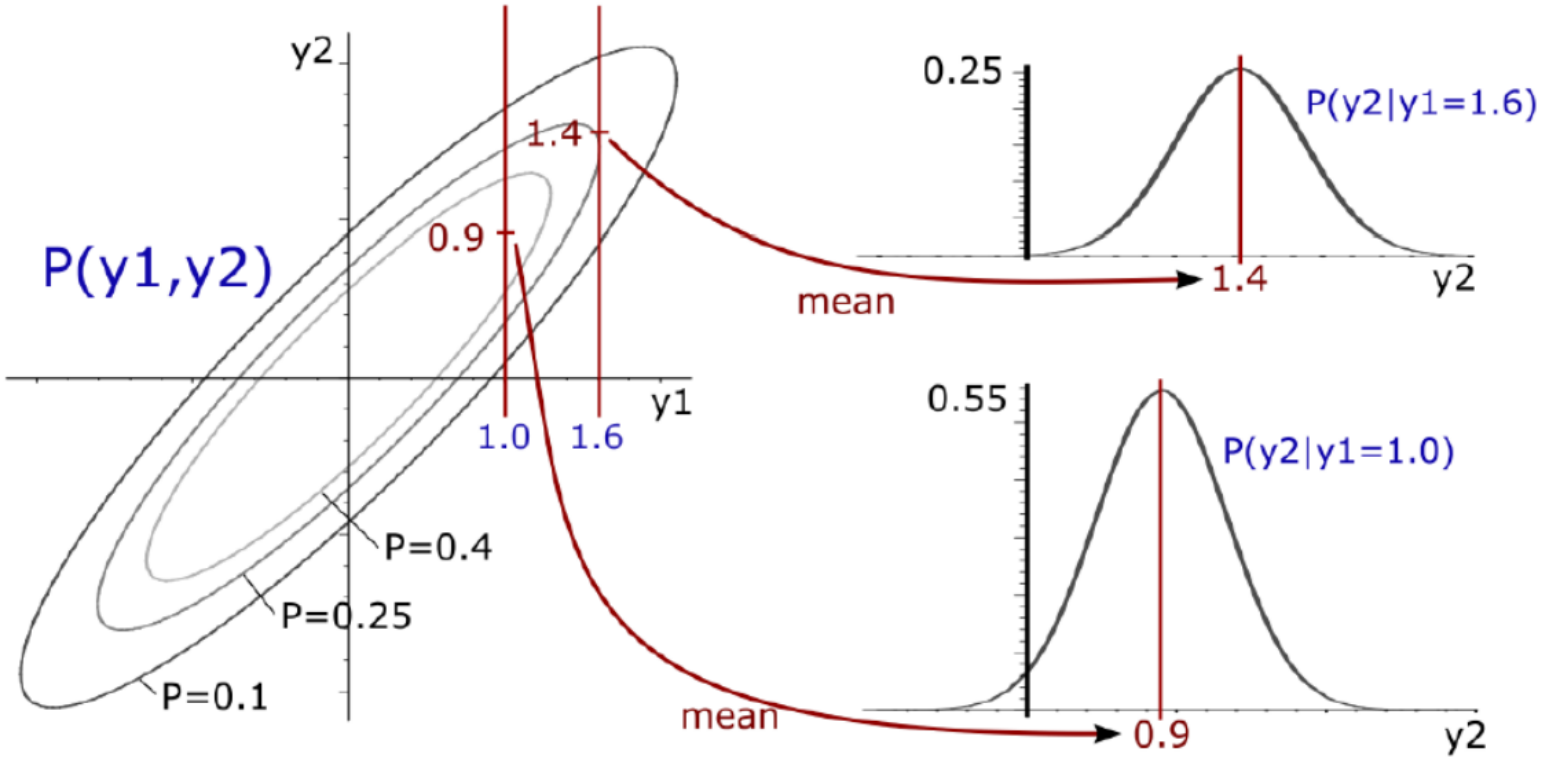

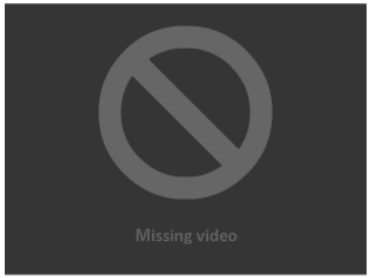

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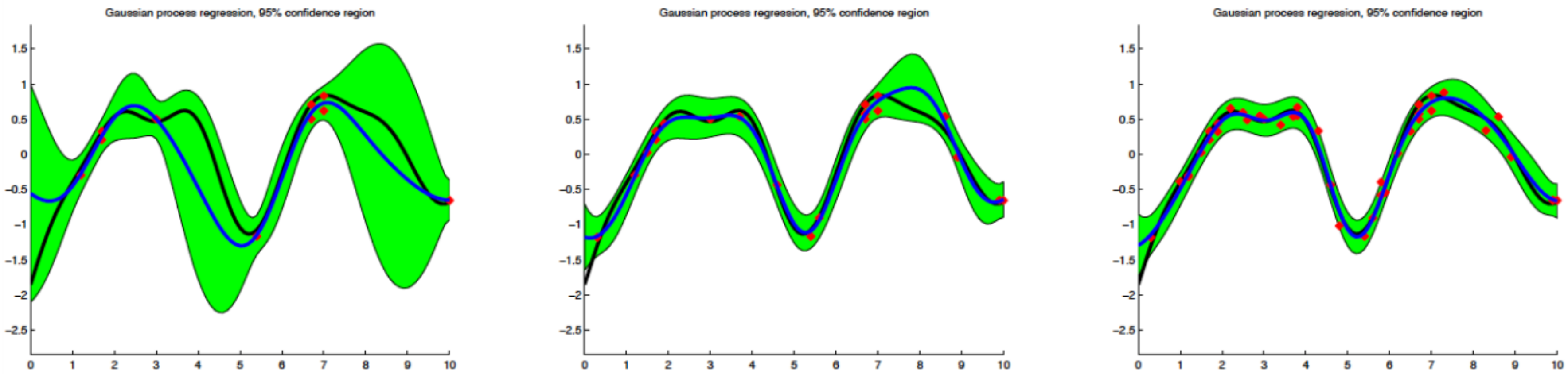

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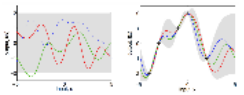

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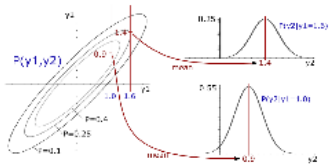

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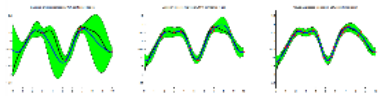

Summary

Gaussian processes are a very powerful approach for performing nonparametric supervised learning.

We can use the kernel trick to allow us to do linear regression effectively using an infinite number of basis functions, while retaining analytic tractability.

The main challenge is the computational scaling; it is cubic in the number of observations.

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Lecture 6

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