A Gentle Introduction to Gaussian Processes

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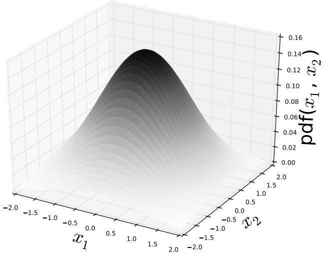

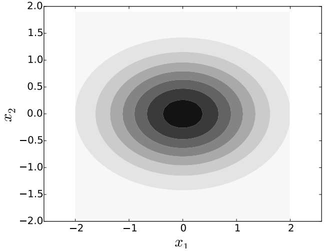

Overview

- Motivation
- The Gaussian Distribution
- Gaussian Processes
- Gaussian Process Regression - A Toy Example
- Gaussian Process Regression - CO_2 Concentrations
- Modelling Gene Expression Time-Series

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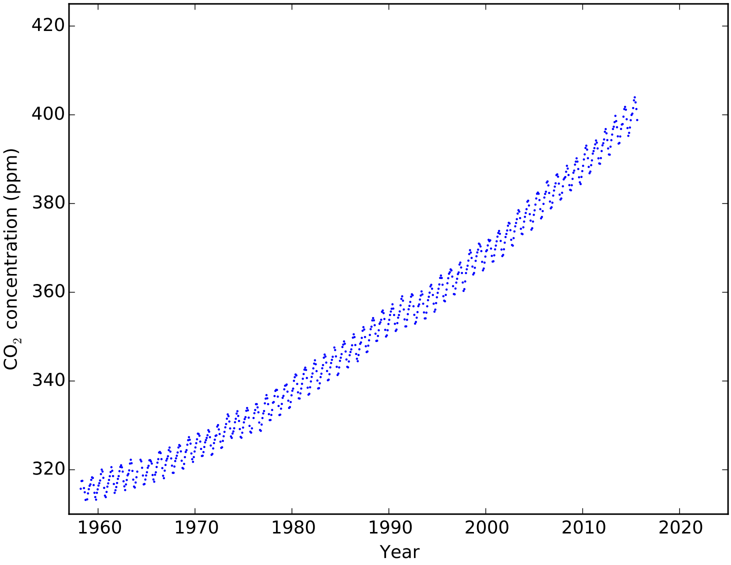

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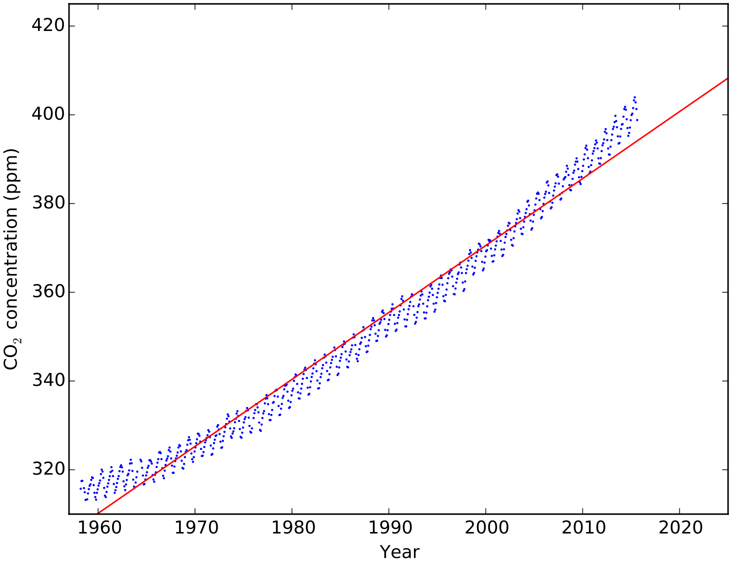
Year
CO2 concentration (ppm)

Motivation



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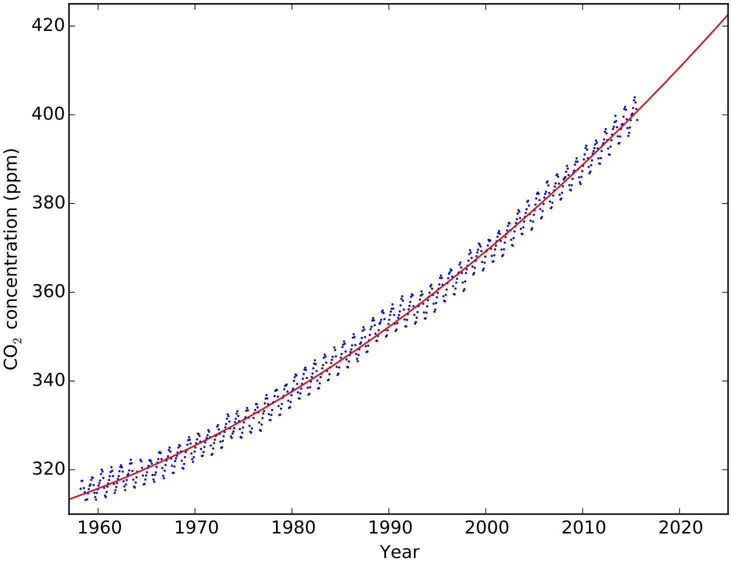

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The Data Modelling Task

- **data**: $\mathbf{x} = \{x_1, \ldots, x_N\}$, $\mathbf{y} = \{y_1, \ldots, y_N\}$
- **model**: $y = f(x) + \epsilon$
- **predictions**: $y^* = f(x^*)$

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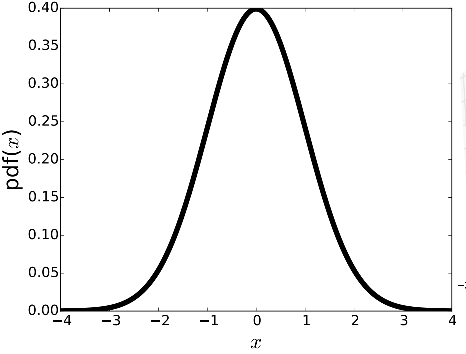
$$f(x)$$

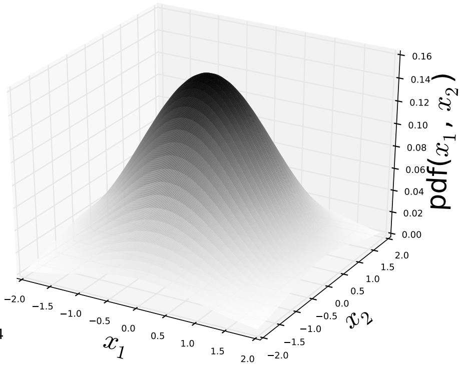
Parametric

e.g $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$

Nonparametric

e.g $f(x) =$ Gaussian Process





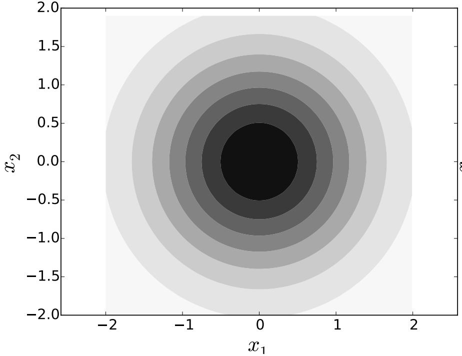
$$\mathcal{N}(\mu,\ \sigma^2)$$

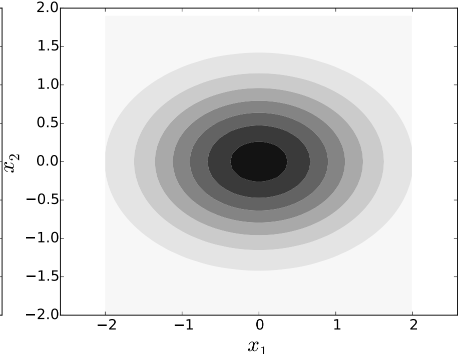
A draw from this distribution is a 1D vector e.g $x = [0.2]$

$$\mathcal{N}(\boldsymbol{\mu},\ \Sigma)$$

A draw from this distribution is a 2D vector e.g $\mathbf{x} = \begin{bmatrix} 0.3 \\ -0.4 \end{bmatrix}$

The Covariance Matrix





Isotropic

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Diagonal

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 0.5 \end{pmatrix}$$

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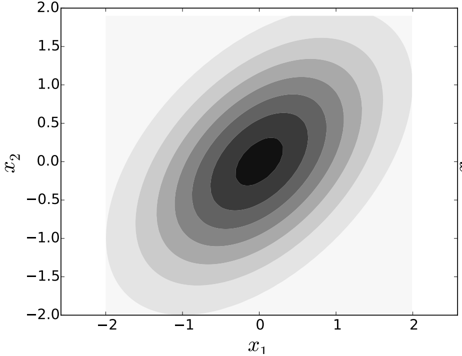

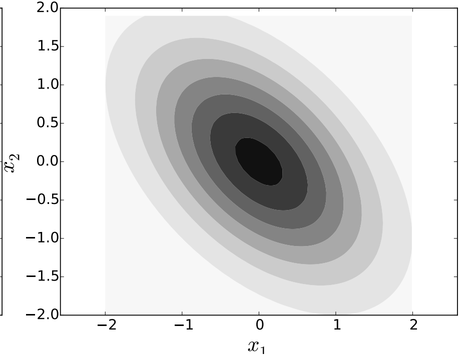

General Form

$$\Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}$$

General Form

$$\Sigma = \begin{pmatrix} 1 & -0.5 \\ -0.5 & 1 \end{pmatrix}$$

Sampling from a Multivariate Gaussian

What does a *single* sample from a 100 dimensional Gaussian look like?

$$\mathbf{x} = \left.\begin{bmatrix} 0.2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ -0.6 \end{bmatrix}\right\} = 100 \Longrightarrow$$

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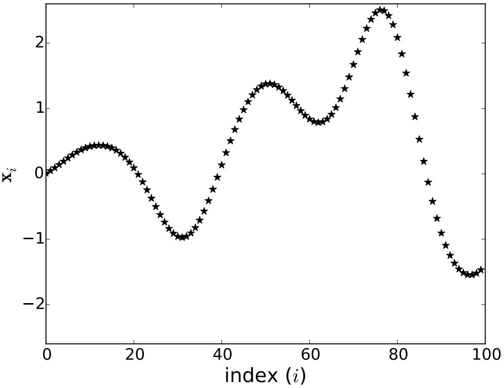

Gaussian Process in a Nutshell

Recall: What we are after is $y = f(x)$

Trick: Think about a function as an infinitely-long vector

$$f(x) = \left.\begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ f_\infty \end{bmatrix}\right\} = \infty \Longrightarrow$$

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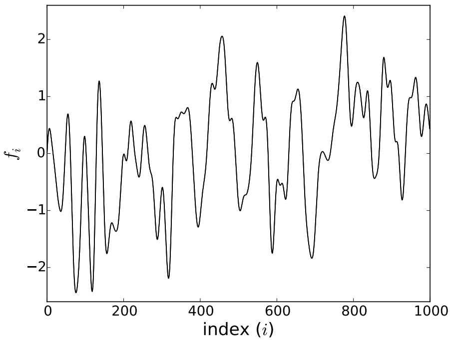

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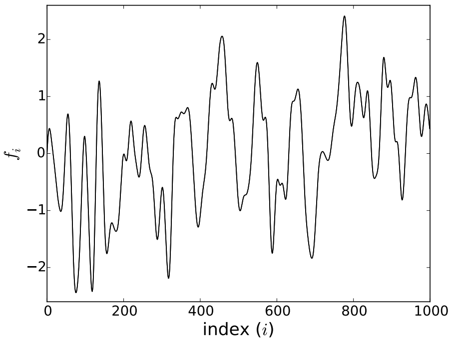

Computational Madness: Ask only for the properties of the function at a *finite* number of points

Gaussian Process in a Nutshell

3 dimensional Gaussian

Mean vector

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix}$$

Covariance matrix

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 \end{pmatrix}$$

∞ dimensional Gaussian

Mean *function*

$$\mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \vdots \\ \mu_\infty \end{pmatrix} = m(\mathbf{x})$$

Covariance *function*

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1\infty} \\ \sigma_{21} & \sigma_2^2 & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \dots & \sigma_\infty^2 \end{pmatrix} = k(\mathbf{x}, \mathbf{x}')$$

Gaussian Process

Definition

A Gaussian Process (GP) is an infinite collection of random variables, any finite number of which have a joint normal distribution.
Essentially an infinite dimension multivariate Gaussian distribution, characterised by a mean function $m(\mathbf{x})$ and a covariance function $k(\mathbf{x}, \mathbf{x}')$

Rationale

Instead of inferring the parameters of a fixed model structure $(\beta_0, \beta_1, \ldots)$, with GPs we model the *correlation* between inputs. That is, inputs $\mathbf{x}$ that are close/similar to each other are likely to give rise to a similar output $f(\mathbf{x})$

$$\begin{aligned} f(\mathbf{x}) &\sim \mathrm{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')) \\ m(\mathbf{x}) &= \mathrm{E}[f(\mathbf{x})] \\ k(\mathbf{x}, \mathbf{x}') &= \mathrm{E}[(f(\mathbf{x}) - m(\mathbf{x})(f(\mathbf{x}') - m(\mathbf{x}')] \end{aligned}$$

Covariance Function

- Vital ingredient in Gaussian Process[1]
- Encodes our assumptions about the function we wish to model (smooth, stationary, etc.)
- Quantifies the *similarity* between two data points; crucial for predicting a test point $\mathbf{x}^*$
- Needs to satisfy a set of mathematical conditions (beyond the scope of this intro)
- A very popular choice is the Squared Exponential:

  (also known as RBF, Gaussian and Exponentiated Quadratic Kernel Function)

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left(\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2l^2}\right)$$

e.g if we set $\alpha = 1$ and $l = 1$ then:
$k(0,0) = e^0 = 1, \quad k(0,1) = e^{-\frac{1}{2}} = 0.6, \quad k(0,2) = e^{-2} = 0.14$

[1] without much loss of generality we can assume that $m(\mathbf{x}) \equiv 0$

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Gaussian Process Regression

- Shift the problem from inferring model parameters to choosing a covariance function and its (hyper)parameters

- Choose $m(\mathbf{x})$ and $k(\mathbf{x}, \mathbf{x}')$ that reflect some prior belief

- This defines a *prior* on the function class itself; it is a prior on a *function* and not parameters of some fixed model structure

- Under a Bayesian framework this prior is "reshaped" by the observed data to obtain a posterior distribution on the *function*

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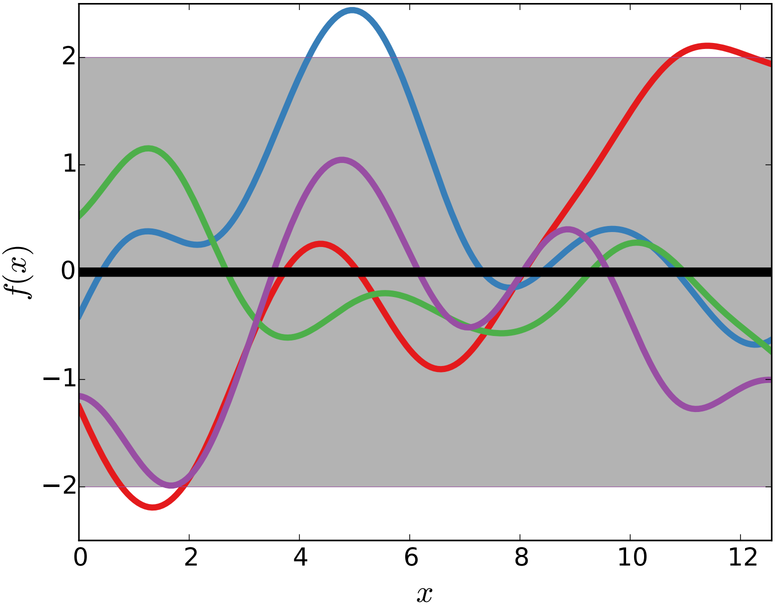

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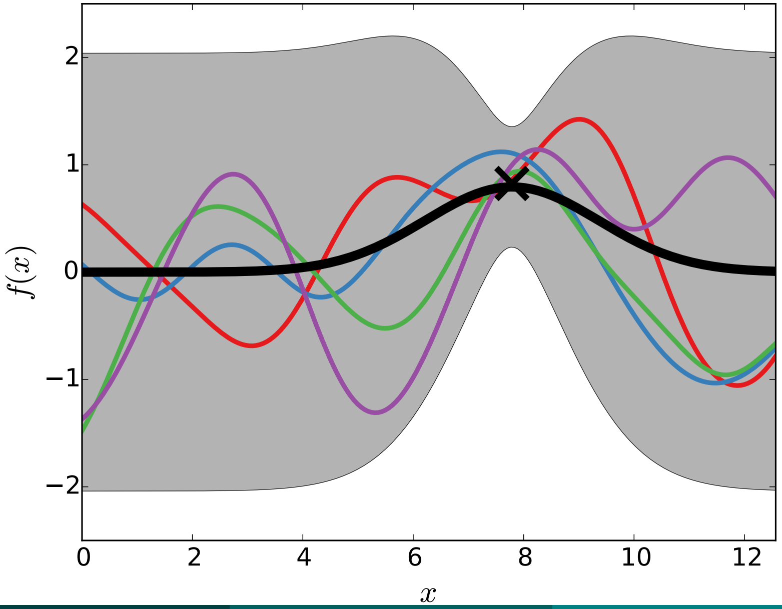

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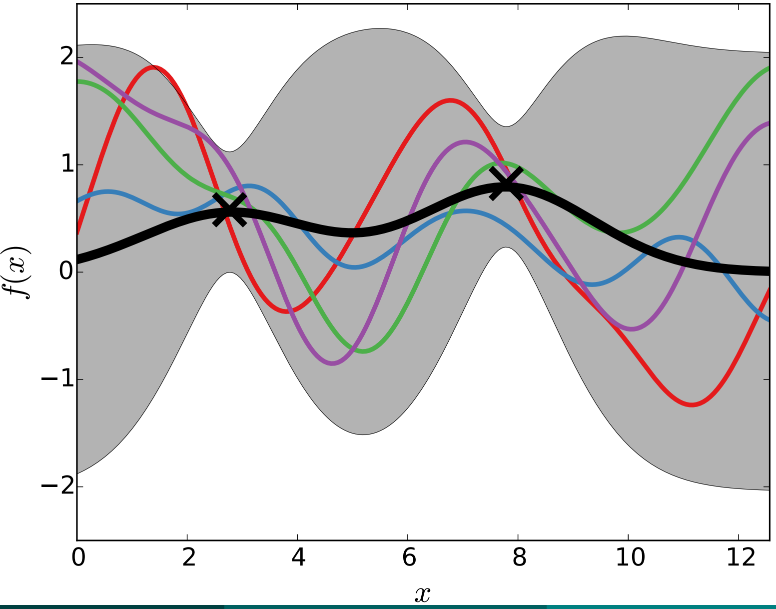

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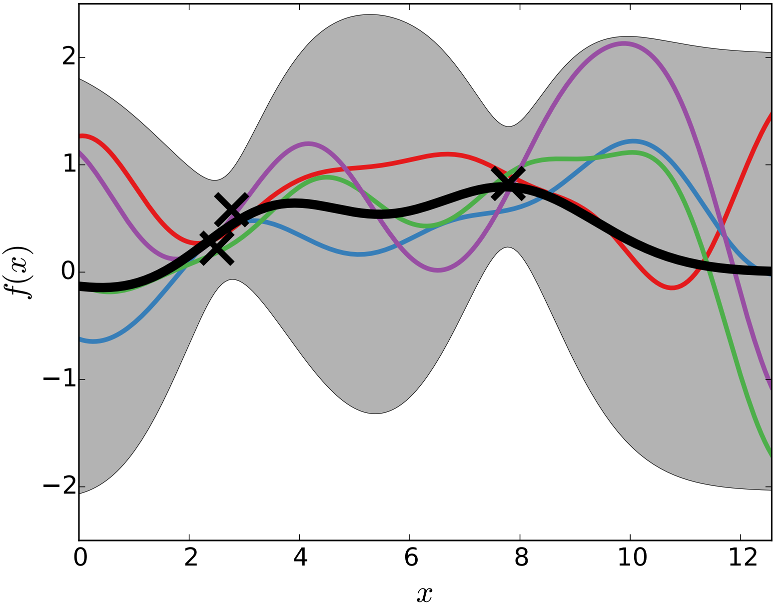

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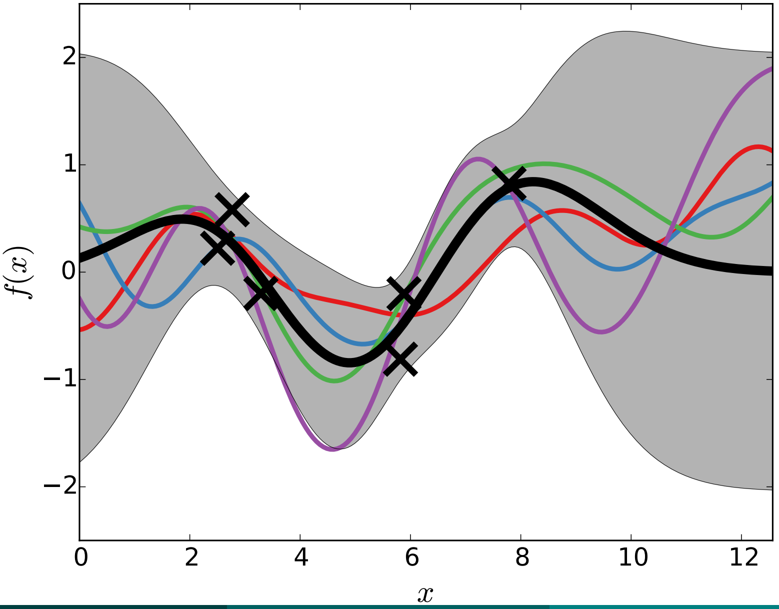

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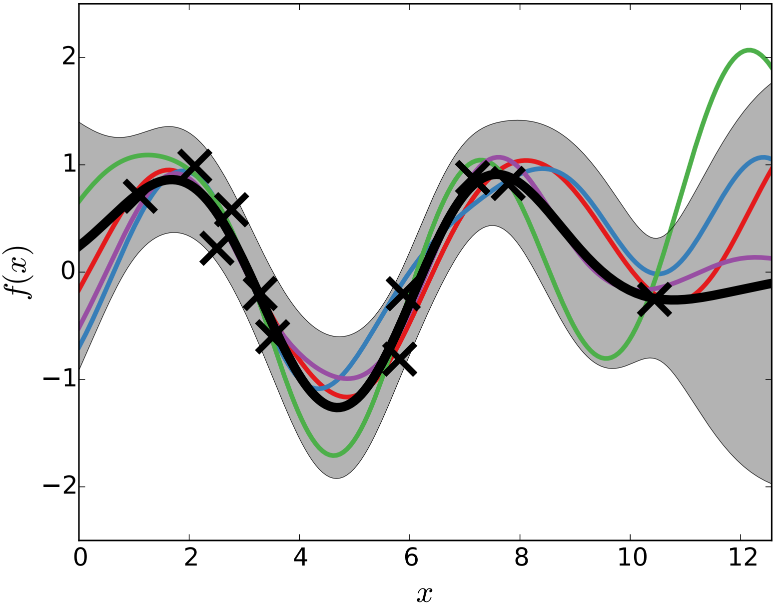

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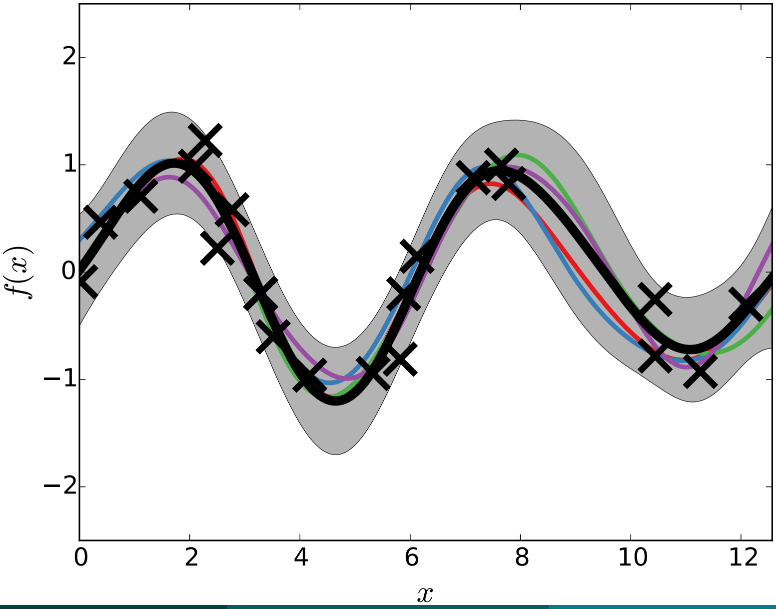

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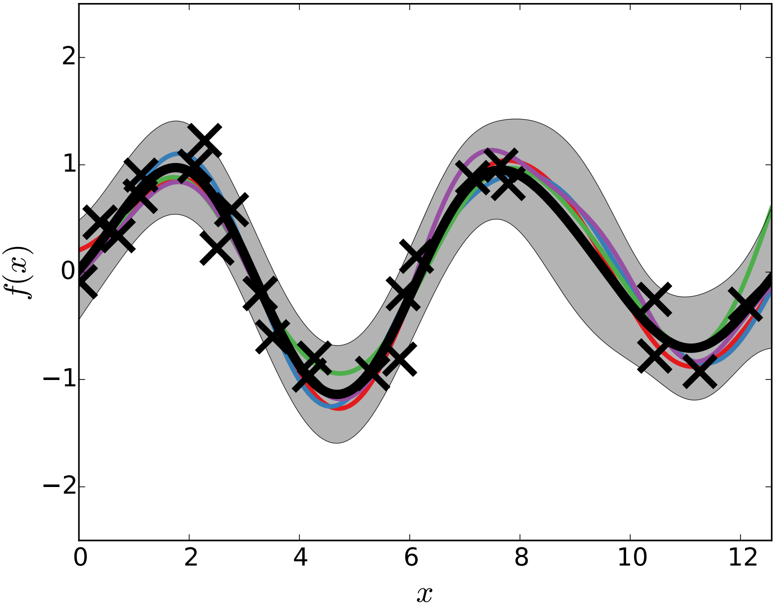

Misspecifying the Covariance Function

- The Squared Exponential covariance function was used in the previous example:

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left(\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2l^2}\right)$$

- Choosing a covariance functions is akin to choosing a model structure; it dictates the class of functions that can be represented by the Gaussian Process[2]

- Misspecifying the covariance function and/or its (hyper)parameters has a detrimental effect on the model fit

- For e.g in the squared exponential case the lengthscale l dictates how much the function is allowed to bend

[2] typically a wider class of functions than in parametric models

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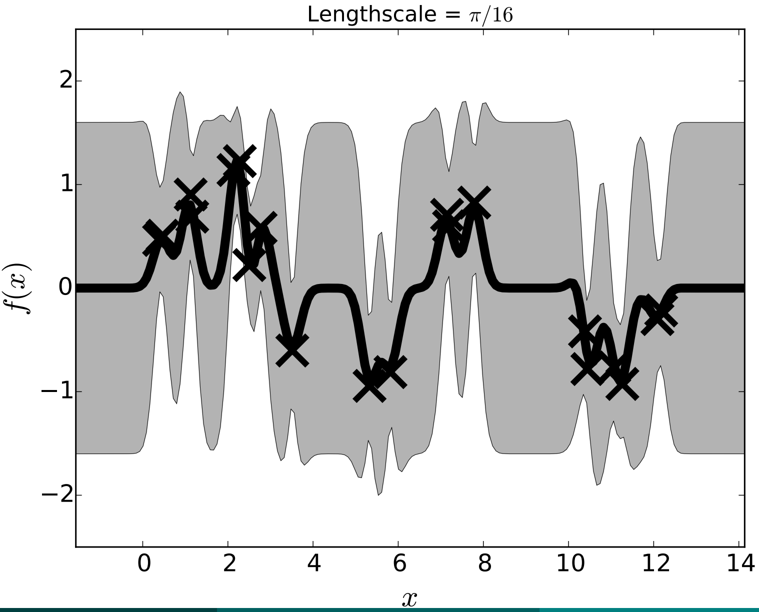
The Effect of Lengthscale on Model Fit



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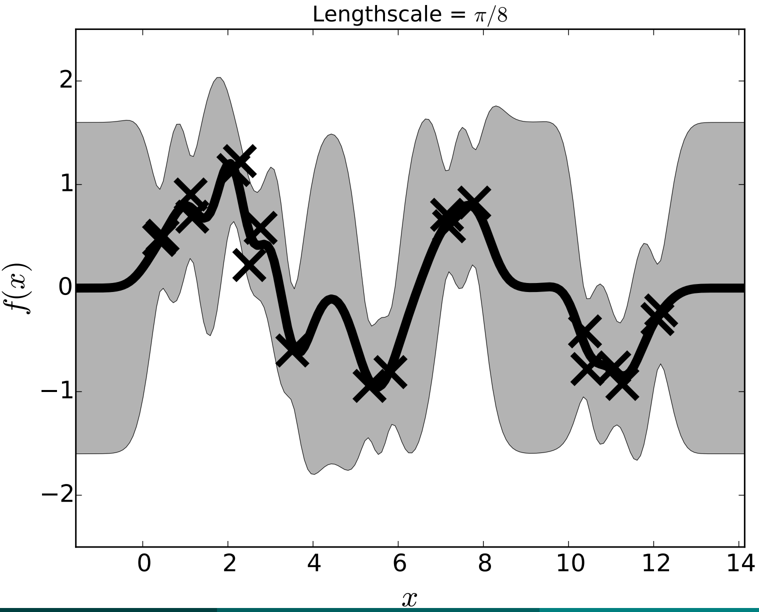

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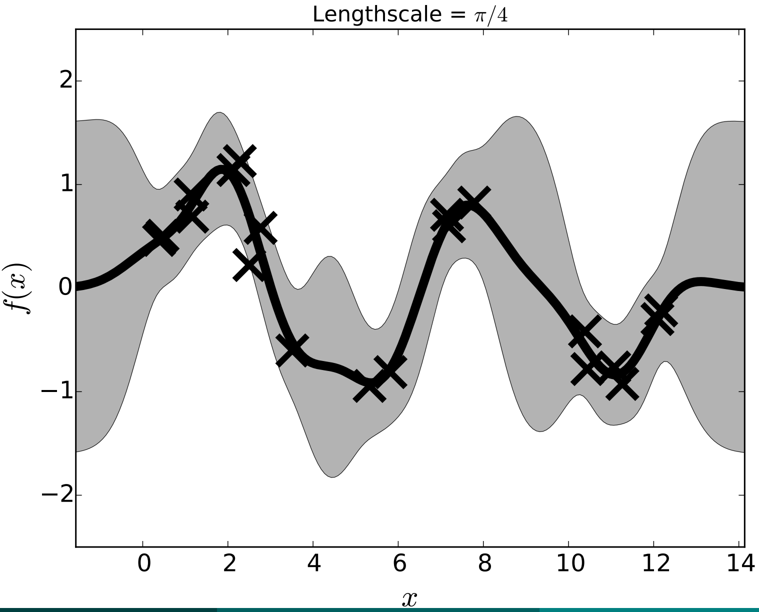

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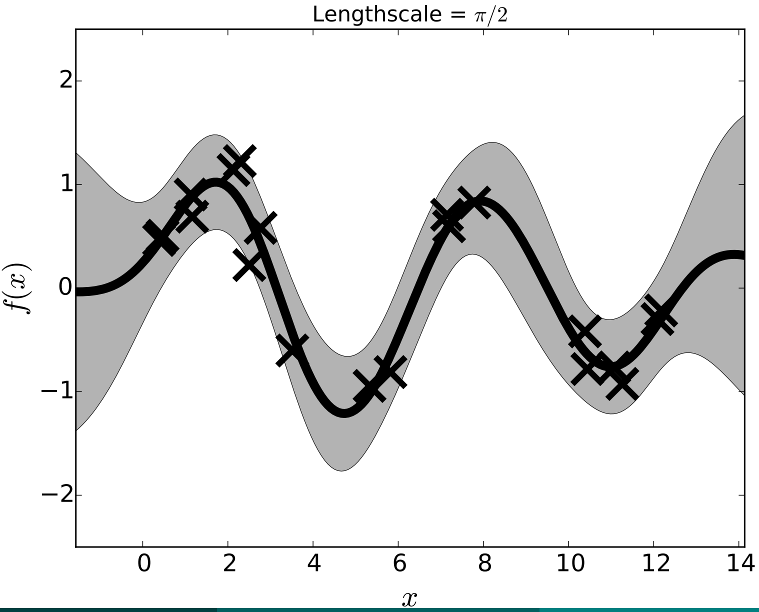

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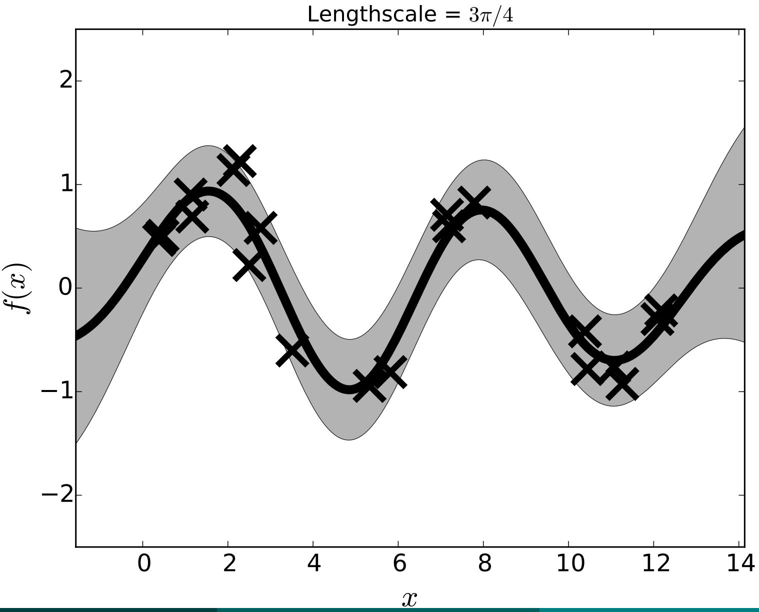

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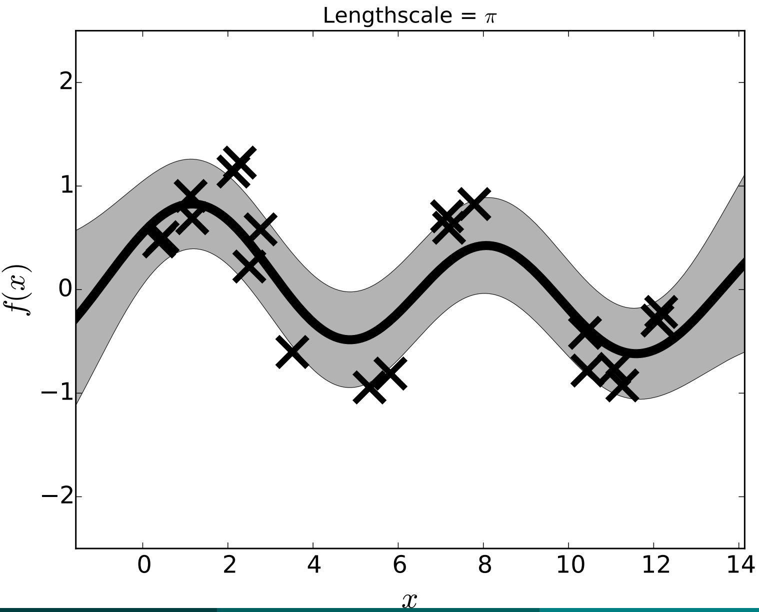

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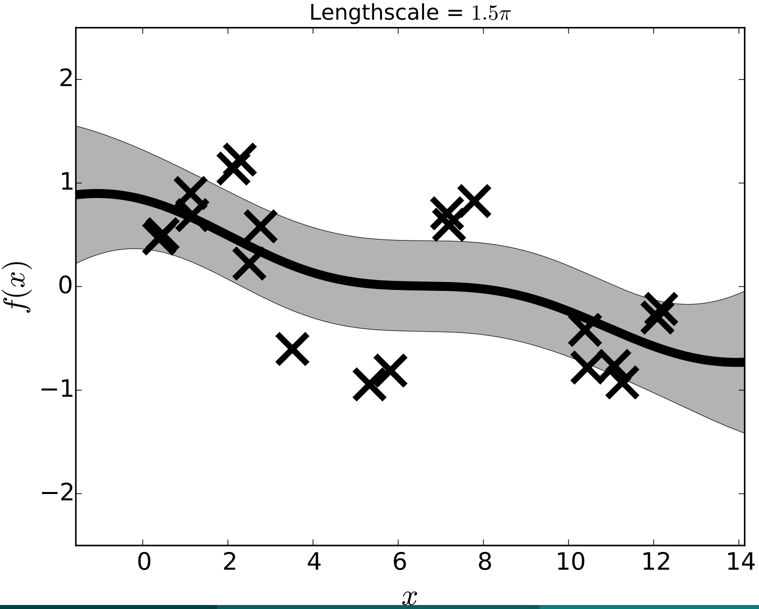

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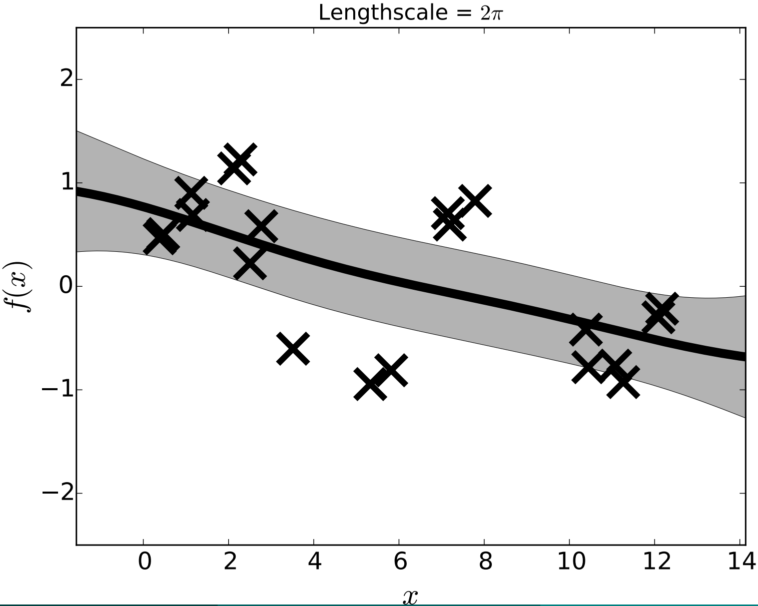

Learning the Covariance Parameters

- Let us define θ as a vector containing all (hyper)parameters e.g $\theta = \{\alpha, l, \sigma_n^2\}$
- We choose θ that maximises the log marginal likelihood, that is:

$$\ln p(y|\mathbf{x}, \theta) = -\frac{1}{2} y^T (k(\mathbf{x}, \mathbf{x}') + \sigma_n^2 I)^{-1} y - \frac{1}{2} \ln |k(\mathbf{x}, \mathbf{x}') + \sigma_n^2 I| - \frac{n}{2} \ln 2\pi$$

- Cannot guarantee a global optimum; try different initial conditions
- Constraint (hyper)parameters to some sensible limits
- **Note**: Choosing the right covariance function (e.g Squared Exponential, Matérn, Rational Quadratic, etc.) is not always easy and should be treated akin to a model selection problem

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- **Note**: Choosing the right covariance function (e.g Squared Exponential, Matérn, Rational Quadratic, etc.) is not always easy and should be treated akin to a model selection problem

Learning the Covariance Parameters

- Let us define θ as a vector containing all (hyper)parameters e.g $\theta = \{\alpha, l, \sigma_n^2\}$
- We choose θ that maximises the log marginal likelihood, that is:

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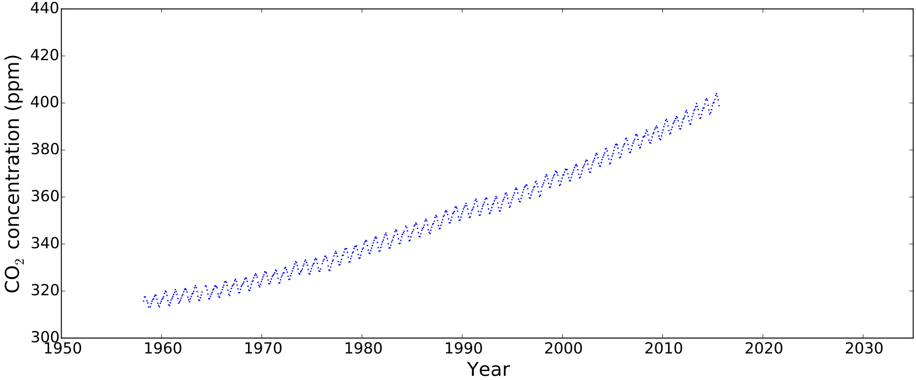
Modelling CO_2 Concentrations



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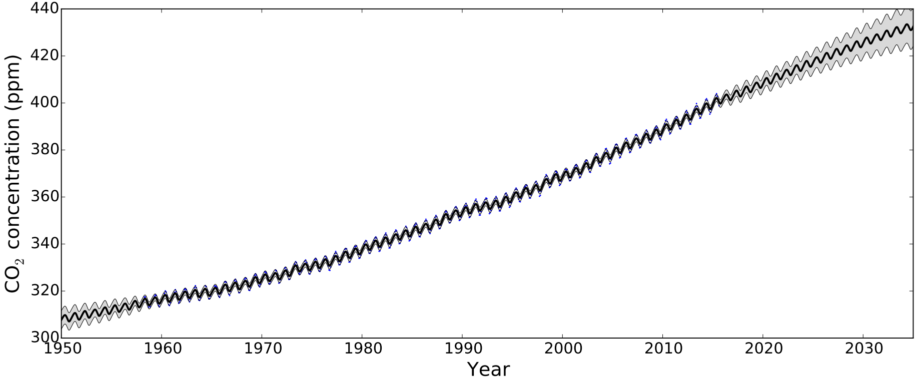
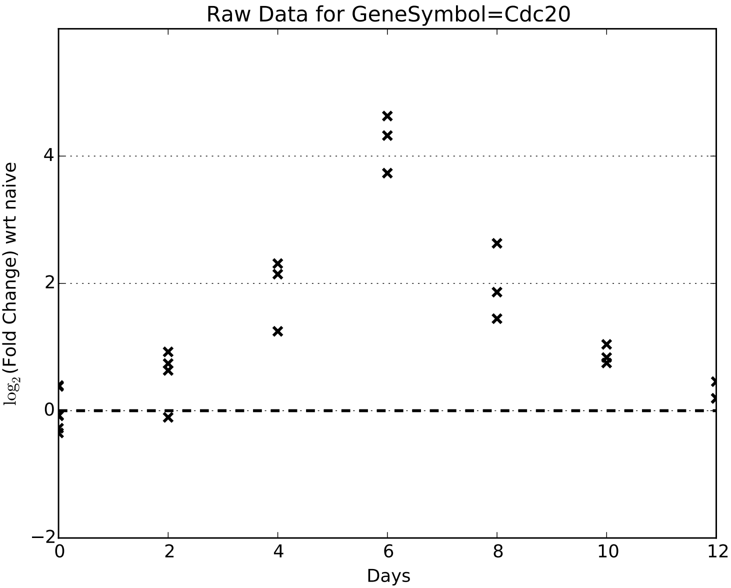
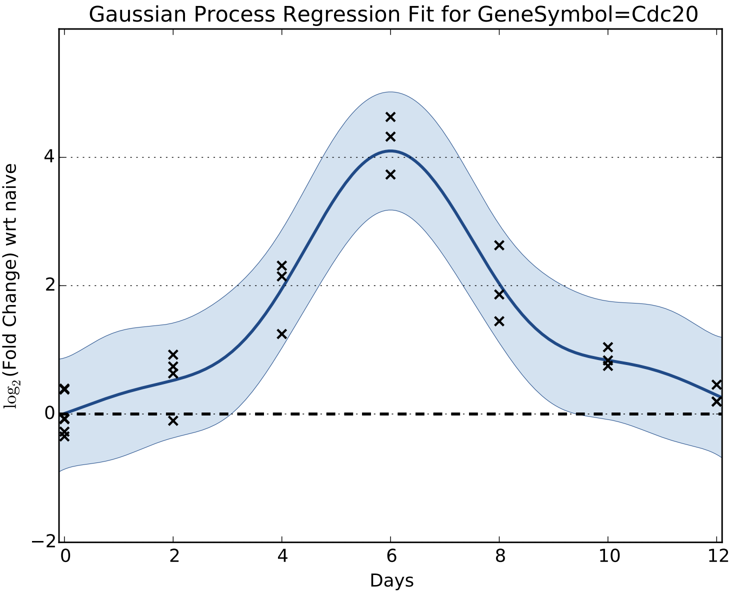
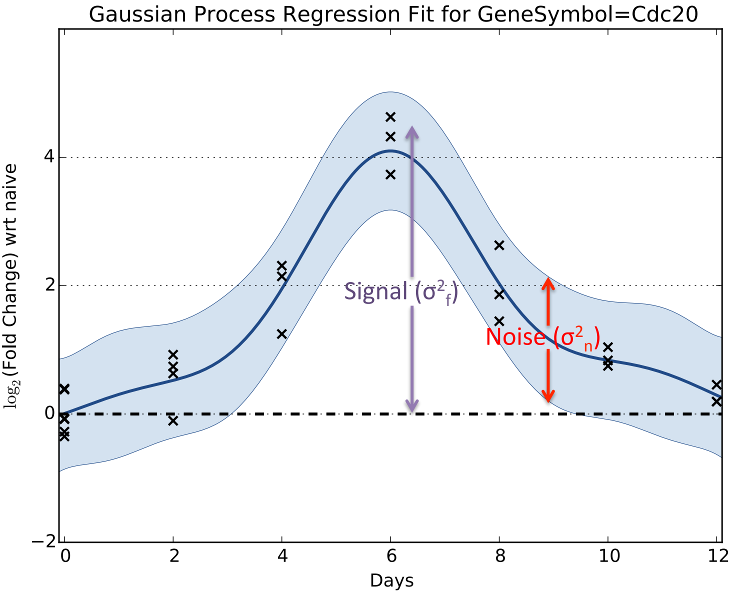



Raw Data for GeneSymbol=Cdc20
$\log_2$(Fold Change) wrt naive
Days
4
2
0
−2
0
2
4
6
8
10
12

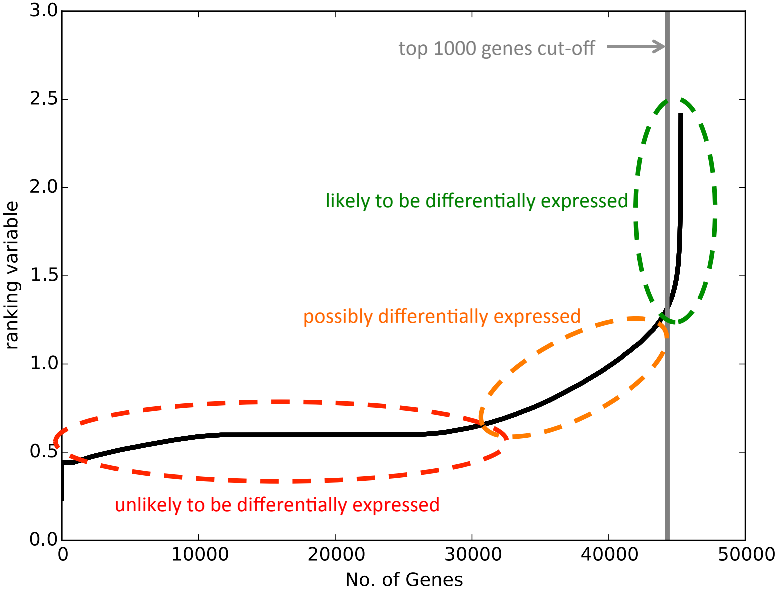
Modelling Gene Expression Time-Series



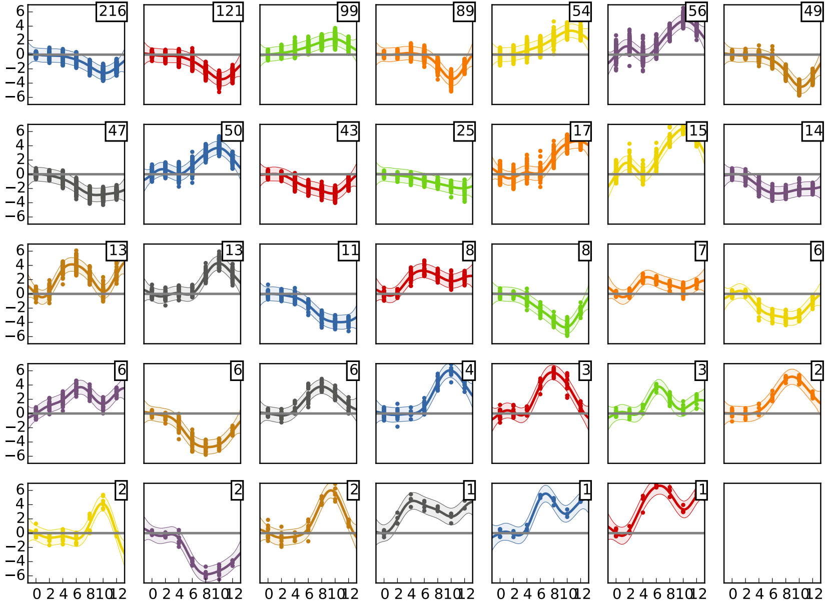
Modelling Gene Expression Time-Series



Ranking Gene Expression Time-Series



Clustering Gene Expression Time-Series

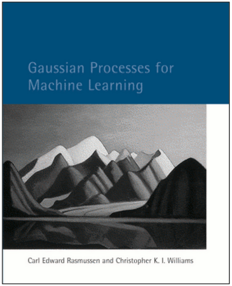


Gaussian Process Resources

- Rasmussen and Williams book

Gaussian Processes for Machine Learning

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



- http://www.gaussianprocess.org/
- The `GPy` Python Module by Neil Lawrence's Sheffield Group: https://github.com/SheffieldML/GPy