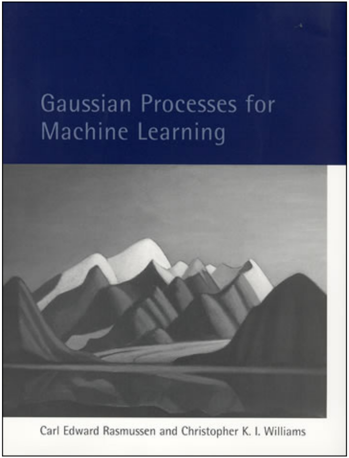
Session 1: Gaussian Processes

Neil D. Lawrence

BioPreDyn Workshop
Barcelona, 12th June 2012

Outline

Book


Gaussian Processes for
Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams

?

Outline

1. The Gaussian Density
2. GP Limitations
3. Gene Expression Examples
4. Conclusions

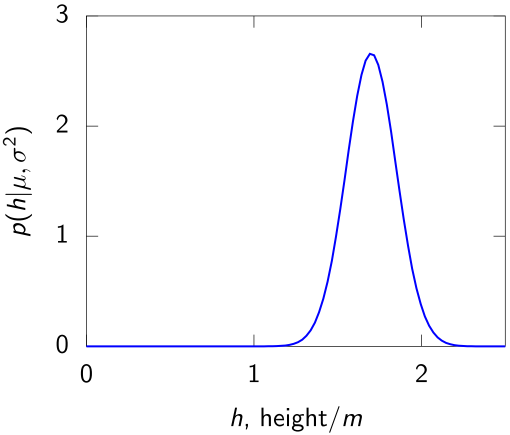
The Gaussian Density

- Perhaps the most common probability density.

$$p(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$
$$= \mathcal{N}\left(y|\mu, \sigma^2\right)$$

- The Gaussian density.

Gaussian Density



The Gaussian PDF with $\mu = 1.7$ and variance $\sigma^2 = 0.0225$. Mean shown as red line. It could represent the heights of a population of students.

Gaussian Density

$$\mathcal{N}\left(y|\mu,\sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

Two Important Gaussian Properties

1. Sum of Gaussian variables is also Gaussian.

$$y_i \sim \mathcal{N}\left(\mu_i, \sigma_i^2\right)$$

$$\sum_{i=1}^{n} y_i \sim \mathcal{N}\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2\right)$$

(*Aside*: As sum increases, sum of non-Gaussian, finite variance variables is also Gaussian [central limit theorem].)

2. Scaling a Gaussian leads to a Gaussian.

$$y \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

$$wy \sim \mathcal{N}\left(w\mu, w^2\sigma^2\right)$$

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Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$
\begin{aligned}
y_1 &= mt_1 + c \\
y_2 &= mt_2 + c
\end{aligned}
$$

Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$y_1 - y_2 = m(t_1 - t_2)$$

Two Simultaneous Equations

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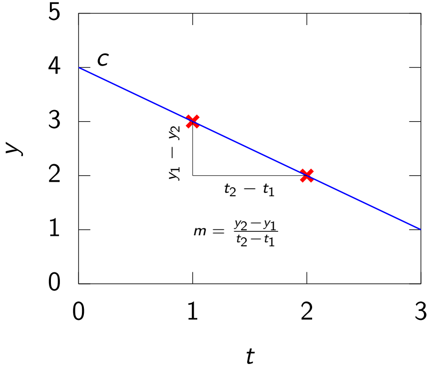
$$\frac{y_1 - y_2}{t_1 - t_2} = m$$

Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$m = \frac{y_2 - y_1}{t_2 - t_1}$$

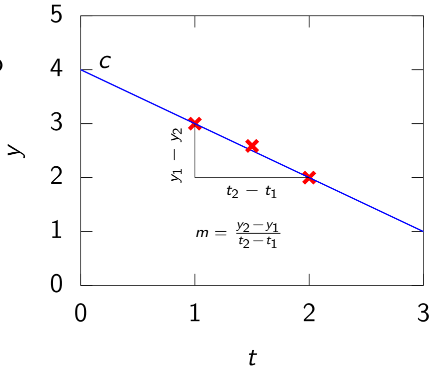
$$c = y_1 - mt_1$$



Two Simultaneous Equations

How do we deal with three simultaneous equations with only two unknowns?

$$y_1 = mt_1 + c$$
$$y_2 = mt_2 + c$$
$$y_3 = mt_3 + c$$



Overdetermined System

- With two unknowns and two observations:

$$\begin{aligned} y_1 =& mt_1 + c \\ y_2 =& mt_2 + c \end{aligned}$$

- Additional observation leads to *overdetermined* system.

$$y_3 = mt_3 + c$$

- This problem is solved through a noise model $\epsilon \sim \mathcal{N}\left(0, \sigma^2\right)$

$$\begin{aligned} y_1 &= mt_1 + c + \epsilon_1 \\ y_2 &= mt_2 + c + \epsilon_2 \\ y_3 &= mt_3 + c + \epsilon_3 \end{aligned}$$

Overdetermined System

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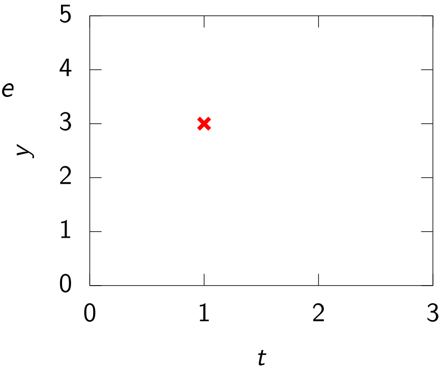
Noise Models

- We aren't modeling entire system.
- Noise model gives mismatch between model and data.
- Gaussian model justified by appeal to central limit theorem.
- Other models also possible (Student-t for heavy tails).
- Maximum likelihood with Gaussian noise leads to *least squares*.

Underdetermined System

What about two unknowns and *one* observation?

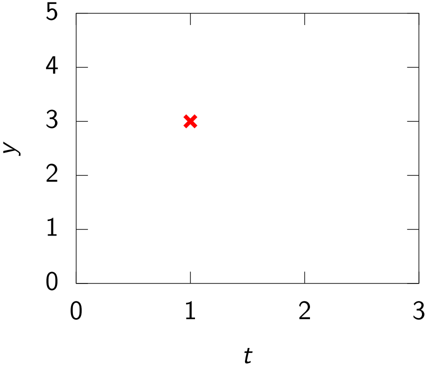
$$y_1 = mt_1 + c$$



Underdetermined System

Can compute m given c.

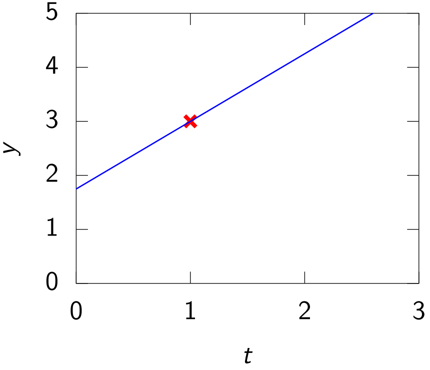
$$m = \frac{y_1 - c}{t}$$



Underdetermined System

Can compute m given c.

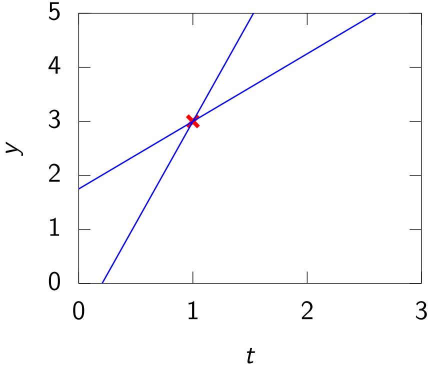
$$c = 1.75 \Longrightarrow m = 1.25$$



Underdetermined System

Can compute m given c.

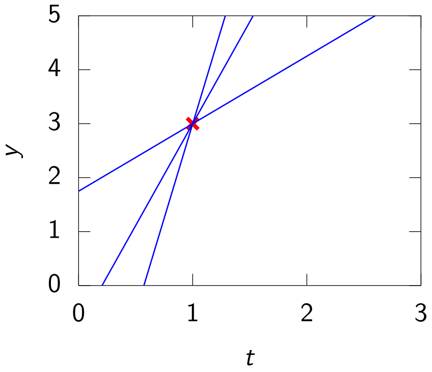
$$c = -0.777 \implies m = 3.78$$



Underdetermined System

Can compute m given c.

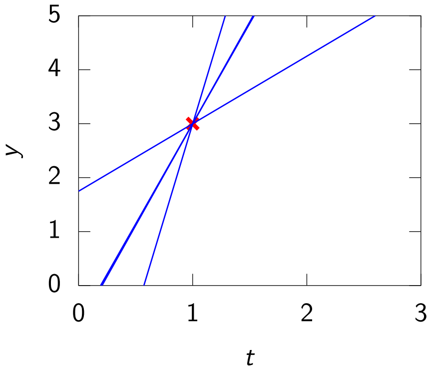
$$c = -4.01 \Longrightarrow m = 7.01$$



Underdetermined System

Can compute m given c.

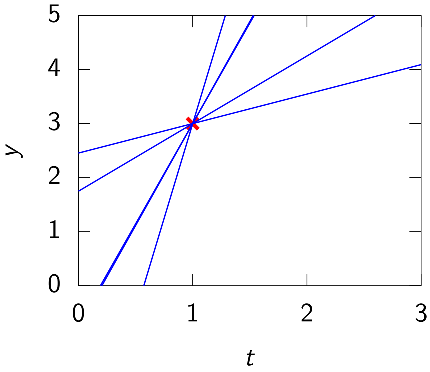
$$c = -0.718 \Longrightarrow m = 3.72$$



Underdetermined System

Can compute m given c.

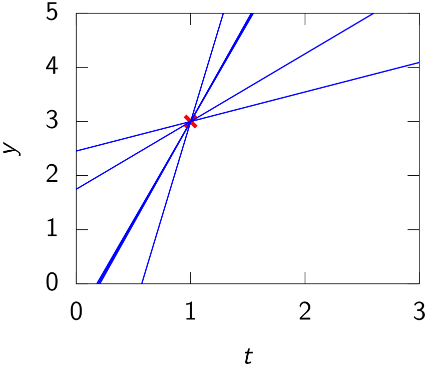
$$c = 2.45 \Longrightarrow m = 0.545$$



Underdetermined System

Can compute m given c.

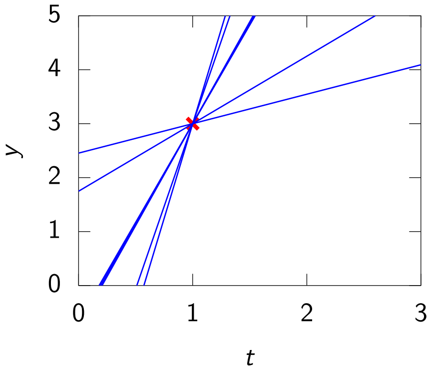
$$c = -0.657 \implies m = 3.66$$



Underdetermined System

Can compute *m* given *c*.

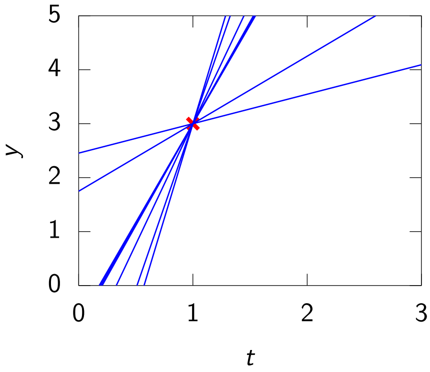
$$c = -3.13 \implies m = 6.13$$



Underdetermined System

Can compute m given c.

$$c = -1.47 \Longrightarrow m = 4.47$$

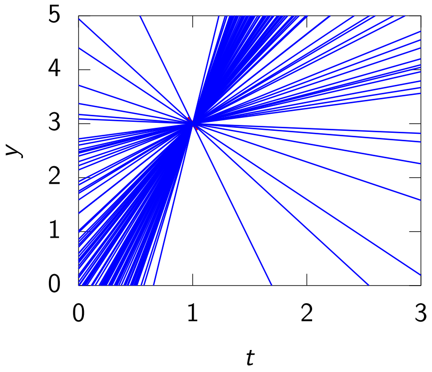


Underdetermined System

Can compute m given c.
Assume

$$c \sim \mathcal{N}(0, 4),$$

we find a distribution of solutions.



Probability for Under- and Overdetermined

- To deal with overdetermined introduced probability distribution for 'variable', ϵ_i.
- For underdetermined system introduced probability distribution for 'parameter', c.
- This is known as a Bayesian treatment.

- For general Bayesian inference need multivariate priors.
- E.g. for multivariate linear regression:

$$y_i = \sum_i w_j t_{i,j} + \epsilon_i$$

(where we've dropped c for convenience), we need a prior over $\mathbf{w}$.
- This motivates a *multivariate* Gaussian density.
- We will use the multivariate Gaussian to put a prior *directly* on the function (a Gaussian process).

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Two Dimensional Gaussian

- Consider height, h/m and weight, w/kg.
- Could sample height from a distribution:

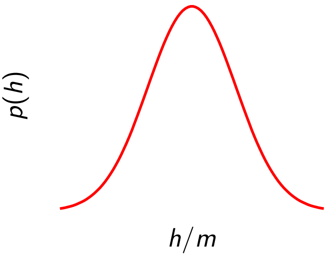
$$p(h) \sim \mathcal{N}(1.7, 0.0225)$$

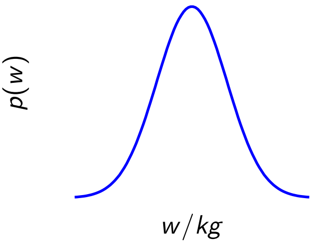
- And similarly weight:

$$p(w) \sim \mathcal{N}(75, 36)$$

Height and Weight Models

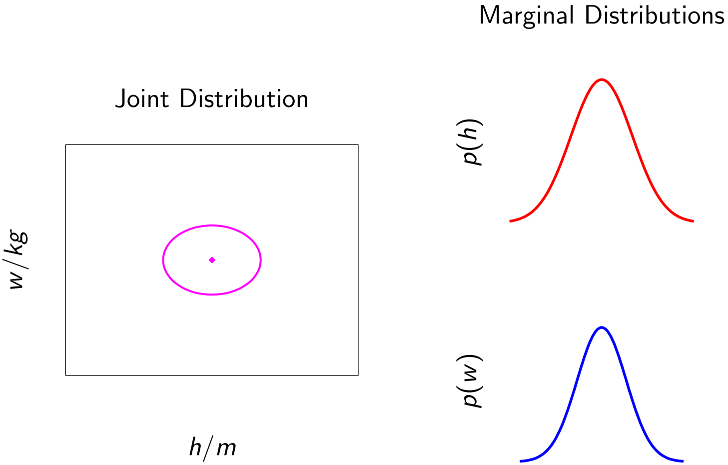
Marginal Distributions





Gaussian distributions for height and weight.

Sampling Two Dimensional Variables



Sample height and weight one after the other and plot against each other.

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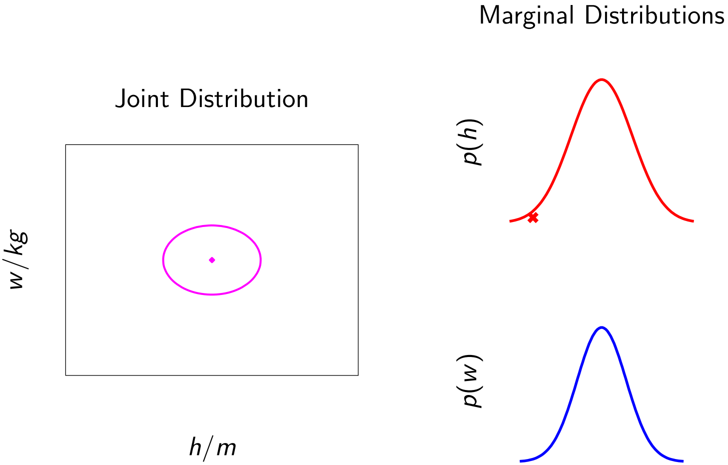

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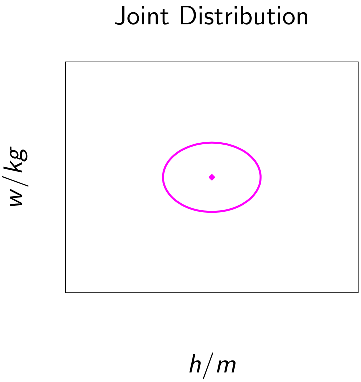

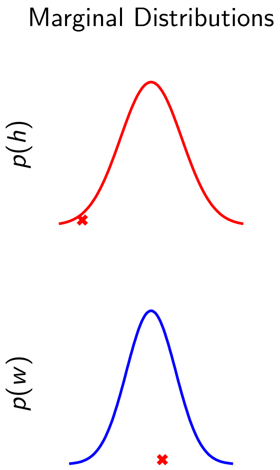

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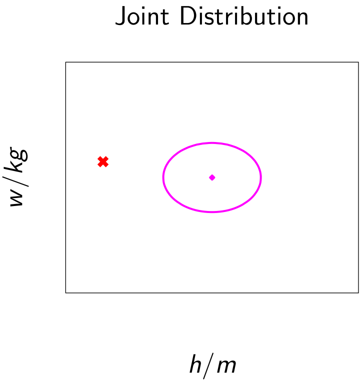

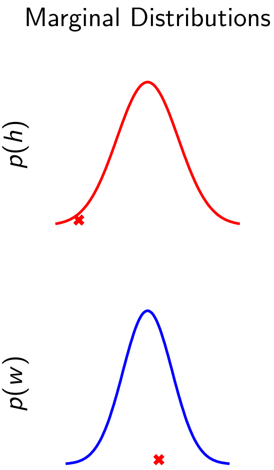

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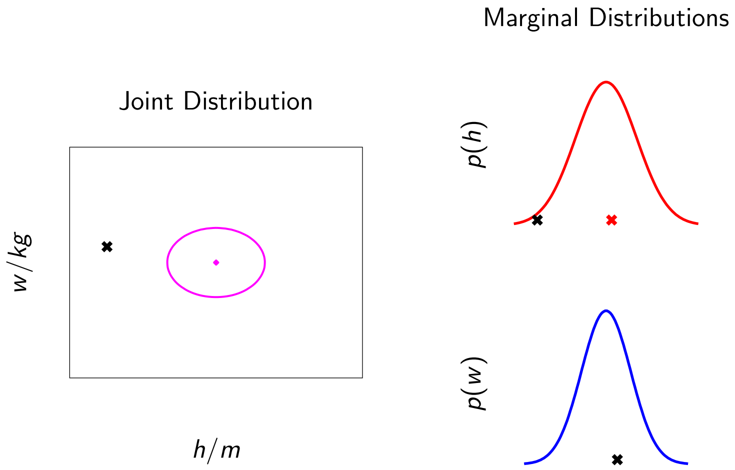

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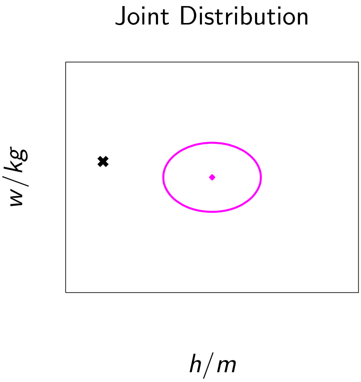

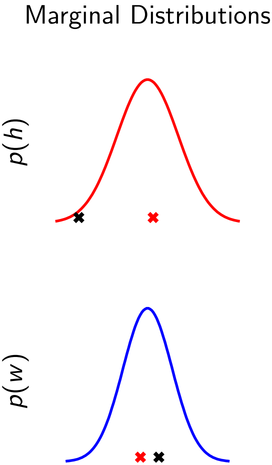

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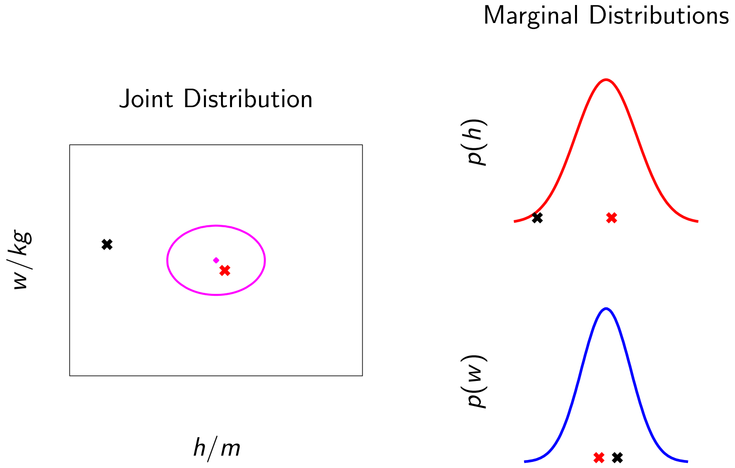

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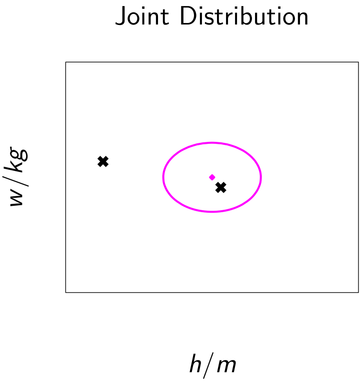

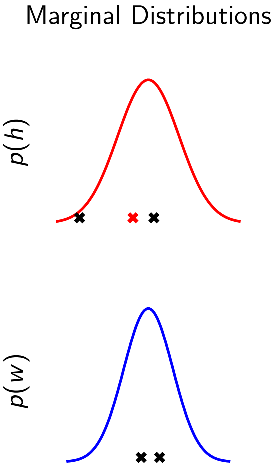

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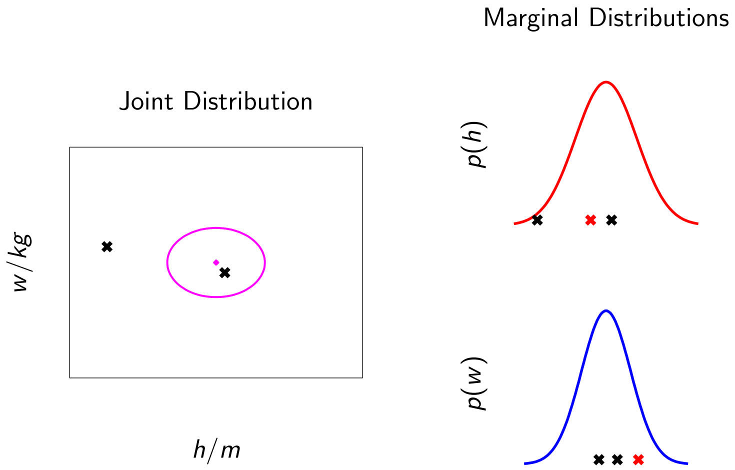

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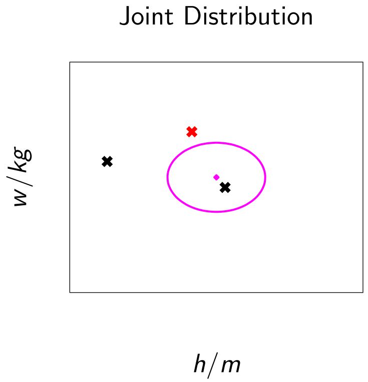

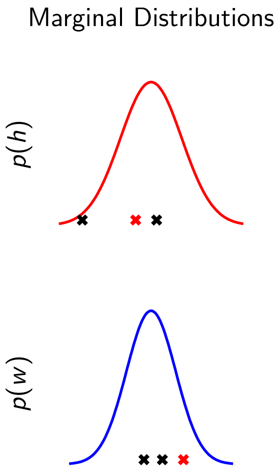

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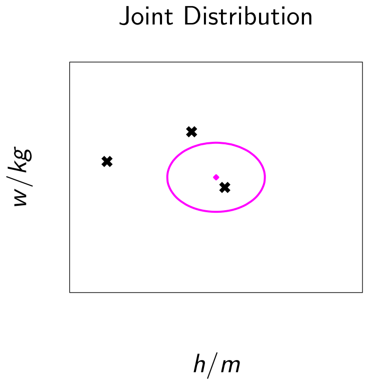

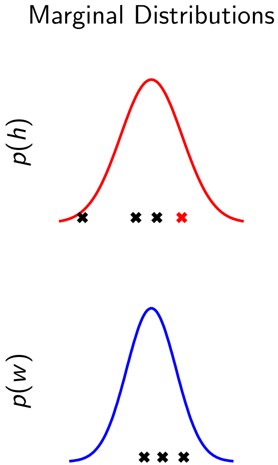

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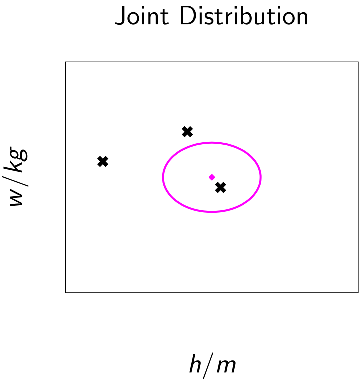

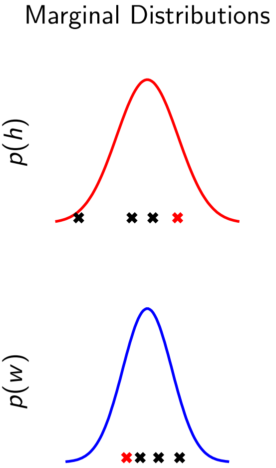

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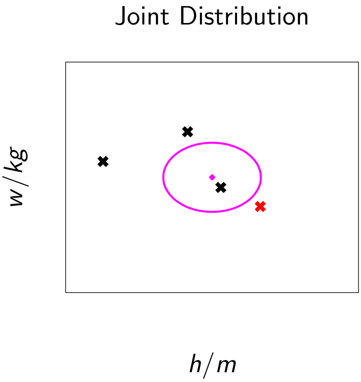

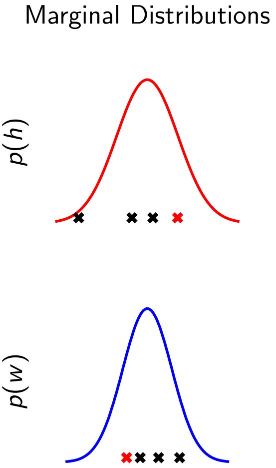

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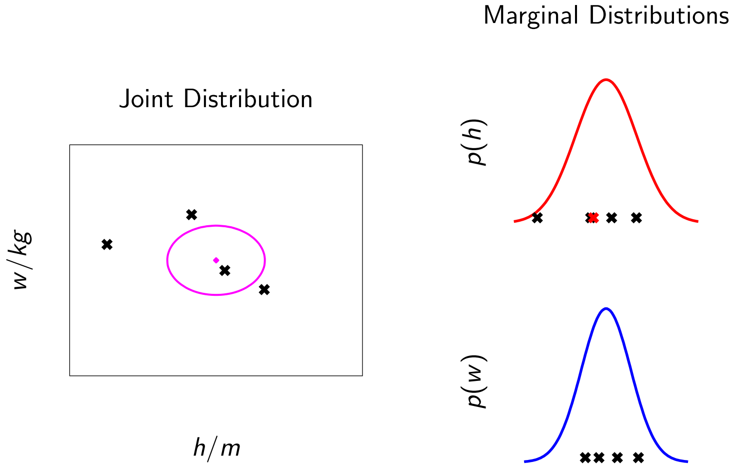

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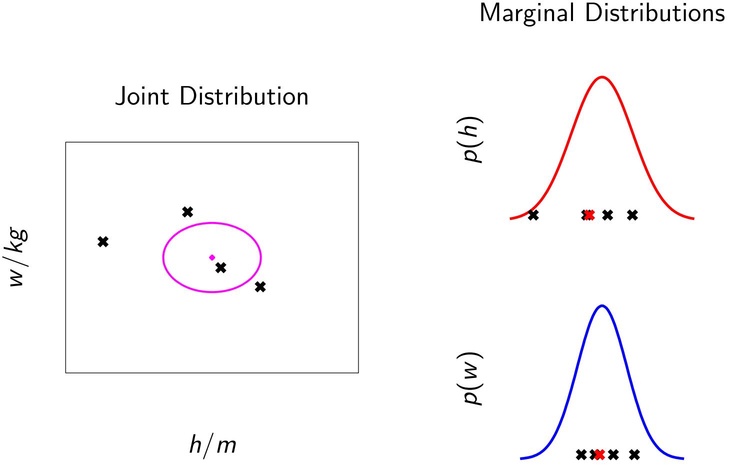

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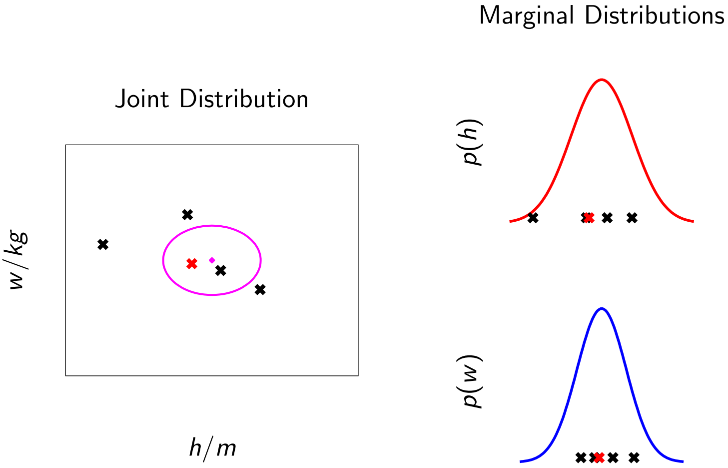

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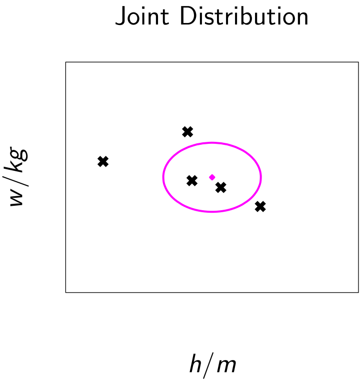

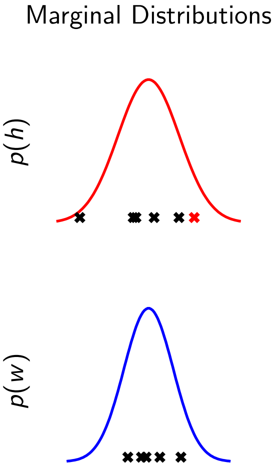

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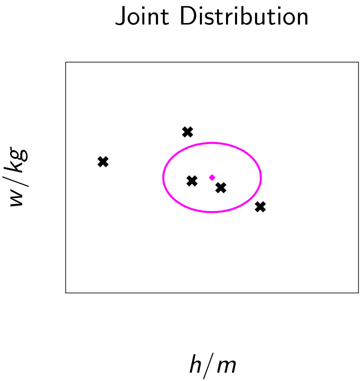

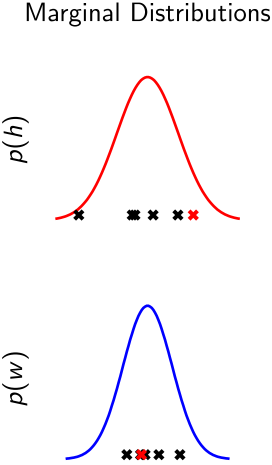

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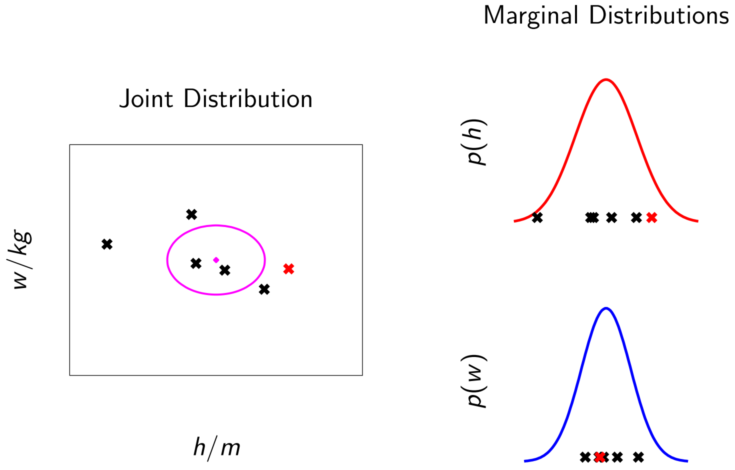
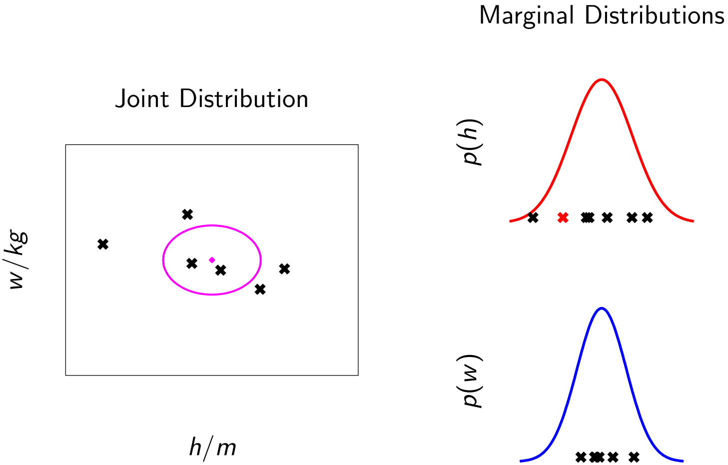


Sample height and weight one after the other and plot against each other.

Sampling Two Dimensional Variables



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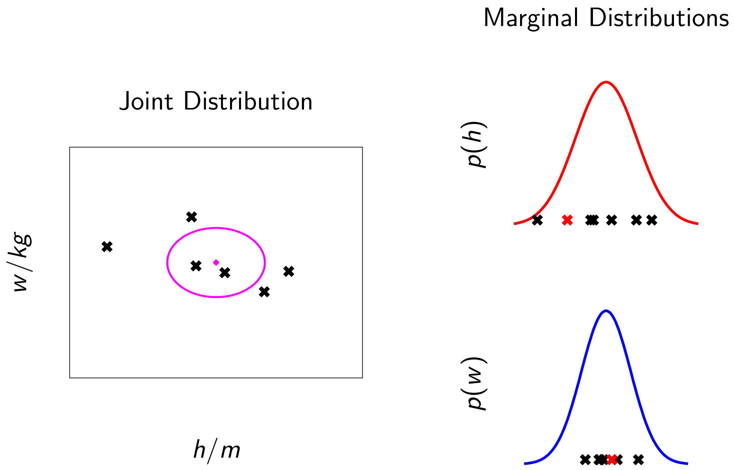

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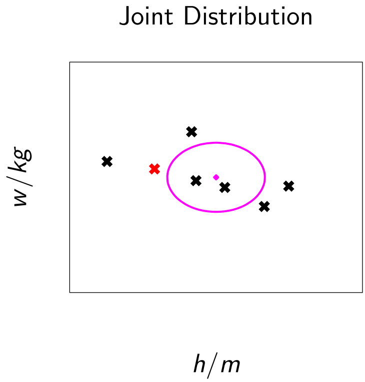

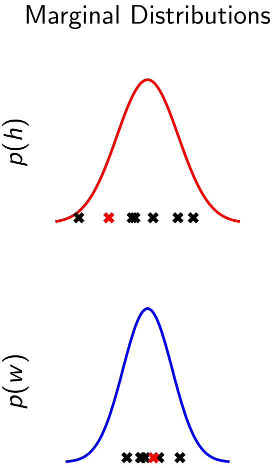

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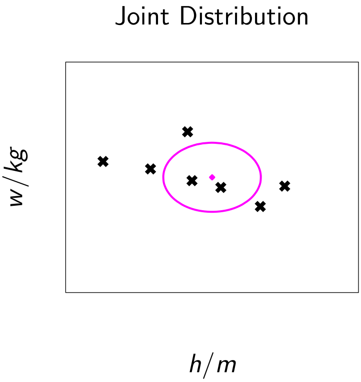
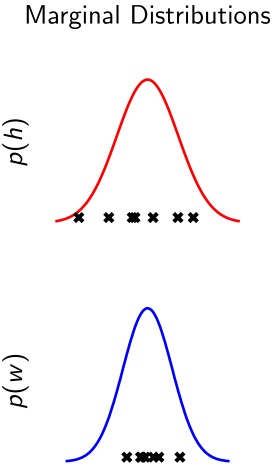




Sample height and weight one after the other and plot against each other.

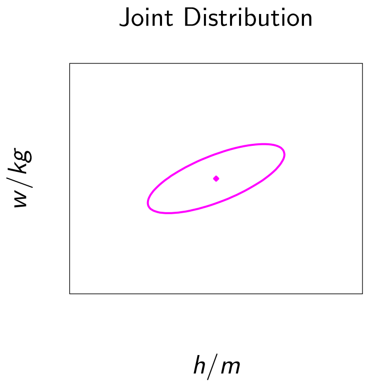
Independence Assumption

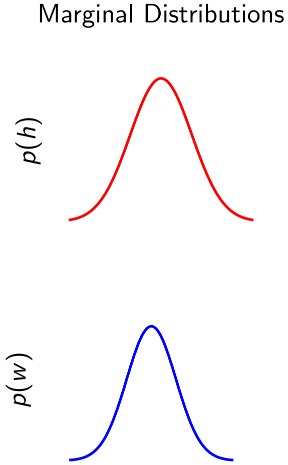
- This assumes height and weight are independent.

$$p(h, w) = p(h)p(w)$$

- In reality they are dependent (body mass index) $= \frac{w}{h^2}$.

Sampling Two Dimensional Variables





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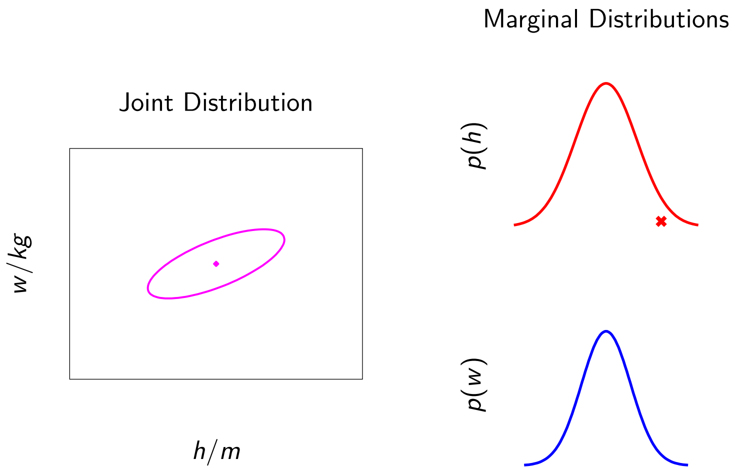

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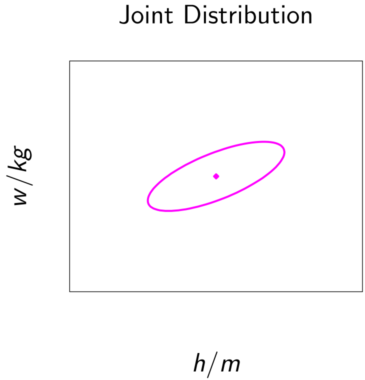

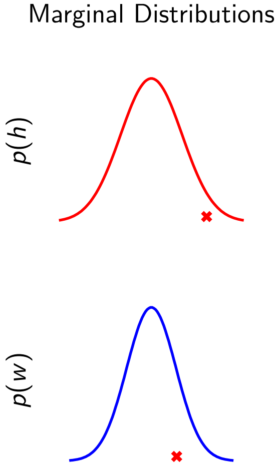

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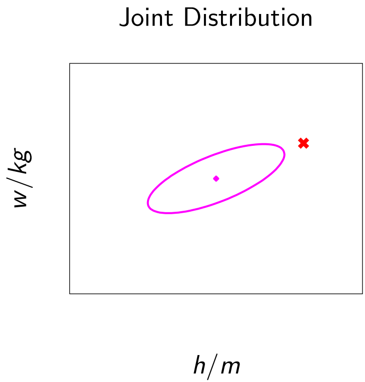

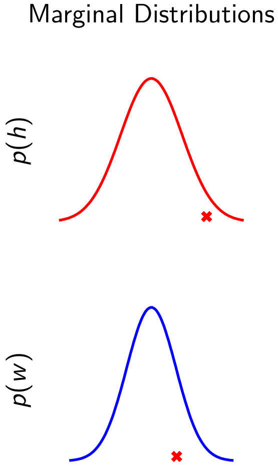

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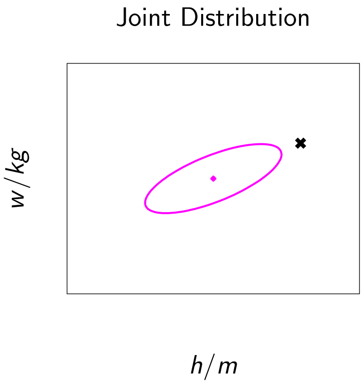

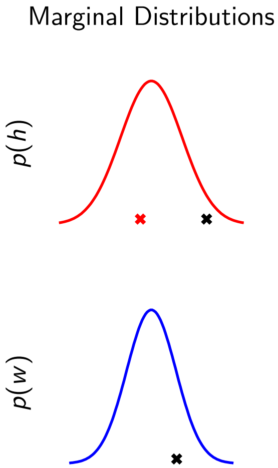

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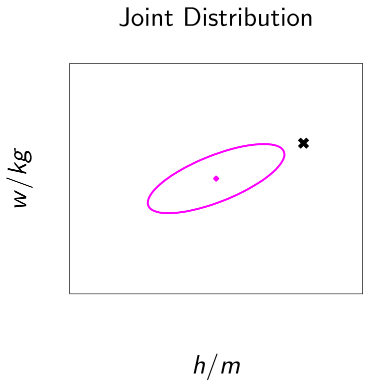

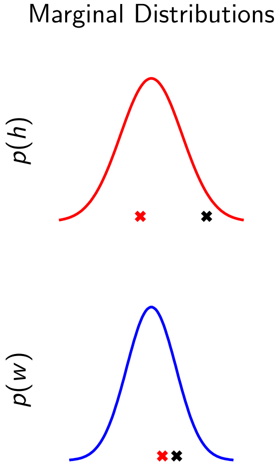

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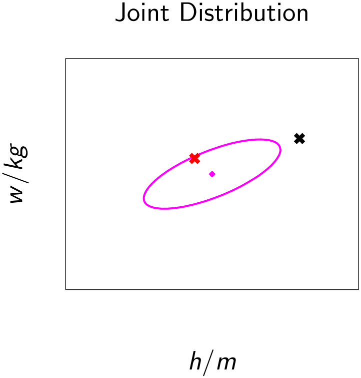

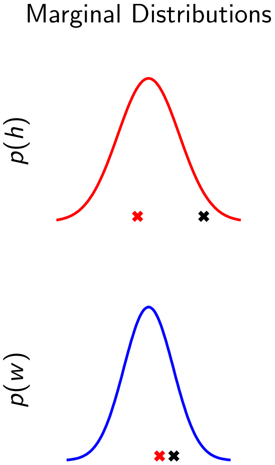

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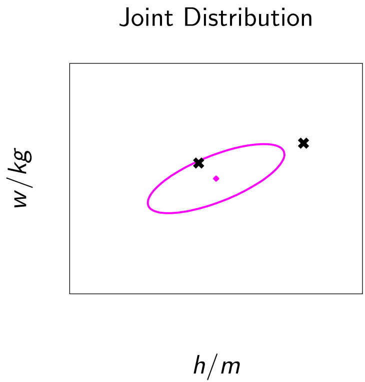

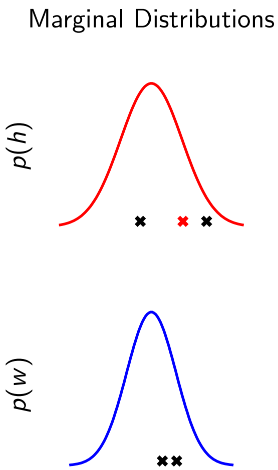

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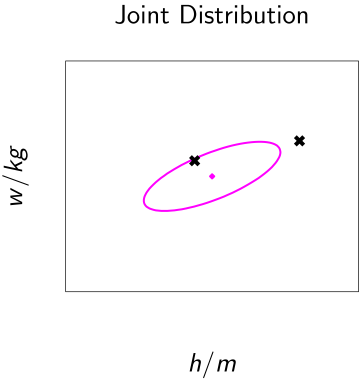

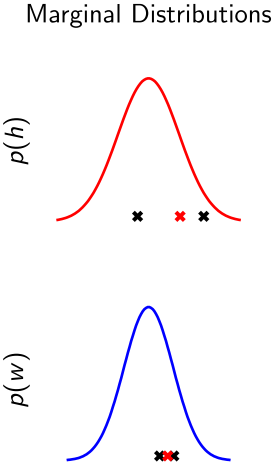

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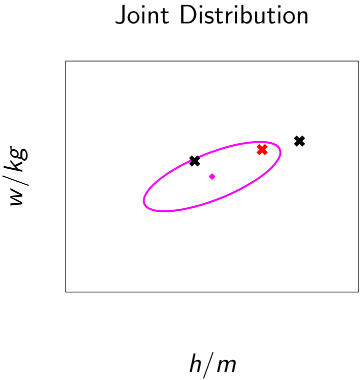

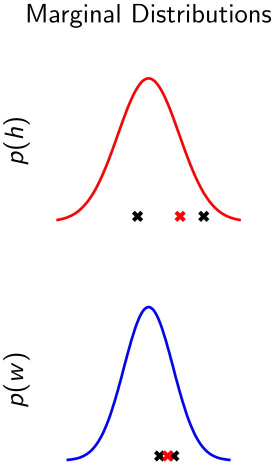

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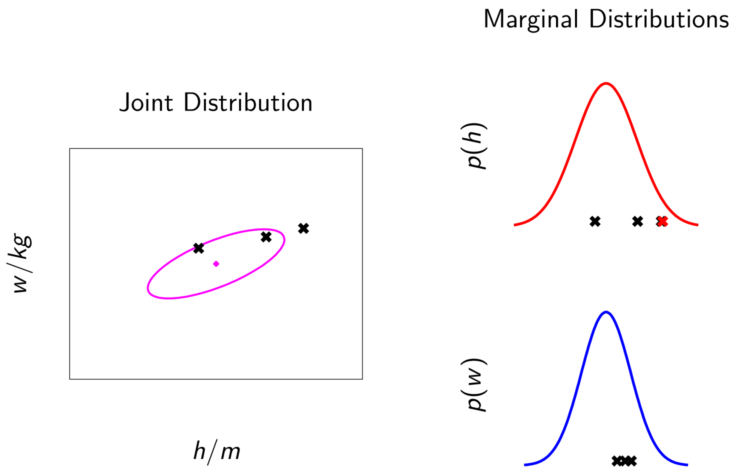

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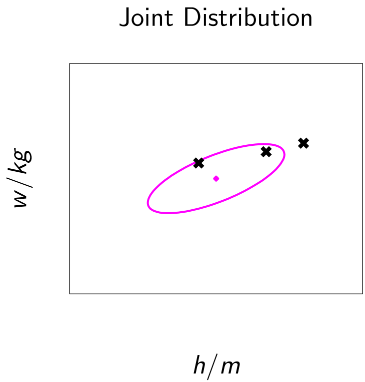

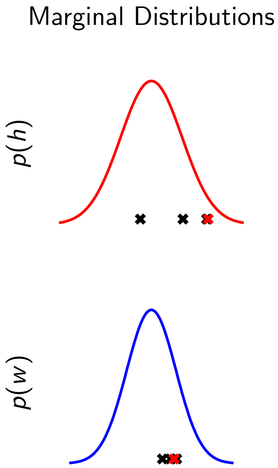

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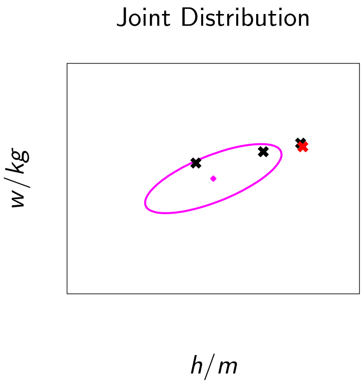

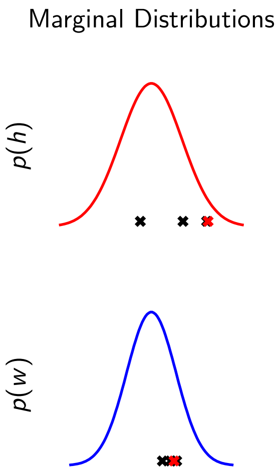

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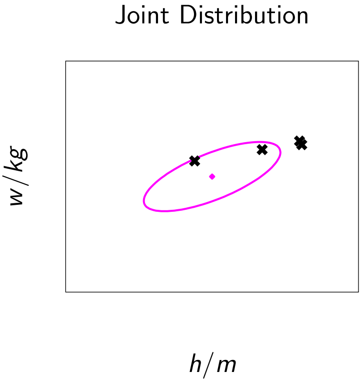

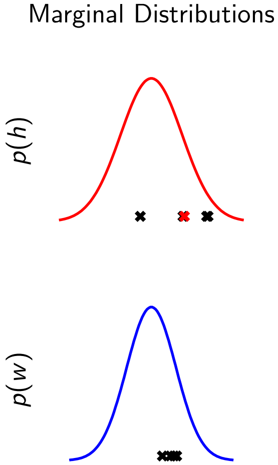

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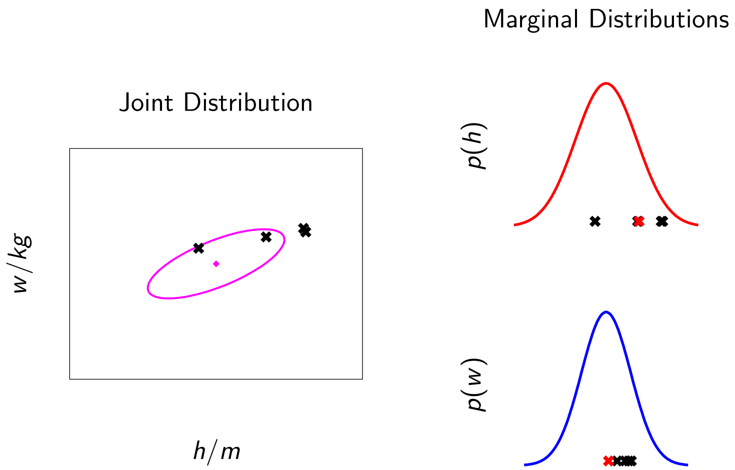

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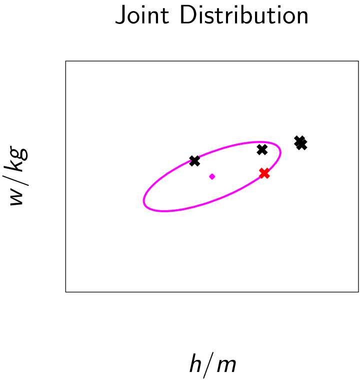

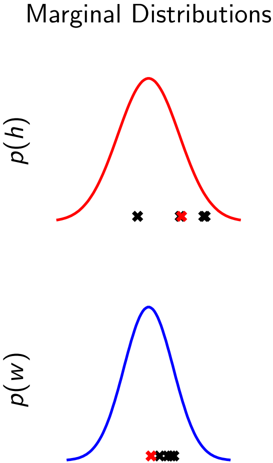

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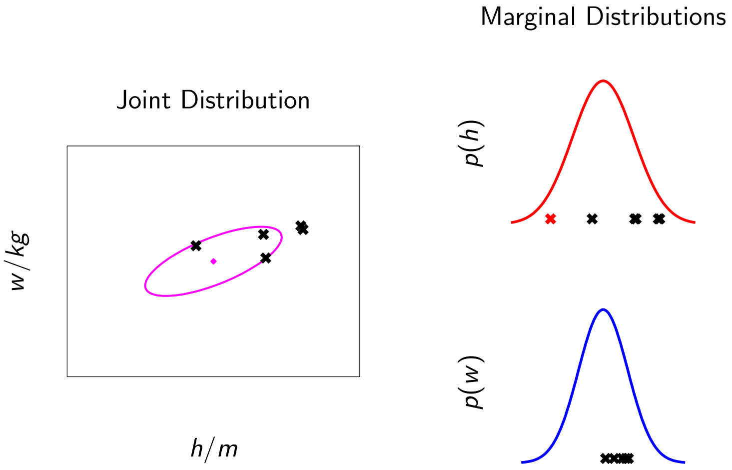

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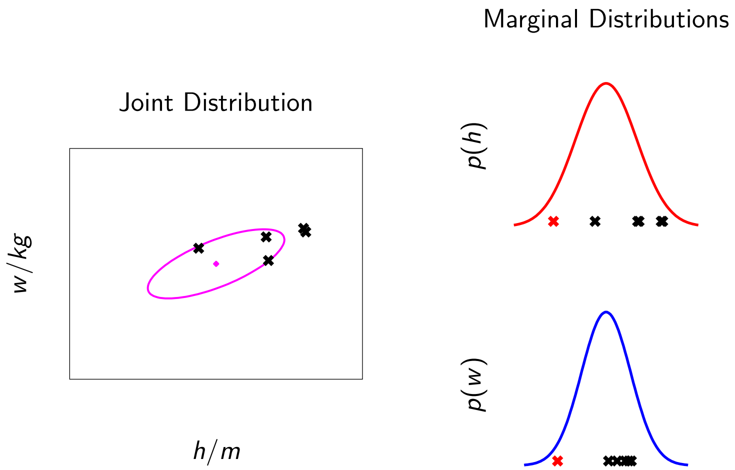

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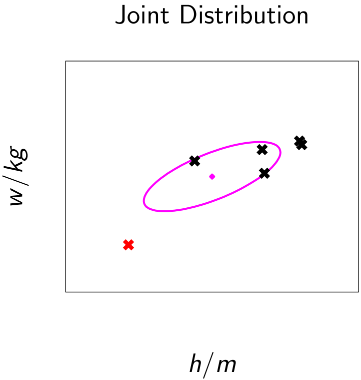

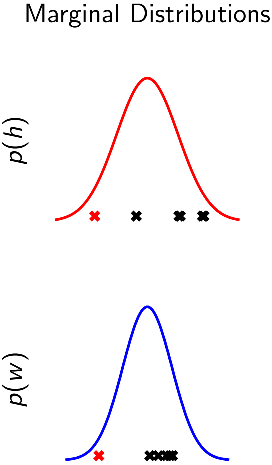

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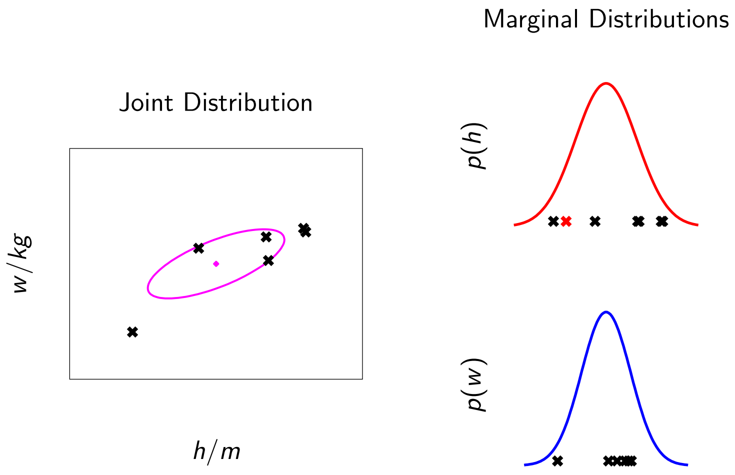

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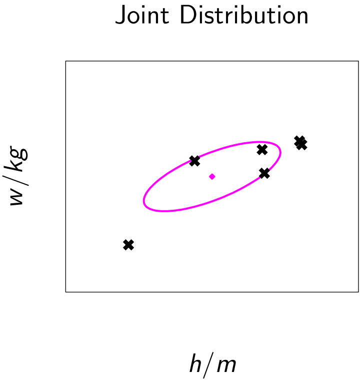

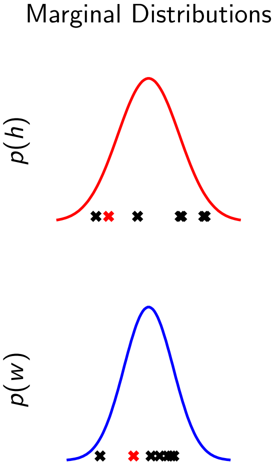

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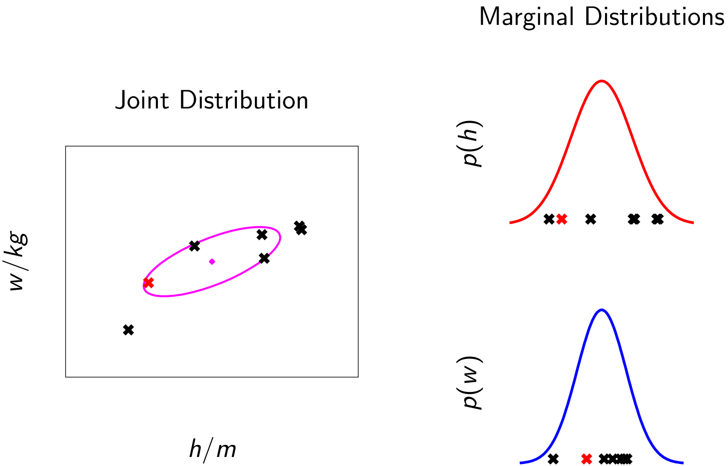

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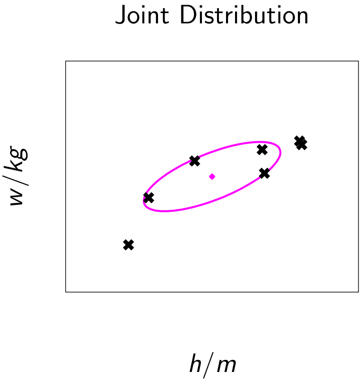

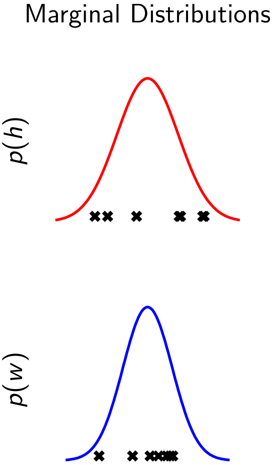

Independent Gaussians

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$$p(w, h) = \frac{1}{\sqrt{2\pi\sigma_1^2}\sqrt{2\pi\sigma_2^2}} \exp\left(-\frac{1}{2}\left(\frac{(w-\mu_1)^2}{\sigma_1^2} + \frac{(h-\mu_2)^2}{\sigma_2^2}\right)\right)$$

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Independent Gaussians

$$p(\mathbf{y}) = \frac{1}{2\pi \left|\mathbf{D}\right|} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^{\top}\mathbf{D}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right)$$

Correlated Gaussian

Form correlated from original by rotating the data space using matrix **R**.

$$p(\mathbf{y}) = \frac{1}{2\pi \left|\mathbf{D}\right|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{y} - \boldsymbol{\mu})^{\top}\mathbf{D}^{-1}(\mathbf{y} - \boldsymbol{\mu})\right)$$

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this gives a covariance matrix:

$$\mathbf{C}^{-1} = \mathbf{R}\mathbf{D}^{-1}\mathbf{R}^\top$$

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Recall Univariate Gaussian Properties

1. Sum of Gaussian variables is also Gaussian.

$$y_i \sim \mathcal{N}\left(\mu_i, \sigma_i^2\right)$$

$$\sum_{i=1}^{n} y_i \sim \mathcal{N}\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2\right)$$

2. Scaling a Gaussian leads to a Gaussian.

$$y \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

$$wy \sim \mathcal{N}\left(w\mu, w^2\sigma^2\right)$$

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Multivariate Consequence

- If

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

- And

$$\mathbf{y} = \mathbf{W}\mathbf{t}$$

- Then

$$\mathbf{y} \sim \mathcal{N}\left(\mathbf{W}\mu, \mathbf{W}\Sigma\mathbf{W}^{\top}\right)$$

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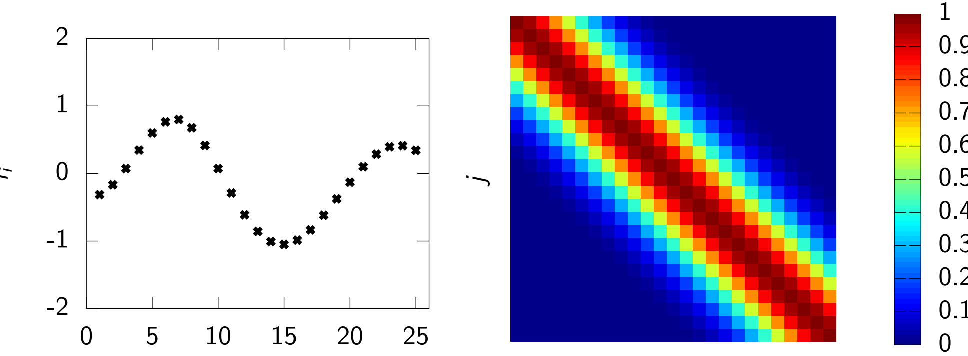
Sampling a Function

Multi-variate Gaussians

- We will consider a Gaussian with a particular structure of covariance matrix.
- Generate a single sample from this 25 dimensional Gaussian distribution, $\mathbf{f} = [f_1, f_2 \ldots f_{25}]$.
- We will plot these points against their index.

Gaussian Distribution Sample

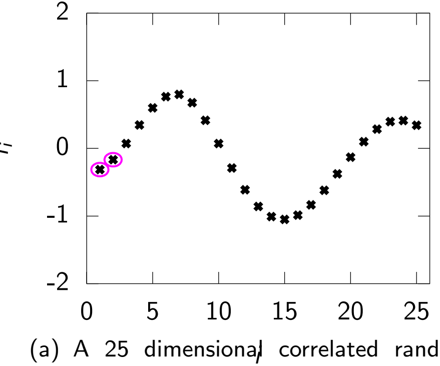


(a) A 25 dimensional correlated random variable (values ploted against index)

(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



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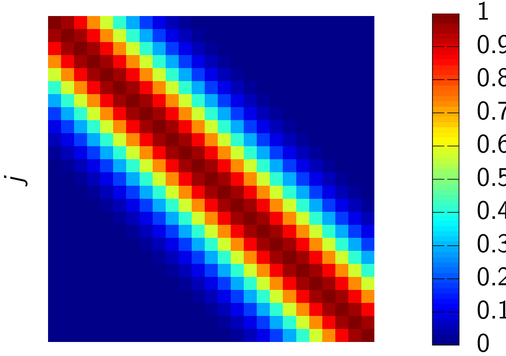

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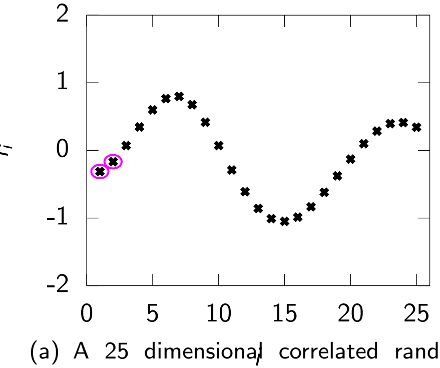

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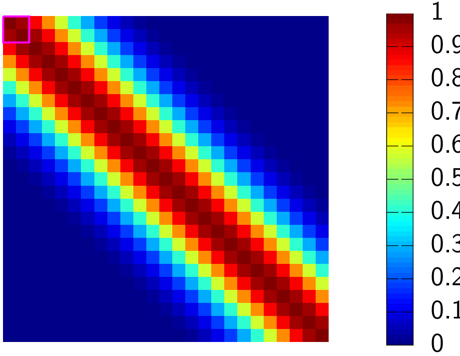

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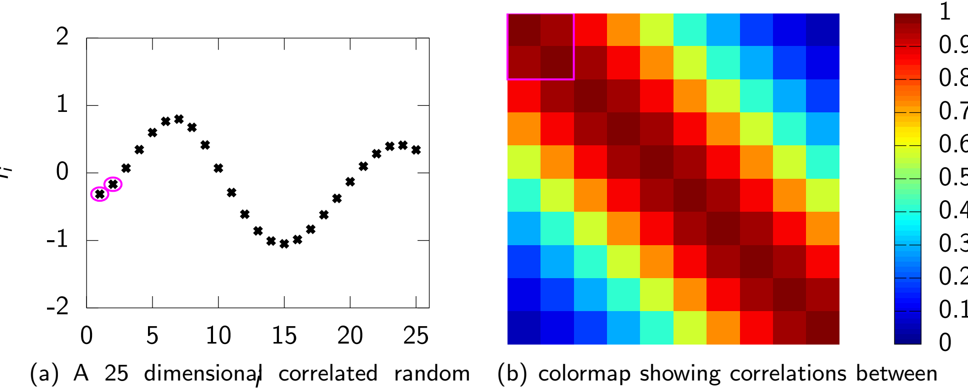

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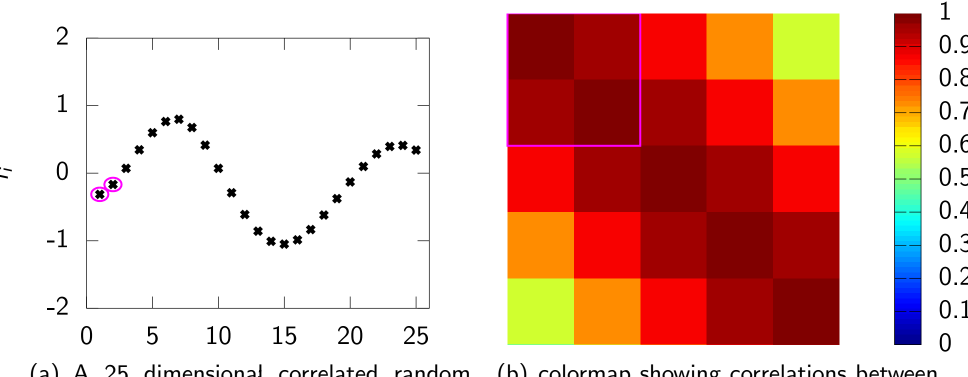

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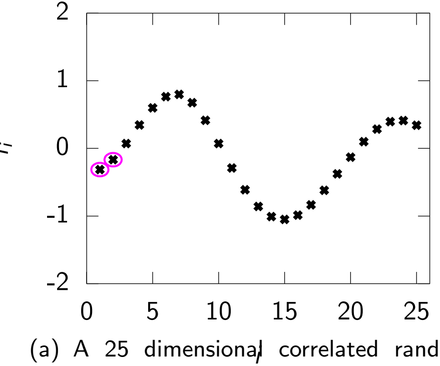
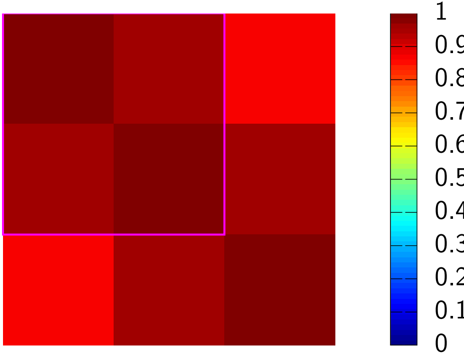
Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



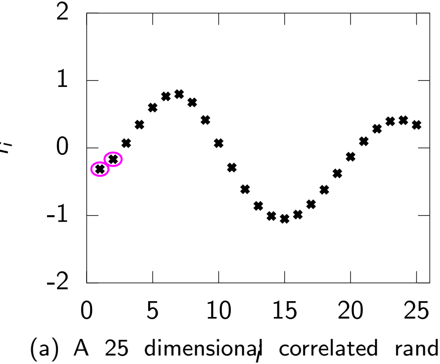
(a) A 25 dimensional correlated random variable (values ploted against index)



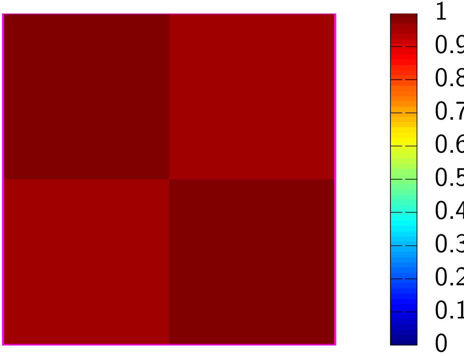
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



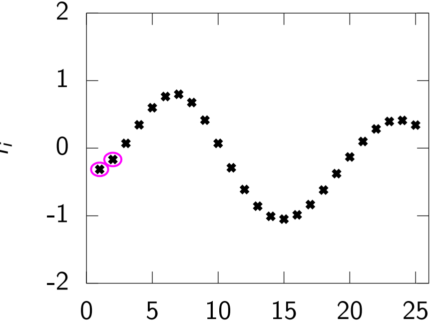
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



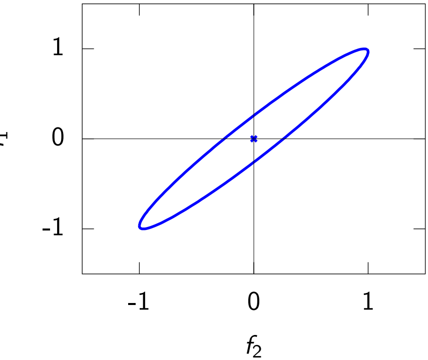
(a) A 25 dimensional correlated random variable (values ploted against index)

$$\begin{bmatrix} 1 & 0.96587 \\ 0.96587 & 1 \end{bmatrix}$$

(b) correlation between f_1 and f_2.

Figure: A sample from a 25 dimensional Gaussian distribution.

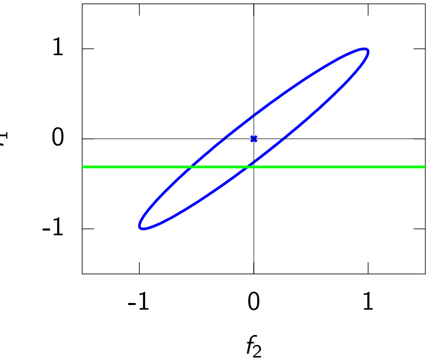
Prediction of f_2 from f_1



$$\begin{bmatrix} 1 & 0.96587 \\ 0.96587 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_2)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_2|f_1 = -0.313)$.

Prediction of f_2 from f_1



$$\begin{bmatrix} 1 & 0.96587 \\ 0.96587 & 1 \end{bmatrix}$$

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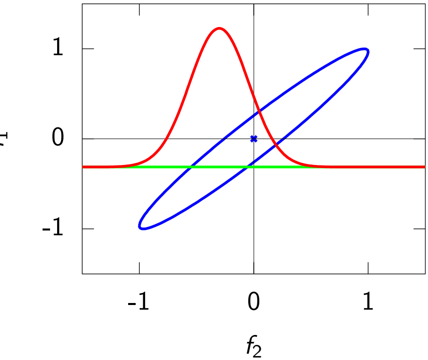

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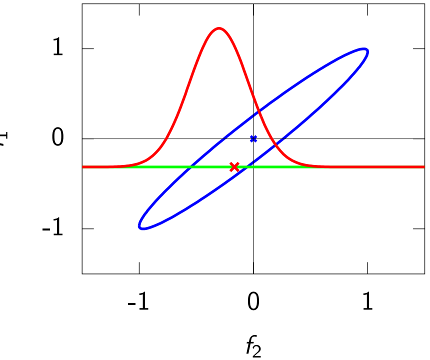
Prediction of f_2 from f_1



$$\begin{bmatrix} 1 & 0.96587 \\ 0.96587 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_2)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_2|f_1 = -0.313)$.

Prediction with Correlated Gaussians

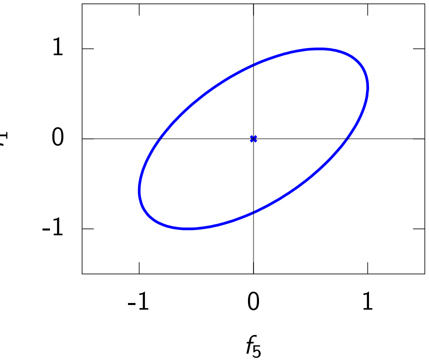
- Prediction of f_2 from f_1 requires *conditional density*.
- Conditional density is *also* Gaussian.

$$p(f_2|f_1) = \mathcal{N}\left(f_2|\frac{k_{1,2}}{k_{1,1}}f_1, k_{2,2} - \frac{k_{1,2}^2}{k_{1,1}}\right)$$

where covariance of joint density is given by

$$\mathbf{K} = \begin{bmatrix} k_{1,1} & k_{1,2} \\ k_{2,1} & k_{2,2} \end{bmatrix}$$

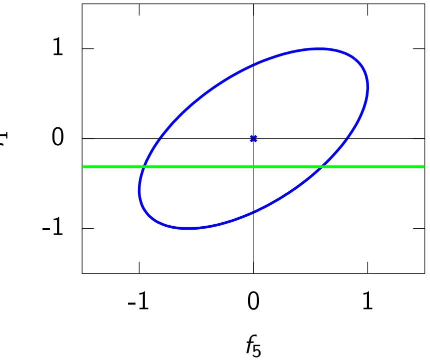
Prediction of f_5 from f_1



$$\begin{bmatrix} 1 & 0.57375 \\ 0.57375 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_5)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_5|f_1 = -0.313)$.

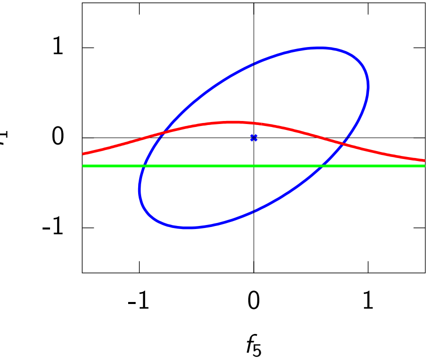
Prediction of f_5 from f_1



$$\begin{bmatrix} 1 & 0.57375 \\ 0.57375 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_5)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_5|f_1 = -0.313)$.

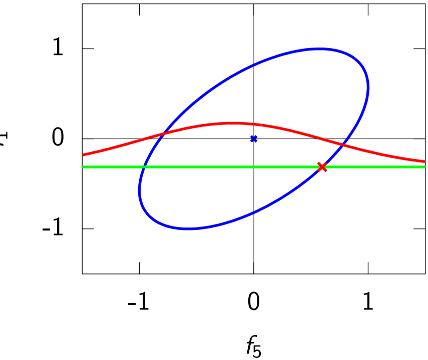
Prediction of f_5 from f_1



$$\begin{bmatrix} 1 & 0.57375 \\ 0.57375 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_5)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_5|f_1 = -0.313)$.

Prediction of f_5 from f_1



$$\begin{bmatrix} 1 & 0.57375 \\ 0.57375 & 1 \end{bmatrix}$$

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_5)$.
- We observe that $f_1 = -0.313$.
- Conditional density: $p(f_5|f_1 = -0.313)$.

Prediction with Correlated Gaussians

- Prediction of $\mathbf{f}_*$ from $\mathbf{f}$ requires multivariate *conditional density*.
- Multivariate conditional density is *also* Gaussian.

$$p(\mathbf{f}_*|\mathbf{f}) = \mathcal{N}\left(\mathbf{f}_*|\mathbf{K}_{*,\mathbf{f}}\mathbf{K}_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{f}, \mathbf{K}_{*,*} - \mathbf{K}_{*,\mathbf{f}}\mathbf{K}_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{K}_{\mathbf{f},*}\right)$$

- Here covariance of joint density is given by

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{\mathbf{f},\mathbf{f}} & \mathbf{K}_{*,\mathbf{f}} \\ \mathbf{K}_{\mathbf{f},*} & \mathbf{K}_{*,*} \end{bmatrix}$$

Prediction with Correlated Gaussians

- Prediction of $\mathbf{f}_*$ from $\mathbf{f}$ requires multivariate *conditional density*.
- Multivariate conditional density is *also* Gaussian.

$$p(\mathbf{f}_*|\mathbf{f}) = \mathcal{N}\left(\mathbf{f}_*|\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$
$$\boldsymbol{\mu} = \mathbf{K}_{*,\mathbf{f}}\mathbf{K}_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{f}$$
$$\boldsymbol{\Sigma} = \mathbf{K}_{*,*} - \mathbf{K}_{*,\mathbf{f}}\mathbf{K}_{\mathbf{f},\mathbf{f}}^{-1}\mathbf{K}_{\mathbf{f},*}$$

- Here covariance of joint density is given by

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{\mathbf{f},\mathbf{f}} & \mathbf{K}_{*,\mathbf{f}} \\ \mathbf{K}_{\mathbf{f},*} & \mathbf{K}_{*,*} \end{bmatrix}$$

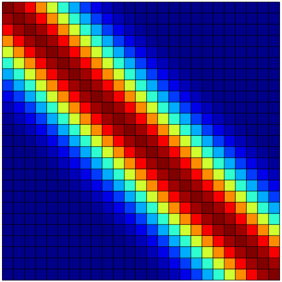
Covariance Functions

Where did this covariance matrix come from?

Exponentiated Quadratic Kernel Function (RBF, Squared Exponential, Gaussian)

$$k\left(t, t'\right) = \alpha \exp\left(-\frac{\left\|t - t'\right\|_2^2}{2\ell^2}\right)$$

- Covariance matrix is built using the *inputs* to the function t.
- For the example above it was based on Euclidean distance.
- The covariance function is also know as a kernel.



Covariance Functions

Where did this covariance matrix come from?

Exponentiated Quadratic Kernel Function (RBF, Squared Exponential, Gaussian)

$$k\left(t, t'\right) = \alpha \exp\left(-\frac{\|t - t'\|_2^2}{2\ell^2}\right)$$

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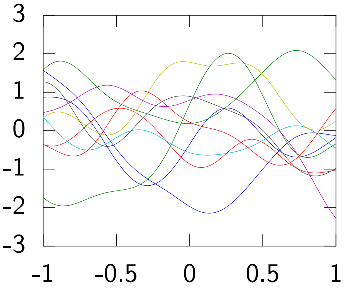


Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left\|t_i - t_j\right\|^2}{2\ell^2}\right)$$

$$t_1 = -3.0, \; t_1 = -3.0$$

$$k_{1,1} = 1.00 \times \exp\left(-\frac{(-3.0 - -3.0)^2}{2 \times 2.00^2}\right)$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_1 = -3.0, \; t_1 = -3.0$$

$$k_{1,1} = 1.00 \times \exp\left(-\frac{(-3.0 - -3.0)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & & \\ & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_1 = -3.0$$

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & & \\ & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_1 = -3.0$$

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & & \\ \boxed{0.110} & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_2 = 1.20,\ t_1 = -3.0$

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20-1.20)^2}{2\times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & \\ 0.110 & & \\ & & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_2 = 1.20$$

$$k_{2,2} = 1.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & \\ 0.110 & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_2 = 1.20$$

$$k_{2,2} = 1.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & \\ 0.110 & \boxed{1.00} & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left\|t_i - t_j\right\|^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_1 = -3.0$$

$$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & \\ 0.110 & 1.00 & \\ & & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.40, \; t_1 = -3.0$

$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40-1.40)^2}{2\times 2.00^2}\right)$

$$\begin{bmatrix} 1.00 & 0.110 & \\ 0.110 & 1.00 & \\ 0.0889 & & \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left\|t_i - t_j\right\|^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_1 = -3.0$$

$$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40-1.40)^2}{2\times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & \\ 0.0889 & & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \ t_2 = 1.20$$

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & \\ 0.0889 & & \end{bmatrix}$$

$t_1 = -3.0, \ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_2 = 1.20$$

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & \\ 0.0889 & \boxed{0.995} & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_2 = 1.20$$

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & 0.995 \\ 0.0889 & 0.995 & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.40, \; t_3 = 1.40$

$$k_{3,3} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & 0.995 \\ 0.0889 & 0.995 & \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left\|t_i - t_j\right\|^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_3 = 1.40$$

$$k_{3,3} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$

$$\begin{bmatrix} 1.00 & 0.110 & 0.0889 \\ 0.110 & 1.00 & 0.995 \\ 0.0889 & 0.995 & \boxed{1.00} \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

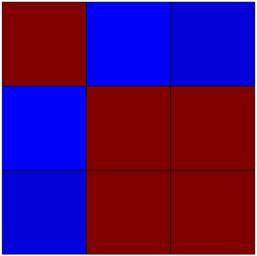
Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left|\left|t_i - t_j\right|\right|^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_3 = 1.40$$

$$k_{3,3} = 1.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 2.00^2}\right)$$



$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left|\left|t_i - t_j\right|\right|^2}{2\ell^2}\right)$$

$$t_1 = -3,\ t_1 = -3$$

$$k_{1,1} = 1.0 \times \exp\left(-\frac{(-3 - -3)^2}{2 \times 2.0^2}\right)$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_1 = -3, \; t_1 = -3$$

$$k_{1,1} = 1.0 \times \exp\left(-\frac{(-3 - -3)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} \boxed{1.0} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.2,\ t_1 = -3$$

$$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2-1.2)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.2,\ t_1 = -3$$

$$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2 - 1.2)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & & & \\ 0.11 & & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_2 = 1.2,\ t_1 = -3$

$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2-1.2)^2}{2\times 2.0^2}\right)$

$$\begin{bmatrix} 1.0 & 0.11 & & \\ 0.11 & & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.2,\ t_2 = 1.2$$

$$k_{2,2} = 1.0 \times \exp\left(-\frac{(1.2-1.2)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & & \\ 0.11 & & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4,$ and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.2,\; t_2 = 1.2$$

$$k_{2,2} = 1.0 \times \exp\left(-\frac{(1.2-1.2)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & & \\ 0.11 & \boxed{1.0} & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\; t_2 = 1.2,\; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.4, \; t_1 = -3$$

$$k_{3,1} = 1.0 \times \exp\left(-\frac{(1.4 - 1.4)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & & \\ 0.11 & 1.0 & & \\ & & & \\ & & & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.4,\ t_1 = -3$$

$$k_{3,1} = 1.0 \times \exp\left(-\frac{(1.4 - 1.4)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & & \\ 0.11 & 1.0 & & \\ 0.089 & & & \\ & & & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.4, \; t_1 = -3$$

$$k_{3,1} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & & \\ 0.089 & & & \\ & & & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.4,\ t_2 = 1.2$

$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2\times 2.0^2}\right)$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & & \\ 0.089 & & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4,$ and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.4,\ t_2 = 1.2$

$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2\times 2.0^2}\right)$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & & \\ 0.089 & \boxed{1.0} & & \\ & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.4, \; t_2 = 1.2$

$$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & & \\ & & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.4, \ t_3 = 1.4$$

$$k_{3,3} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & & \\ & & & \end{bmatrix}$$

$t_1 = -3, \ t_2 = 1.2, \ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.4, \ t_3 = 1.4$

$$k_{3,3} = 1.0 \times \exp\left(-\frac{(1.4-1.4)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 \\ 0.11 & 1.0 & 1.0 \\ 0.089 & 1.0 & \boxed{1.0} \end{bmatrix}$$

$t_1 = -3, \ t_2 = 1.2, \ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \; t_1 = -3$$

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0 - 2.0)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & 1.0 & \\ & & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4,$ and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0.$

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0,\ t_1 = -3$$

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & 1.0 & \\ \boxed{0.044} & & & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \; t_1 = -3$$

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0,\ t_2 = 1.2$$

$$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & & & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_4 = 2.0, \; t_2 = 1.2$

$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & \boxed{0.92} & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \ t_2 = 1.2$$

$$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & 0.92 & & \end{bmatrix}$$

$t_1 = -3, \ t_2 = 1.2, \ t_3 = 1.4,$ and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_4 = 2.0, \; t_3 = 1.4$

$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & 0.92 & & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0,\ t_3 = 1.4$$

$$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & \\ 0.044 & 0.92 & \boxed{0.96} & \end{bmatrix}$$

$t_1 = -3,\ t_2 = 1.2,\ t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \; t_3 = 1.4$$

$$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & 0.96 \\ 0.044 & 0.92 & 0.96 & \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \; t_4 = 2.0$$

$$k_{4,4} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2\times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & 0.96 \\ 0.044 & 0.92 & 0.96 & \end{bmatrix}$$

$t_1 = -3$, $t_2 = 1.2$, $t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_4 = 2.0, \; t_4 = 2.0$$

$$k_{4,4} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2 \times 2.0^2}\right)$$

$$\begin{bmatrix} 1.0 & 0.11 & 0.089 & 0.044 \\ 0.11 & 1.0 & 1.0 & 0.92 \\ 0.089 & 1.0 & 1.0 & 0.96 \\ 0.044 & 0.92 & 0.96 & \boxed{1.0} \end{bmatrix}$$

$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

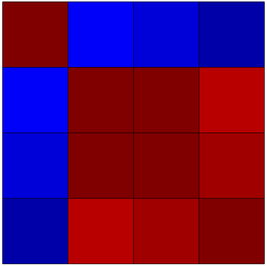
Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_4 = 2.0, \; t_4 = 2.0$

$$k_{4,4} = 1.0 \times \exp\left(-\frac{(2.0-2.0)^2}{2 \times 2.0^2}\right)$$



$t_1 = -3, \; t_2 = 1.2, \; t_3 = 1.4$, and $t_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left|\left|t_i - t_j\right|\right|^2}{2\ell^2}\right)$$

$$t_1 = -3.0,\ t_1 = -3.0$$

$$k_{1,1} = 4.00 \times \exp\left(-\frac{(-3.0 - -3.0)^2}{2 \times 5.00^2}\right)$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_1 = -3.0, \; t_1 = -3.0$$

$$k_{1,1} = 4.00 \times \exp\left(-\frac{(-3.0 - -3.0)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} \boxed{4.00} & & \\ & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20,\ t_1 = -3.0$$

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & & \\ & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{\left|\left|t_i - t_j\right|\right|^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_1 = -3.0$$

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & & \\ 2.81 & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20,\ t_1 = -3.0$$

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & \\ 2.81 & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_2 = 1.20$$

$$k_{2,2} = 4.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & \\ 2.81 & & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_2 = 1.20, \; t_2 = 1.20$$

$$k_{2,2} = 4.00 \times \exp\left(-\frac{(1.20 - 1.20)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 \\ 2.81 & \boxed{4.00} \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.40,\ t_1 = -3.0$

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & \\ 2.81 & 4.00 & \\ & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_1 = -3.0$$

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & \\ 2.81 & 4.00 & \\ \boxed{2.72} & & \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.40, \; t_1 = -3.0$

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & \\ 2.72 & & \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_2 = 1.20$$

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & \\ 2.72 & & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_2 = 1.20$$

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & \\ 2.72 & \boxed{4.00} & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40,\ t_2 = 1.20$$

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40-1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & 4.00 \\ 2.72 & 4.00 & \end{bmatrix}$$

$t_1 = -3.0,\ t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_3 = 1.40$$

$$k_{3,3} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & 4.00 \\ 2.72 & 4.00 & \end{bmatrix}$$

$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

$$k(t_i, t_j) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$t_3 = 1.40, \; t_3 = 1.40$

$$k_{3,3} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$

$$\begin{bmatrix} 4.00 & 2.81 & 2.72 \\ 2.81 & 4.00 & 4.00 \\ 2.72 & 4.00 & \boxed{4.00} \end{bmatrix}$$

$t_1 = -3.0, \; t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

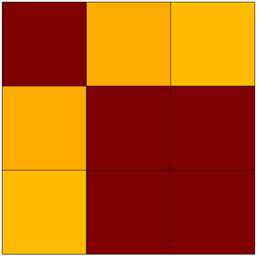
Covariance Functions

Where did this covariance matrix come from?

$$k\left(t_i, t_j\right) = \alpha \exp\left(-\frac{||t_i - t_j||^2}{2\ell^2}\right)$$

$$t_3 = 1.40, \; t_3 = 1.40$$

$$k_{3,3} = 4.00 \times \exp\left(-\frac{(1.40 - 1.40)^2}{2 \times 5.00^2}\right)$$



$t_1 = -3.0$, $t_2 = 1.20$, and $t_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Gaussian Process Interpolation

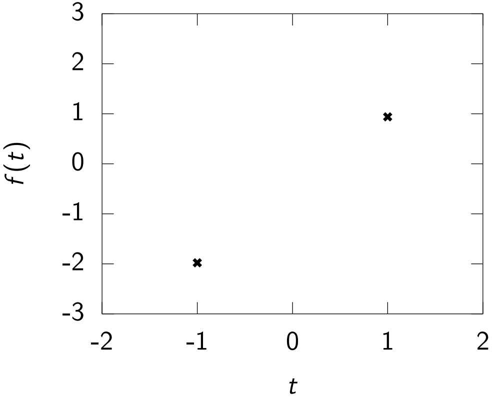
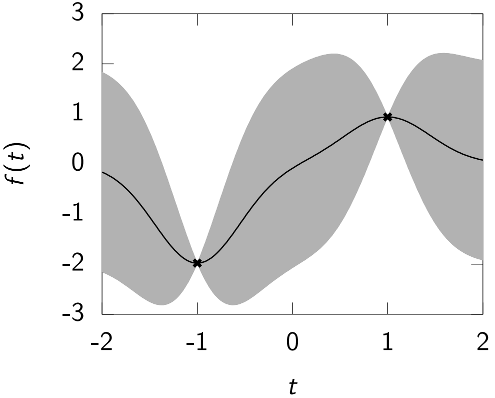


Figure: Real example: BACCO (see *e.g.* (?)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation



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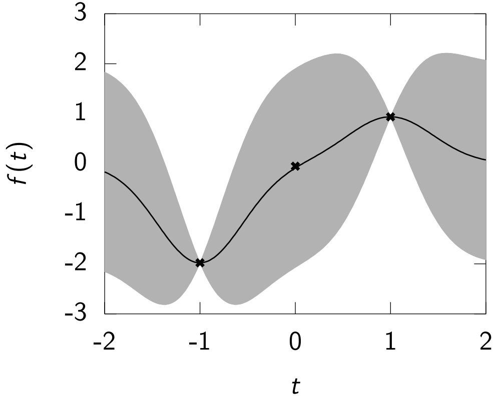

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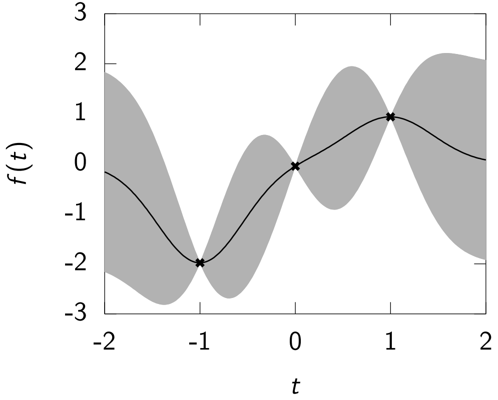

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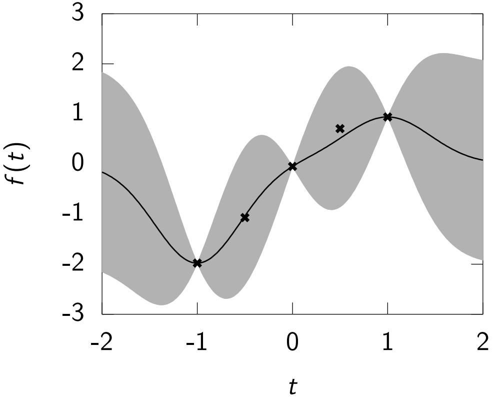

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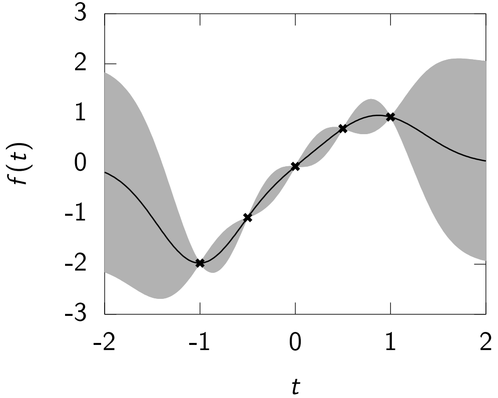

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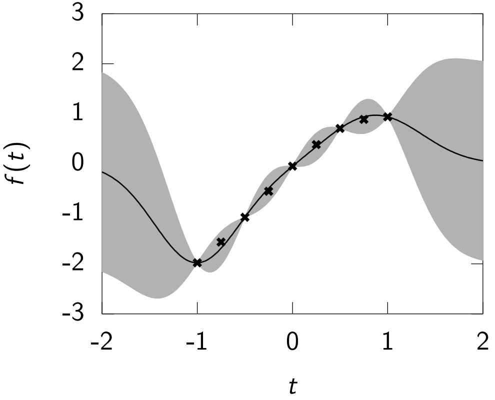

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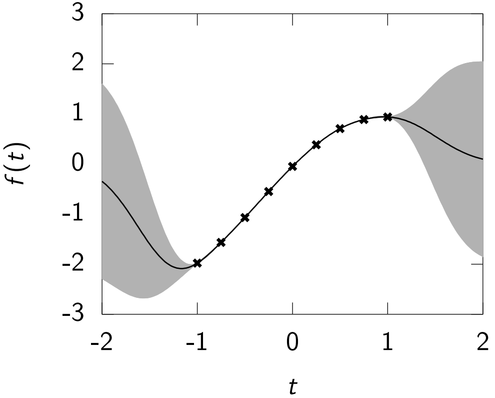

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Noise Models

Graph of a GP

- Relates input variables, $\mathbf{T}$, to vector, $\mathbf{y}$, through $\mathbf{f}$ given kernel parameters $\boldsymbol{\theta}$.
- Plate notation indicates independence of $y_i|f_i$.
- Noise model, $p(y_i|f_i)$ can take several forms.
- Simplest is Gaussian noise.

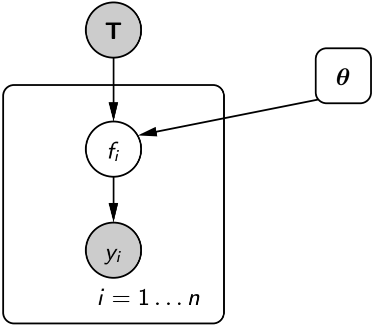


Figure: The Gaussian process depicted graphically.

Gaussian Noise

- Gaussian noise model,

$$p\left(y_i|f_i\right) = \mathcal{N}\left(y_i|f_i, \sigma^2\right)$$

where σ^2 is the variance of the noise.

- Equivalent to a covariance function of the form

$$k(t_i, t_j) = \delta_{i,j}\sigma^2$$

where $\delta_{i,j}$ is the Kronecker delta function.

- Additive nature of Gaussians means we can simply add this term to existing covariance matrices.

Gaussian Process Regression

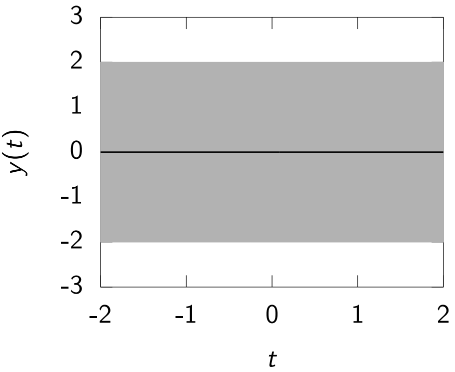
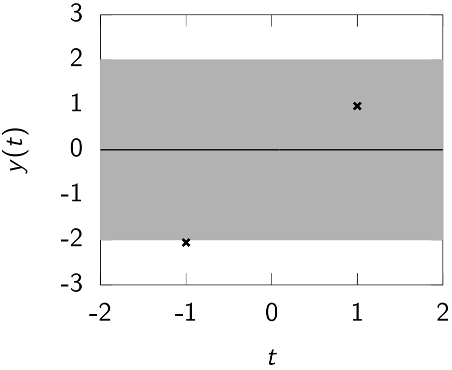


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression



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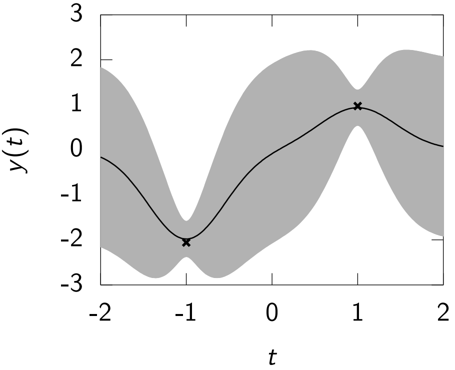

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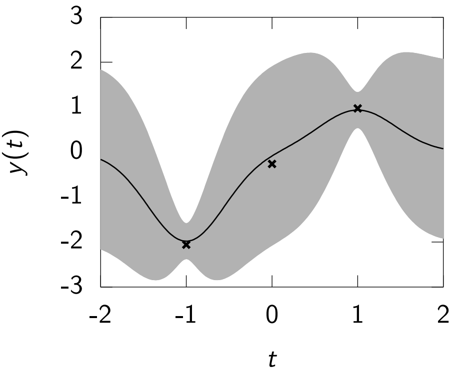

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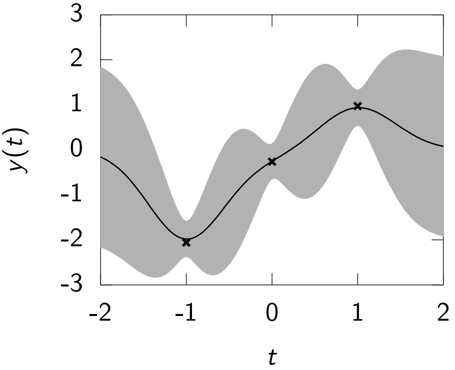

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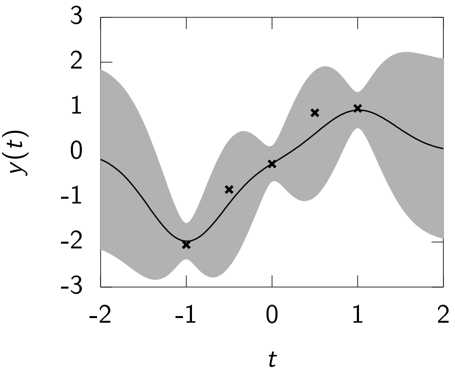

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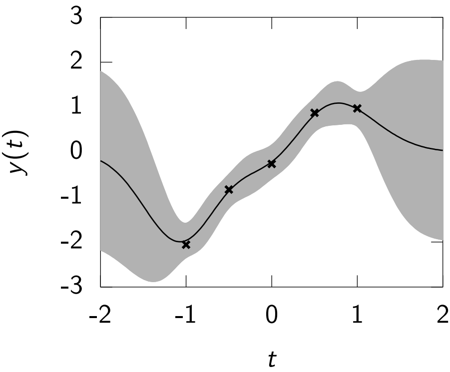

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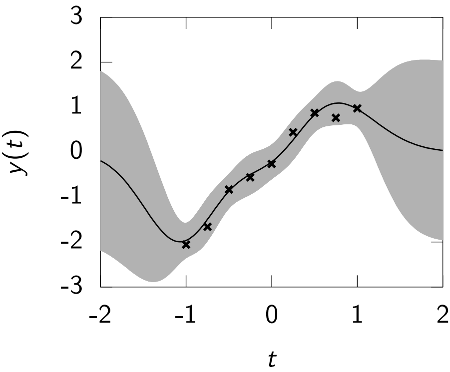

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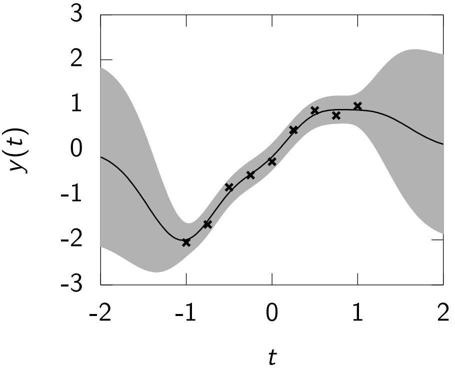

Figure: Examples include WiFi localization, C14 callibration curve.

Learning Covariance Parameters

Can we determine length scales and noise levels from the data?

$$\mathcal{N}\left(\mathbf{y}|\mathbf{0}, \mathbf{K}\right) = \frac{1}{(2\pi)^{\frac{n}{2}}|\mathbf{K}|}\exp\left(-\frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}\right)$$

The parameters are *inside* the covariance function (matrix).

$$k_{i,j} = k(t_i, t_j; \boldsymbol{\theta})$$

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Learning Covariance Parameters

Can we determine length scales and noise levels from the data?

$$\log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}) = -\frac{n}{2}\log 2\pi - \frac{1}{2}\log|\mathbf{K}| - \frac{\mathbf{y}^\top \mathbf{K}^{-1}\mathbf{y}}{2}$$

The parameters are *inside* the covariance function (matrix).

$$k_{i,j} = k(t_i, t_j; \boldsymbol{\theta})$$

Learning Covariance Parameters

Can we determine length scales and noise levels from the data?

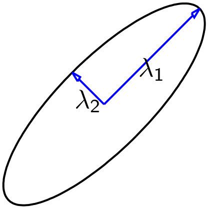
$$E(\boldsymbol{\theta}) = \frac{1}{2}\log|\mathbf{K}| + \frac{\mathbf{y}^\top\mathbf{K}^{-1}\mathbf{y}}{2}$$

The parameters are *inside* the covariance function (matrix).

$$k_{i,j} = k(t_i, t_j; \boldsymbol{\theta})$$

Eigendecomposition of Covariance

$$\mathbf{K} = \mathbf{R}\boldsymbol{\Lambda}^2\mathbf{R}^\top$$

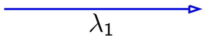


where $\boldsymbol{\Lambda}$ is a *diagonal* matrix and $\mathbf{R}^\top\mathbf{R} = \mathbf{I}$.

Useful representation since $|\mathbf{K}| = \left|\boldsymbol{\Lambda}^2\right| = |\boldsymbol{\Lambda}|^2$.

Capacity control: $\log |\mathbf{K}|$

$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$



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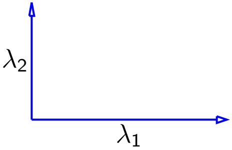

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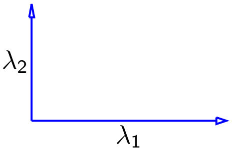

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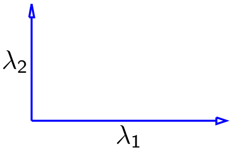

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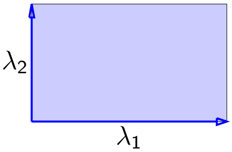

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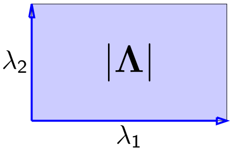
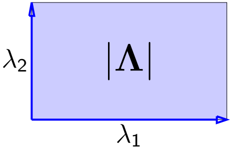


$$|\mathbf{\Lambda}| = \lambda_1 \lambda_2$$

Capacity control: $\log |\mathbf{K}|$

$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$



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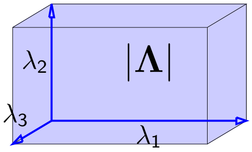

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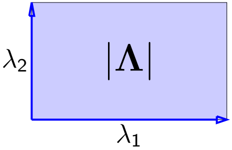
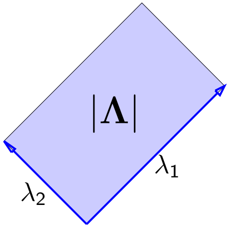


$$|\mathbf{\Lambda}| = \lambda_1 \lambda_2$$

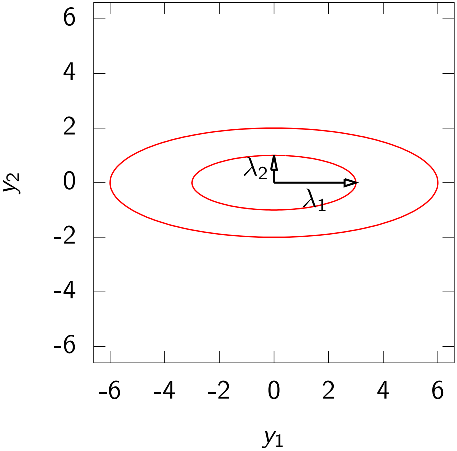
Capacity control: $\log |\mathbf{K}|$

$$\mathbf{R\Lambda} = \begin{bmatrix} w_{1,1} & w_{1,2} \\ w_{2,1} & w_{2,2} \end{bmatrix}$$



$$|\mathbf{R\Lambda}| = \lambda_1 \lambda_2$$

Data Fit: $\frac{\mathbf{y}^{-1}\mathbf{K}^{-1}\mathbf{y}}{2}$



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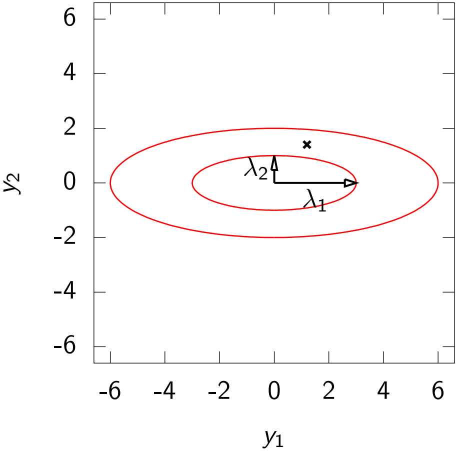

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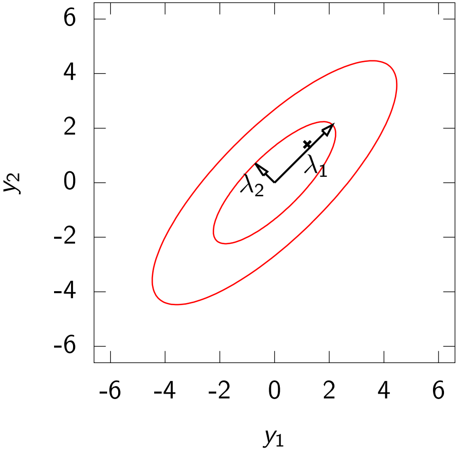
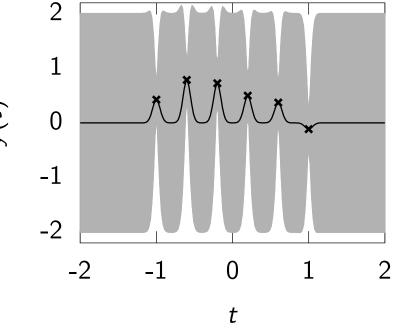
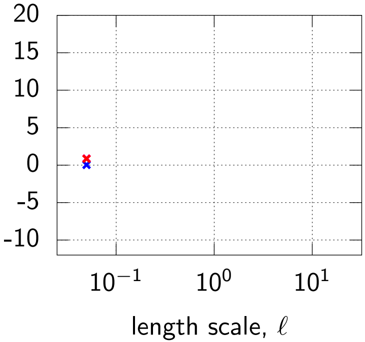


Learning Covariance Parameters

Can we determine length scales and noise levels from the data?





$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

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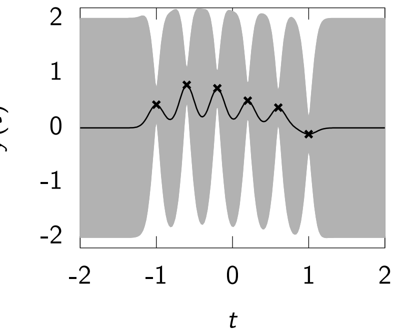

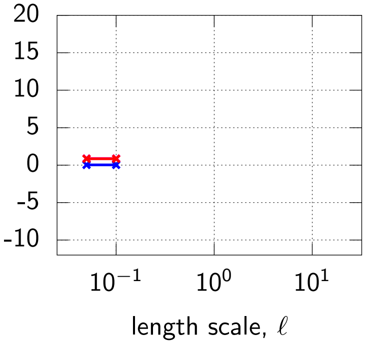

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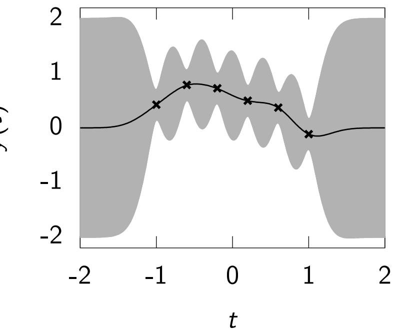

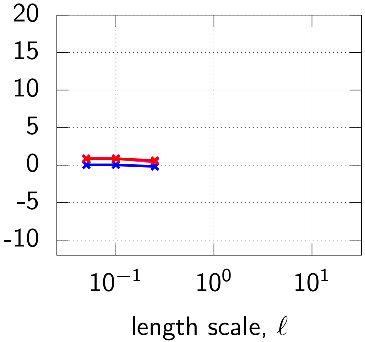

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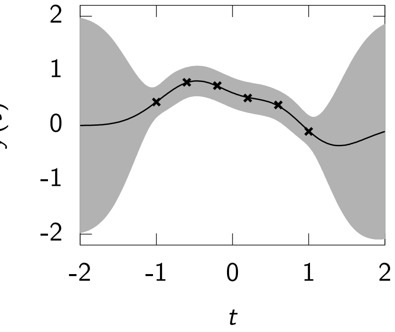

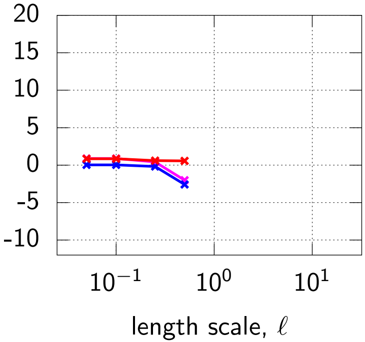

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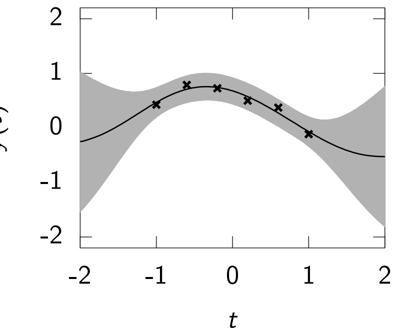

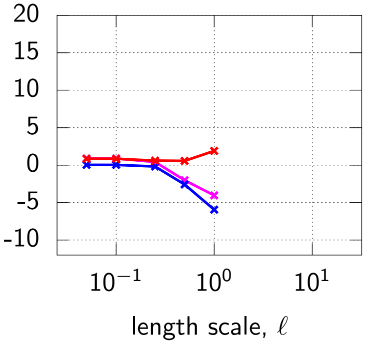

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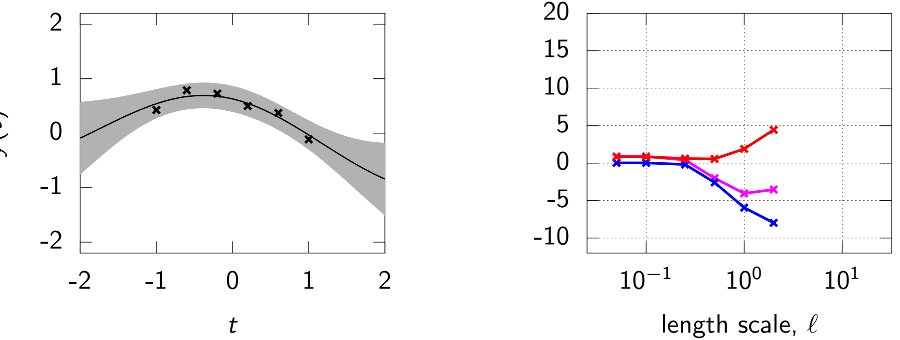

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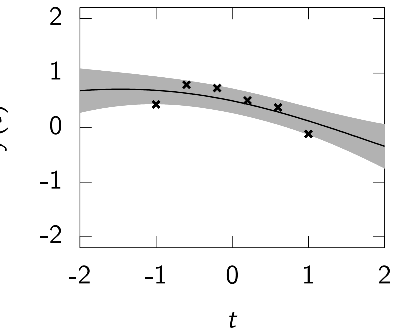

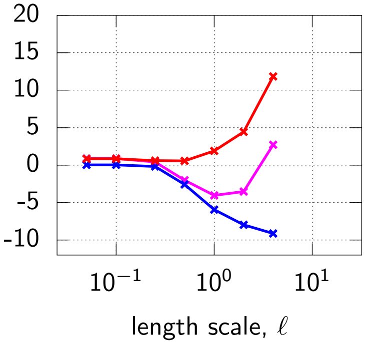

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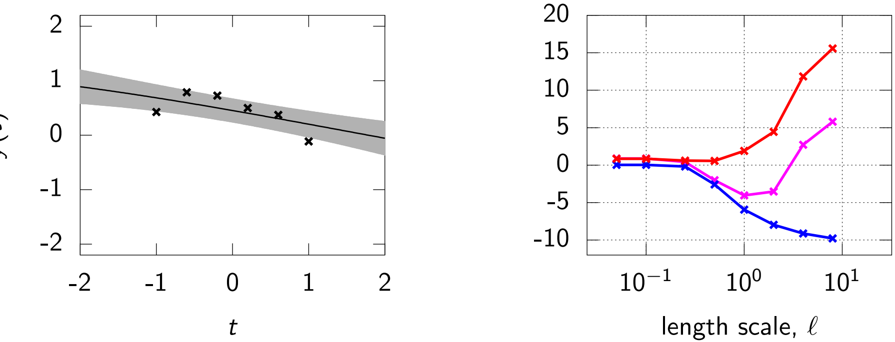

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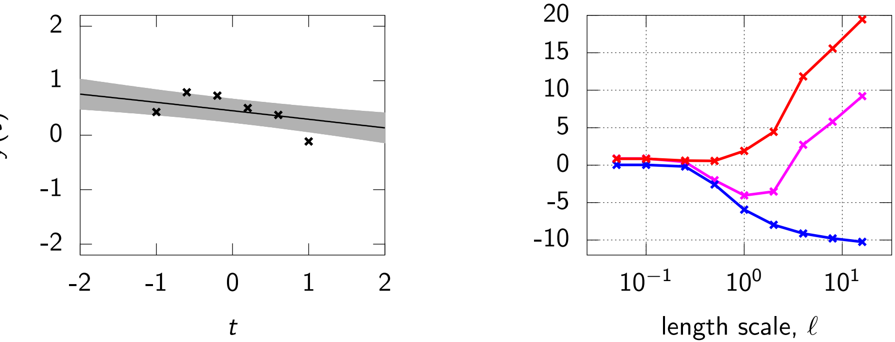

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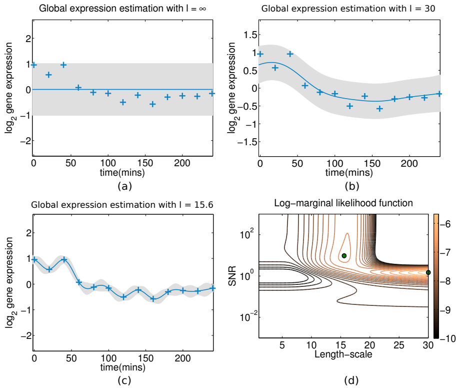
Gene Expression Example



Data from **?**. Figure from **?**.

Outline

Limitations of Gaussian Processes

- Inference is $O(n^3)$ due to matrix inverse (in practice use Cholesky).
- Gaussian processes don't deal well with discontinuities (financial crises, phosphorylation, collisions, edges in images).
- Widely used exponentiated quadratic covariance (RBF) can be too smooth in practice (but there are many alternatives!!).

Outline

Gene Expression Example

Kalaitzis and Lawrence *BMC Bioinformatics* 2011, **12**:180
http://www.biomedcentral.com/1471-2105/12/180

BMC Bioinformatics

RESEARCH ARTICLE Open Access

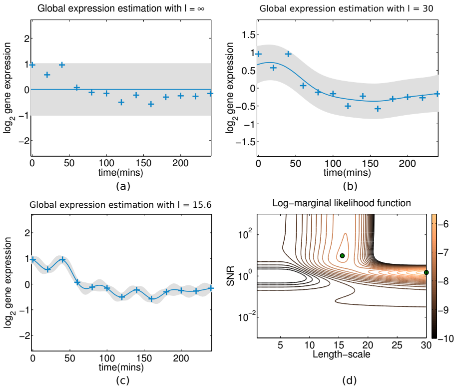
A Simple Approach to Ranking Differentially Expressed Gene Expression Time Courses through Gaussian Process Regression

Alfredo A Kalaitzis* and Neil D Lawrence*

Gene Expression Example

- Detect ‘quiet genes’ in time series.
- `http://www.bioconductor.org/packages/release/bioc/html/gprege.html` (Alfredo Kalaitzis is the maintainer).

Gene Expression Example



Data from **?**. Figure from **?**.

Summary

- Flexible method for probability densities over functions.
- Covariance function is key: defines how different data interrelate.
- Problems occur if there are discontinuities in the function.

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