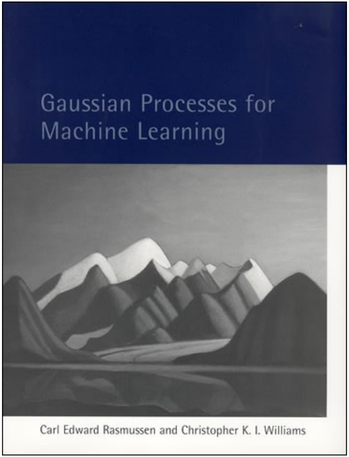
A Brief Introduction to Gaussian Processes

Neil D. Lawrence

UCLA
27th July 2012

Book



Rasmussen and Williams (2006)

Outline

1. The Gaussian Density
2. Constructing Covariance
3. GP Limitations
4. Conclusions

Outline

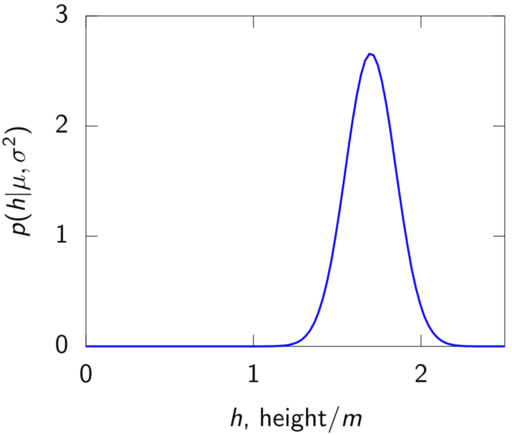
The Gaussian Density

- 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.

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

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

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.

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

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

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.

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

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

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.

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

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

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.

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

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

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.

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

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

Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$

Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$y_1 - y_2 = m(x_1 - x_2)$$

Two Simultaneous Equations

A system of two differential equations with two unknowns.

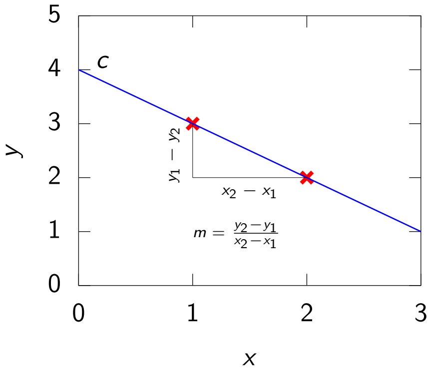
$$\frac{y_1 - y_2}{x_1 - x_2} = m$$

Two Simultaneous Equations

A system of two differential equations with two unknowns.

$$m = \frac{y_2 - y_1}{x_2 - x_1}$$

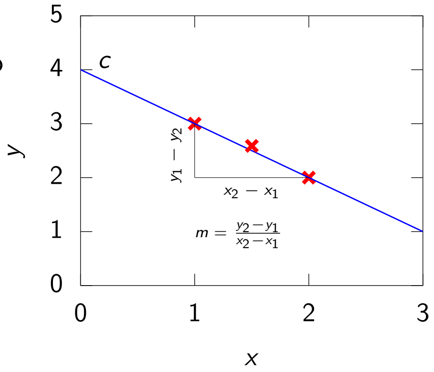
$$c = y_1 - m x_1$$



Two Simultaneous Equations

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

$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$
$$y_3 = mx_3 + c$$



Overdetermined System

- With two unknowns and two observations:

$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$

- Additional observation leads to *overdetermined* system.

$$y_3 = mx_3 + c$$

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

$$y_1 = mx_1 + c + \epsilon_1$$
$$y_2 = mx_2 + c + \epsilon_2$$
$$y_3 = mx_3 + c + \epsilon_3$$

Overdetermined System

- With two unknowns and two observations:

$$
\begin{aligned}
y_1 &= mx_1 + c \\
y_2 &= mx_2 + c
\end{aligned}
$$

- Additional observation leads to *overdetermined* system.

$$y_3 = mx_3 + c$$

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

$$
\begin{aligned}
y_1 &= mx_1 + c + \epsilon_1 \\
y_2 &= mx_2 + c + \epsilon_2 \\
y_3 &= mx_3 + c + \epsilon_3
\end{aligned}
$$

Overdetermined System

- With two unknowns and two observations:

$$y_1 = mx_1 + c$$
$$y_2 = mx_2 + c$$

- Additional observation leads to *overdetermined* system.

$$y_3 = mx_3 + c$$

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

$$y_1 = mx_1 + c + \epsilon_1$$
$$y_2 = mx_2 + c + \epsilon_2$$
$$y_3 = mx_3 + c + \epsilon_3$$

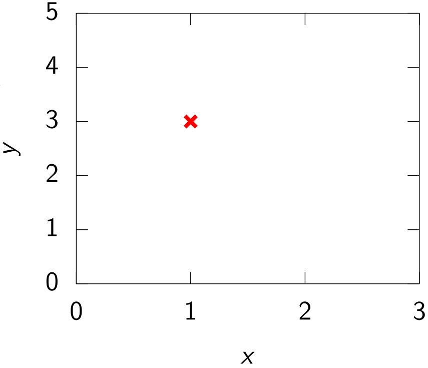
Noise Models

- 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?

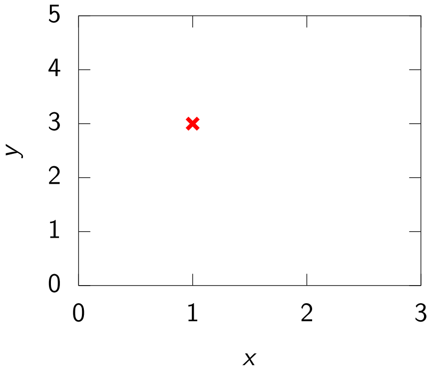
$$y_1 = mx_1 + c$$



Underdetermined System

Can compute m given c.

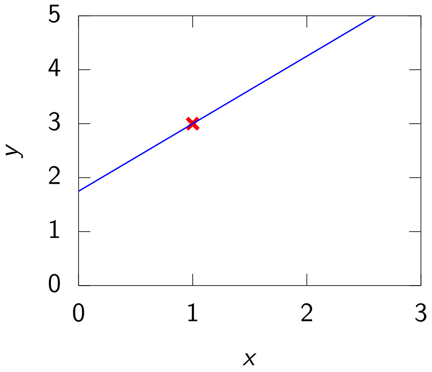
$$m = \frac{y_1 - c}{x}$$



Underdetermined System

Can compute m given c.

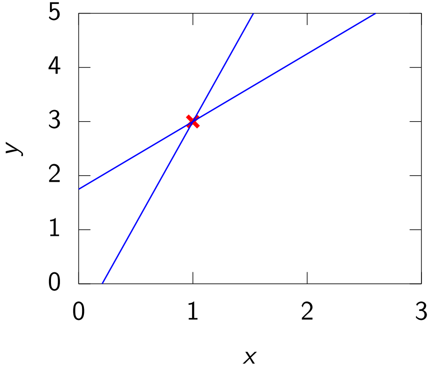
$$c = 1.75 \implies m = 1.25$$



Underdetermined System

Can compute m given c.

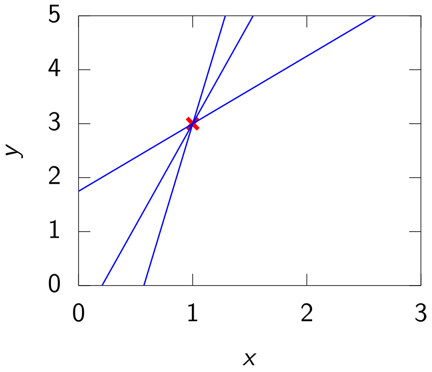
$$c = -0.777 \Longrightarrow m = 3.78$$



Underdetermined System

Can compute m given c.

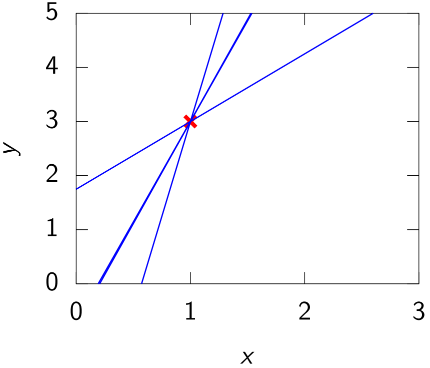
$$c = -4.01 \Longrightarrow m = 7.01$$



Underdetermined System

Can compute m given c.

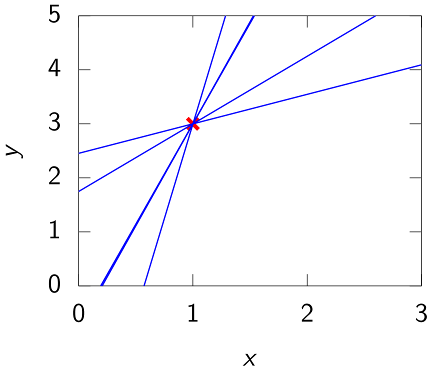
$$c = -0.718 \implies m = 3.72$$



Underdetermined System

Can compute m given c.

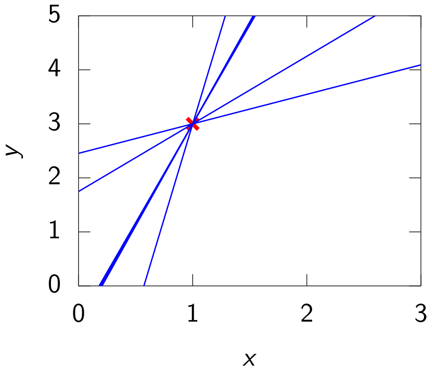
$$c = 2.45 \implies m = 0.545$$



Underdetermined System

Can compute m given c.

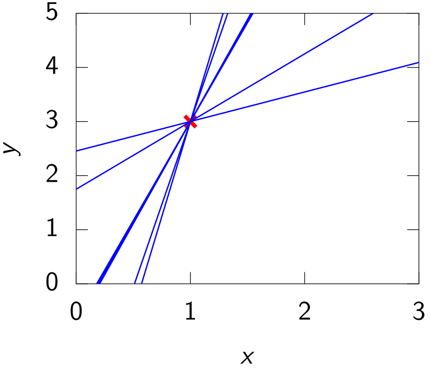
$$c = -0.657 \implies m = 3.66$$



Underdetermined System

Can compute m given c.

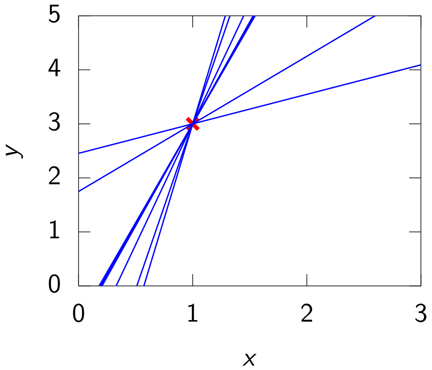
$$c = -3.13 \Longrightarrow m = 6.13$$



Underdetermined System

Can compute m given c.

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

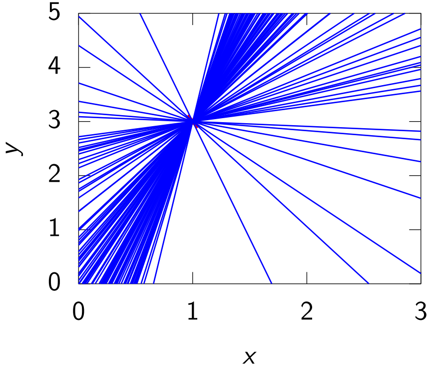


Underdetermined System

Can compute m given c.
Assume

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

we find a distribution of solutions.



Probability for Under- and Overdetermined

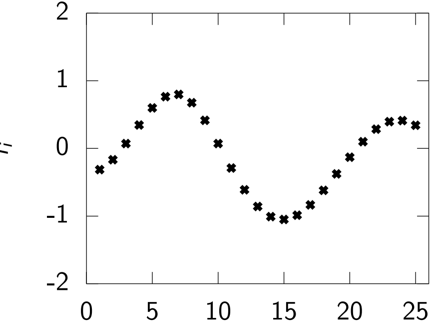
- To deal with overdetermined introduced probability distribution for 'variable', ϵ_i.
- For underdetermined system introduced probability distribution for 'parameter', c.
- This is known as a Bayesian treatment.

Sampling a Function

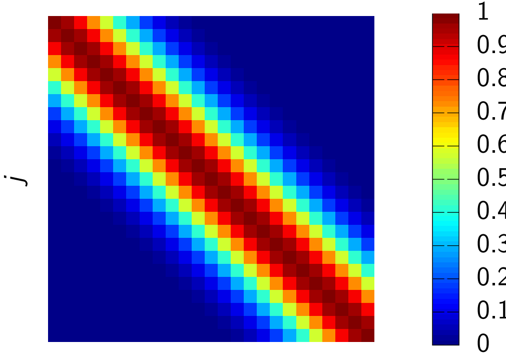
Multi-variate Gaussians

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

Gaussian Distribution Sample



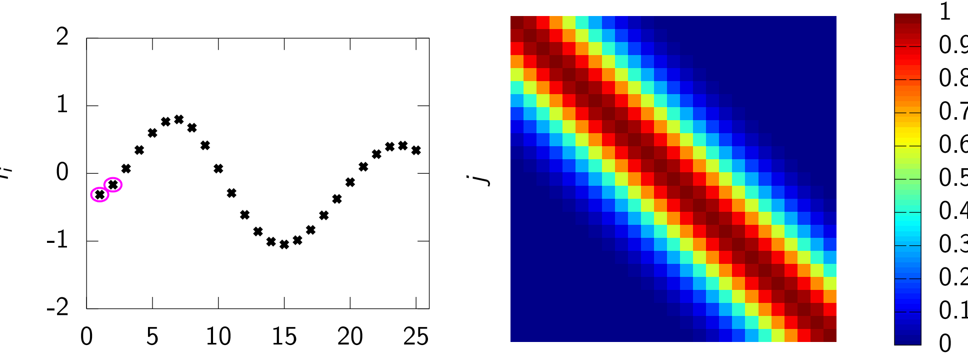
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample

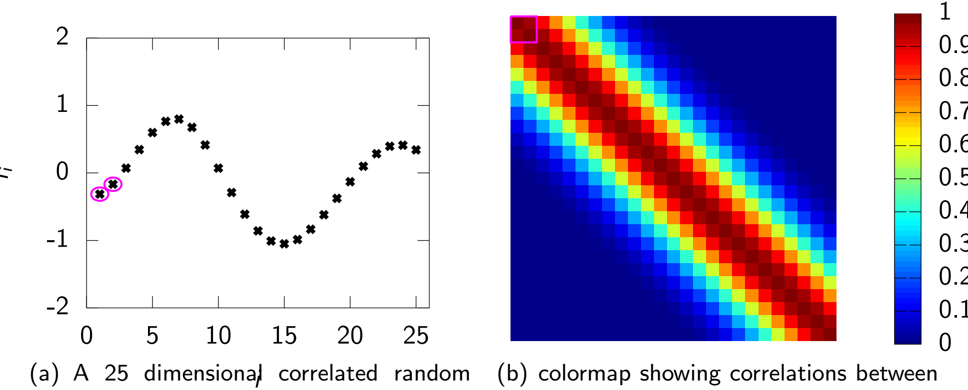


(a) A 25 dimensional correlated random variable (values ploted against index)

(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample

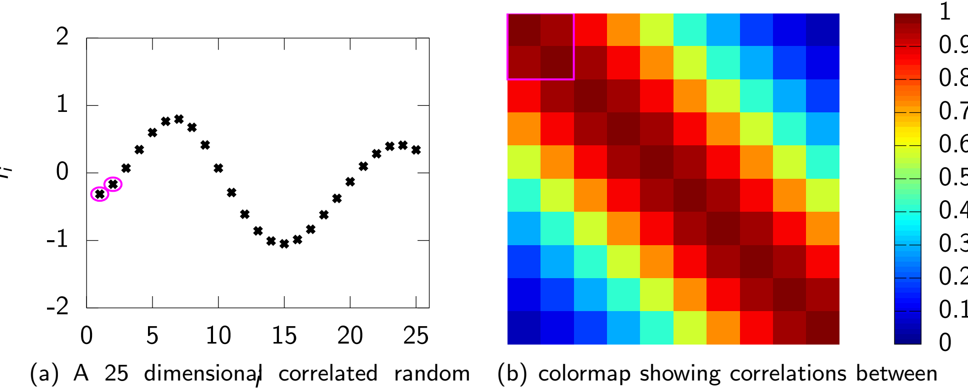


(a) A 25 dimensional correlated random variable (values ploted against index)

(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample

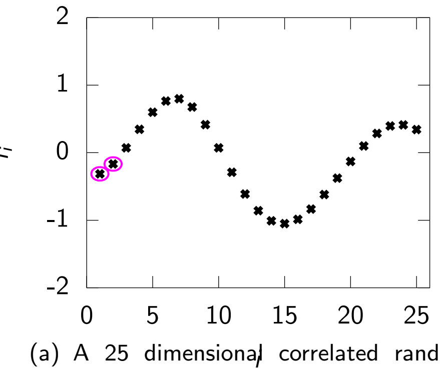


(a) A 25 dimensional correlated random variable (values ploted against index)

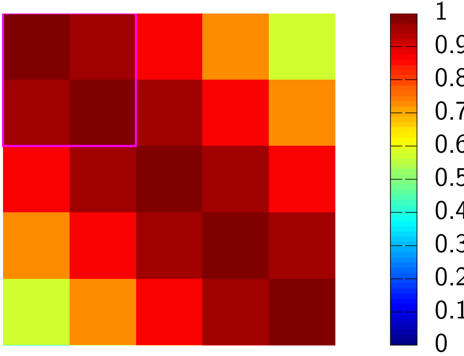
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



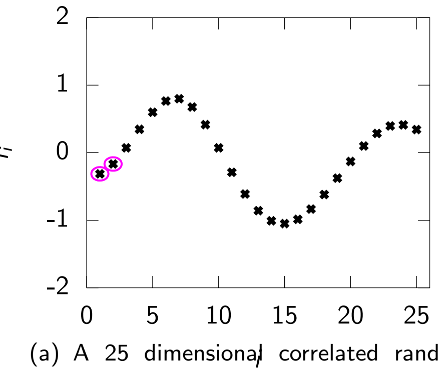
(a) A 25 dimensional correlated random variable (values ploted against index)



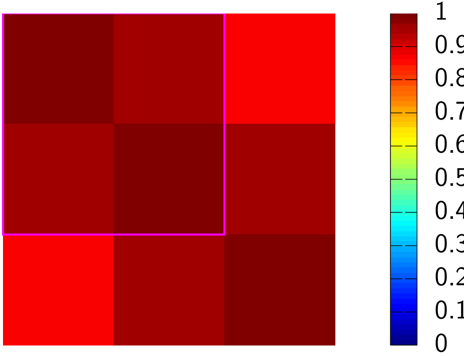
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



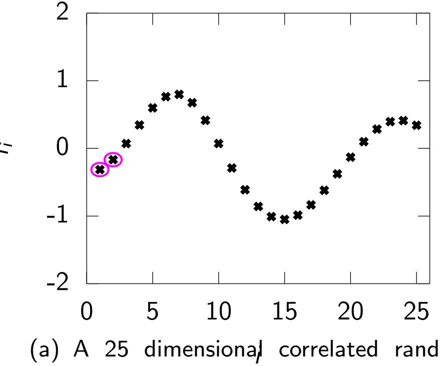
(a) A 25 dimensional correlated random variable (values ploted against index)



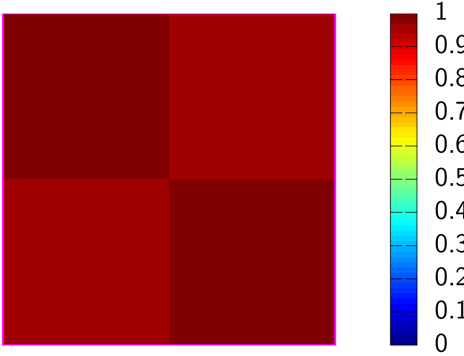
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



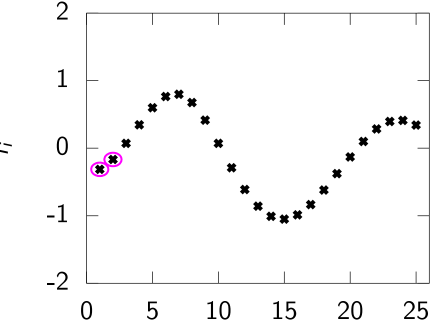
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



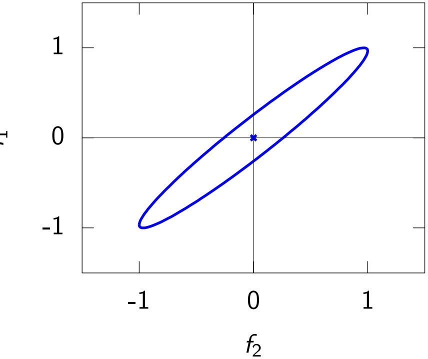
(a) A 25 dimensional correlated random variable (values ploted against index)

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

(b) correlation between f_1 and f_2.

Figure: A sample from a 25 dimensional Gaussian distribution.

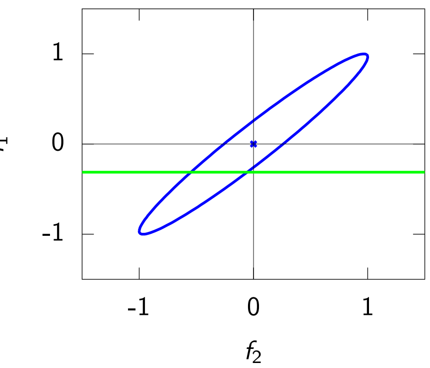
Prediction of f_2 from f_1



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

- 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: $p(f_2 | f_1 = -0.313)$.

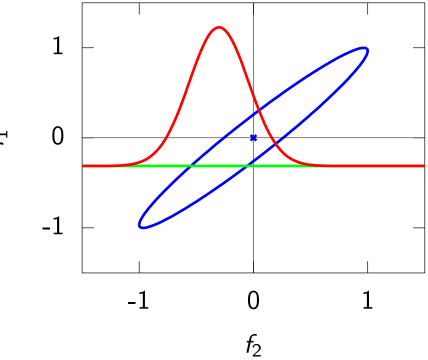
Prediction of f_2 from f_1



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

- 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: $p(f_2|f_1 = -0.313)$.

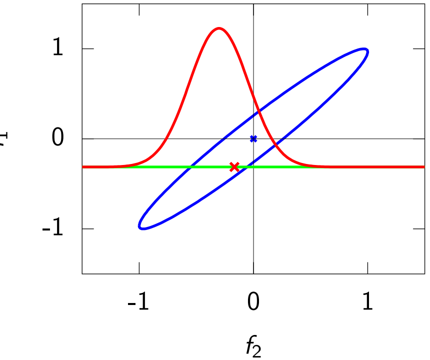
Prediction of f_2 from f_1



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

- 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



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

- 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

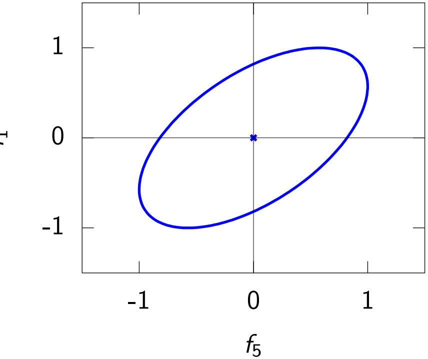
- Prediction of f_2 from f_1 requires *conditional density*.
- Conditional density is *also* Gaussian.

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

where covariance of joint density is given by

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

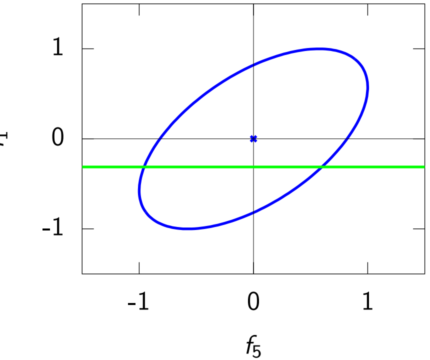
Prediction of f_5 from f_1



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

- 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: $p(f_5 | f_1 = -0.313)$.

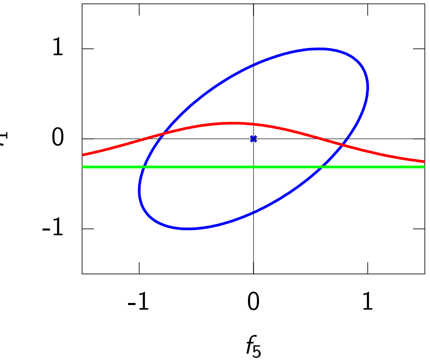
Prediction of f_5 from f_1



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

- 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: $p(f_5|f_1 = -0.313)$.

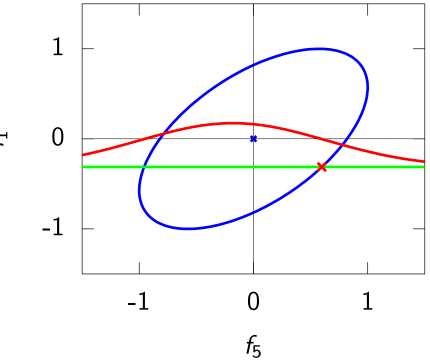
Prediction of f_5 from f_1



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

- 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

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

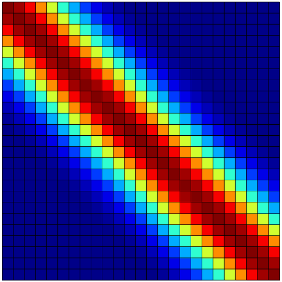
Covariance Functions

Where did this covariance matrix come from?

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

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|_2^2}{2\ell^2}\right)$$

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



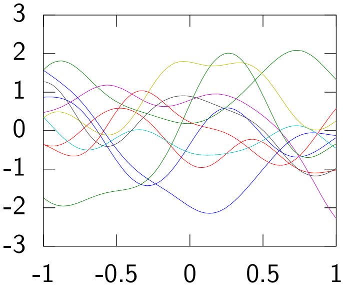
Covariance Functions

Where did this covariance matrix come from?

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

$$k(\mathbf{x}, \mathbf{x}') = \alpha \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|_2^2}{2\ell^2}\right)$$

- Covariance matrix is built using the *inputs* to the function $\mathbf{x}$.
- 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?

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

$$x_1 = -3.0,\ x_1 = -3.0$$

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_1 = -3.0$, $x_1 = -3.0$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20,\ x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20,\ x_1 = -3.0$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20, \; x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20,\ x_2 = 1.20$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20,\ x_2 = 1.20$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40, \; x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_2 = 1.20$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_2 = 1.20$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_2 = 1.20$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_3 = 1.40$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40$, $x_3 = 1.40$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

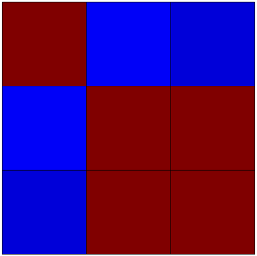
Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_3 = 1.40$

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



$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 2.00$ and $\alpha = 1.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_1 = -3, \; x_1 = -3$$

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_1 = -3,\ x_1 = -3$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.2,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.2,\ x_1 = -3$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.2,\ x_1 = -3$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.2,\ x_2 = 1.2$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.2,\ x_2 = 1.2$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.4,\ x_1 = -3$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.4,\ x_2 = 1.2$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4, \; x_2 = 1.2$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.4,\ x_2 = 1.2$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4, \; x_3 = 1.4$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4,\ x_3 = 1.4$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_1 = -3$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_2 = 1.2$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_2 = 1.2$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_2 = 1.2$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_3 = 1.4$$

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

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		

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_3 = 1.4$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_3 = 1.4$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_4 = 2.0$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0,\ x_4 = 2.0$$

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

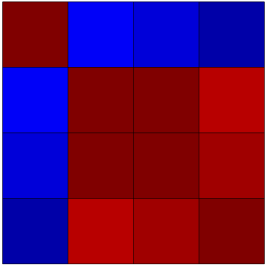
Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_4 = 2.0$

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



$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, and $x_4 = 2.0$ with $\ell = 2.0$ and $\alpha = 1.0$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_1 = -3.0,\ x_1 = -3.0$$

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_1 = -3.0$, $x_1 = -3.0$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20, \; x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20,\ x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20,\; x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20, \; x_2 = 1.20$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20,\ x_2 = 1.20$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_1 = -3.0$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_1 = -3.0$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_1 = -3.0$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_2 = 1.20$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_2 = 1.20$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_2 = 1.20$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40,\ x_3 = 1.40$$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40,\ x_3 = 1.40$

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

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

$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

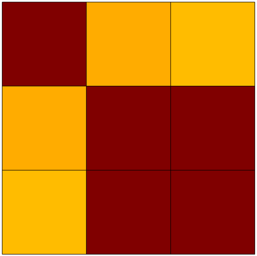
Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40$, $x_3 = 1.40$

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



$x_1 = -3.0$, $x_2 = 1.20$, and $x_3 = 1.40$ with $\ell = 5.00$ and $\alpha = 4.00$.

Outline

Constructing Covariance Functions

- Sum of two covariances is also a covariance function.

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

Constructing Covariance Functions

- Product of two covariances is also a covariance function.

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

Multiply by Deterministic Function

- If $f(\mathbf{x})$ is a Gaussian process.
- $g(\mathbf{x})$ is a deterministic function.
- $h(\mathbf{x}) = f(\mathbf{x})g(\mathbf{x})$
- Then

$$k_h(\mathbf{x}, \mathbf{x}') = g(\mathbf{x})k_f(\mathbf{x}, \mathbf{x}')g(\mathbf{x}')$$

  where k_h is covariance for $h(\cdot)$ and k_f is covariance for $f(\cdot)$.

Covariance Functions

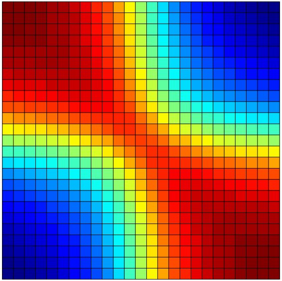
MLP Covariance Function

$$k(\mathbf{x}, \mathbf{x}') = \alpha \text{asin}\left(\frac{w\mathbf{x}^\top\mathbf{x}' + b}{\sqrt{w\mathbf{x}^\top\mathbf{x} + b + 1}\sqrt{w\mathbf{x}'^\top\mathbf{x}' + b + 1}}\right)$$

- Based on infinite neural network model.

$$w = 40$$

$$b = 4$$



Covariance Functions

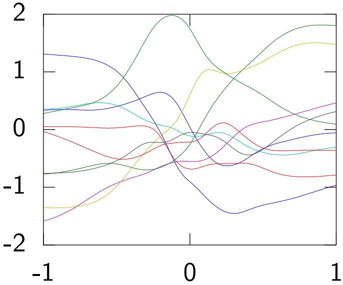
MLP Covariance Function

$$k\left(\mathbf{x}, \mathbf{x}'\right) = \alpha \text{asin}\left(\frac{w\mathbf{x}^\top\mathbf{x}' + b}{\sqrt{w\mathbf{x}^\top\mathbf{x} + b + 1}\sqrt{w\mathbf{x}'^\top\mathbf{x}' + b + 1}}\right)$$

- Based on infinite neural network model.

$$w = 40$$

$$b = 4$$



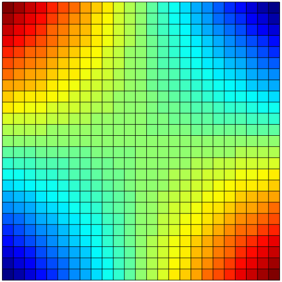
Covariance Functions

Linear Covariance Function

$$k(\mathbf{x}, \mathbf{x}') = \alpha \mathbf{x}^\top \mathbf{x}'$$

- Bayesian linear regression.

$$\alpha = 1$$



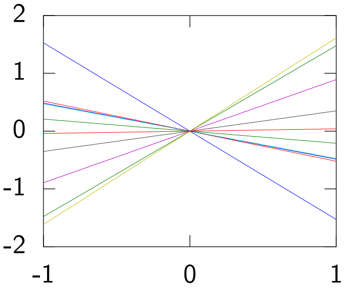
Covariance Functions

Linear Covariance Function

$$k\left(\mathbf{x}, \mathbf{x}'\right) = \alpha \mathbf{x}^{\top}\mathbf{x}'$$

- Bayesian linear regression.

$$\alpha = 1$$



Gaussian Process Interpolation

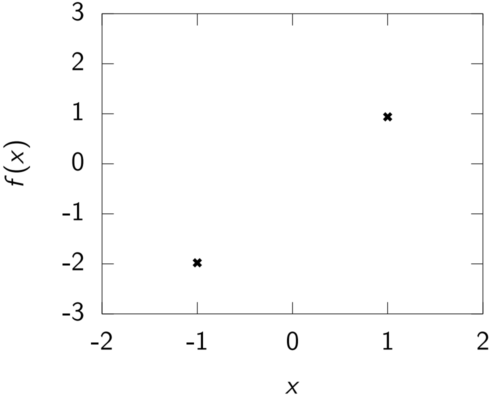


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

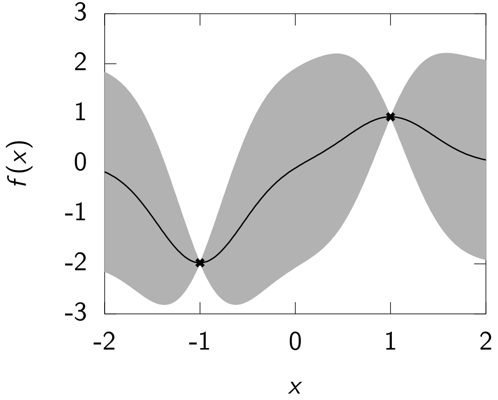


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

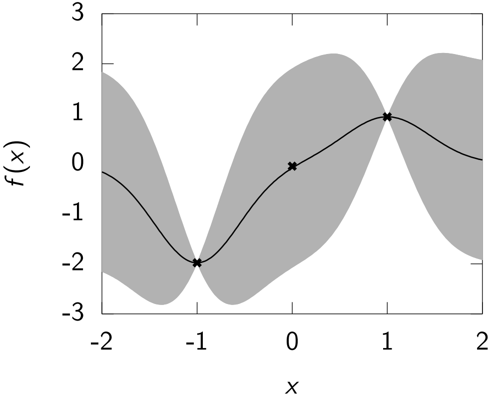


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

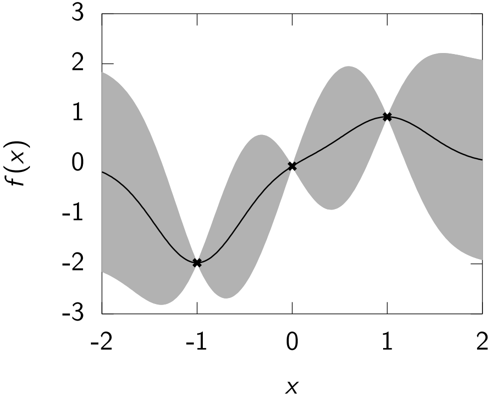


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

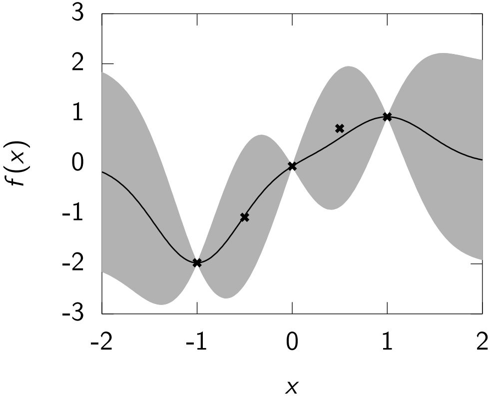


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

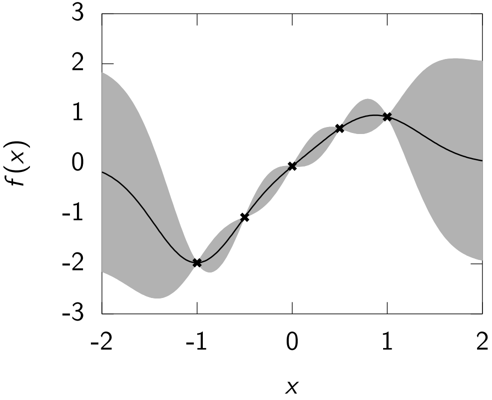


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

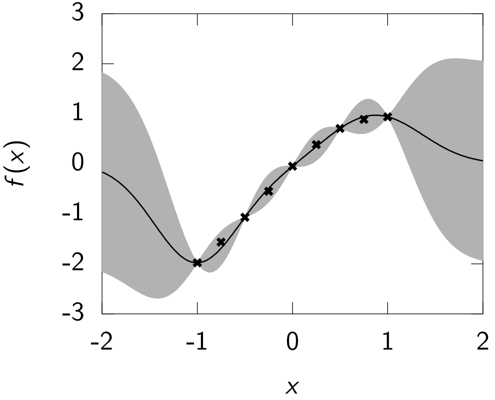


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Gaussian Process Interpolation

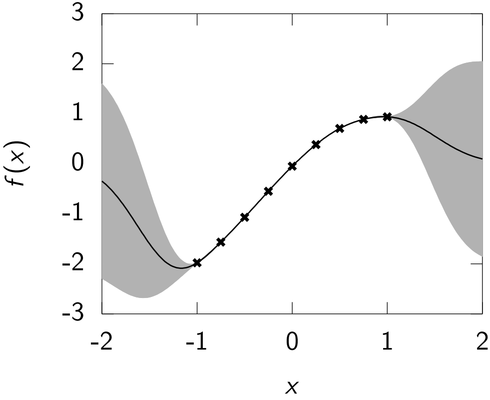


Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

Noise Models

Graph of a GP

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

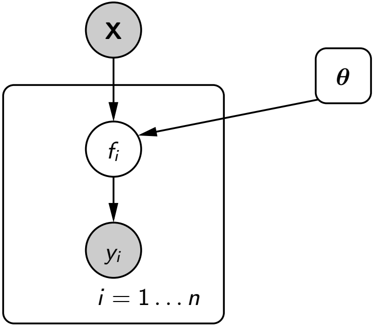


Figure: The Gaussian process depicted graphically.

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

$$k(\mathbf{x}_i, \mathbf{x}_j) = \delta_{i,j}\sigma^2$$

  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

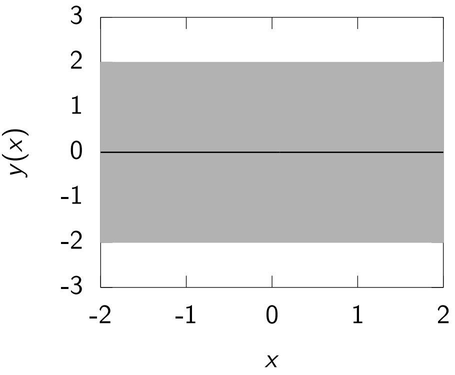


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

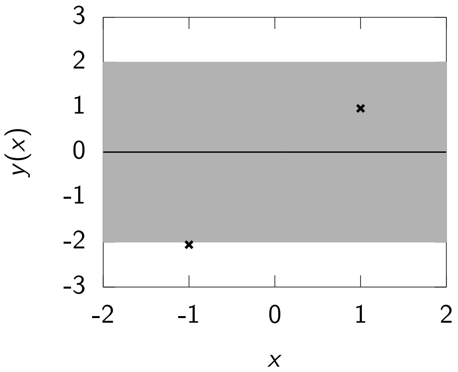


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

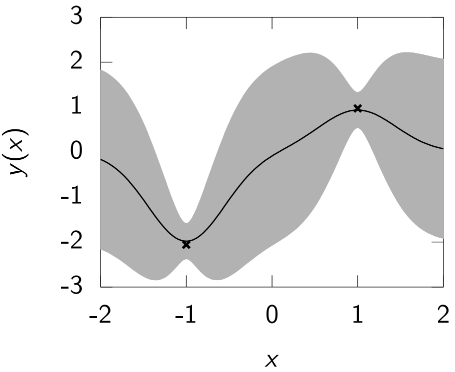


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

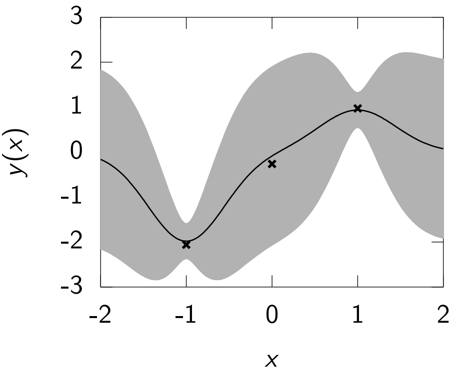


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

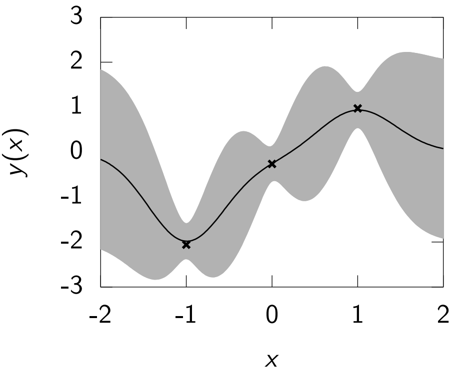


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

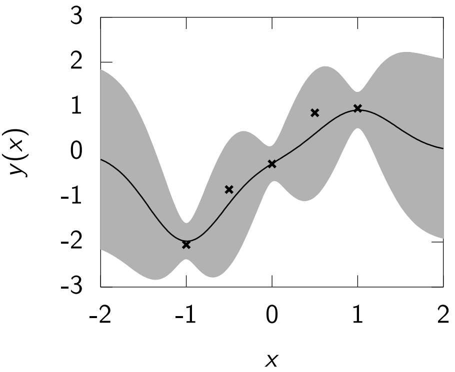


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

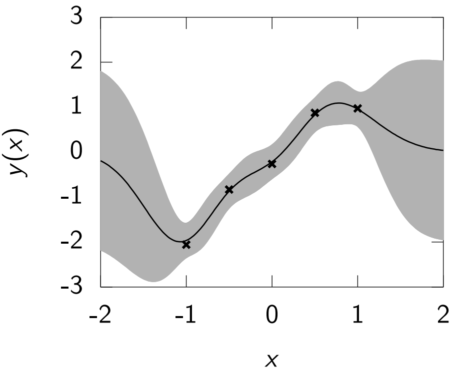


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

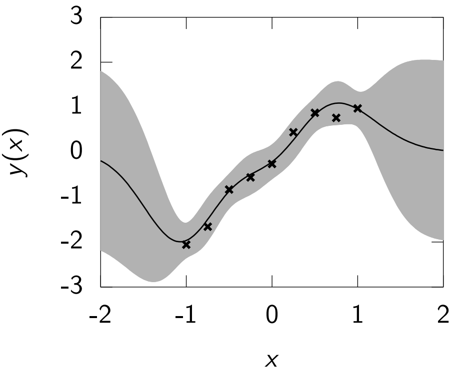


Figure: Examples include WiFi localization, C14 callibration curve.

Gaussian Process Regression

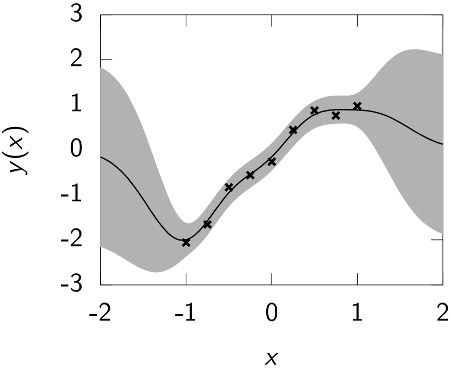


Figure: Examples include WiFi localization, C14 callibration curve.

Learning Covariance Parameters

Can we determine covariance parameters 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).

$$k_{i,j}=k(\mathbf{x}_i,\mathbf{x}_j;\boldsymbol{\theta})$$

Learning Covariance Parameters

Can we determine covariance parameters 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).

$$k_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta})$$

Learning Covariance Parameters

Can we determine covariance parameters 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).

$$k_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta})$$

Learning Covariance Parameters

Can we determine covariance parameters from the data?

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

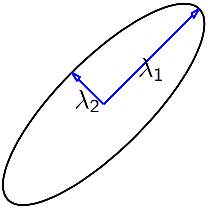
The parameters are *inside* the covariance function (matrix).

$$k_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta})$$

Eigendecomposition of Covariance

A useful decomposition for understanding the objective function.

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



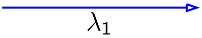
Diagonal of $\mathbf{\Lambda}$ represents distance along axes.
$\mathbf{R}$ gives a rotation of these axes.

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

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

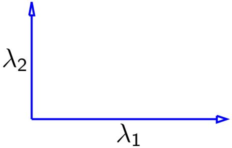
Capacity control: $\log|\mathbf{K}|$

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



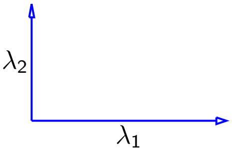
Capacity control: $\log|\mathbf{K}|$

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



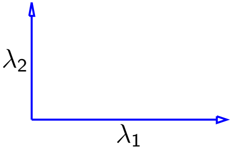
Capacity control: $\log |\mathbf{K}|$

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



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

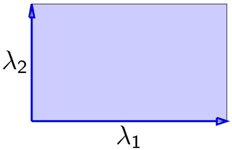
$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$



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

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

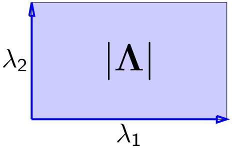
$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$



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

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

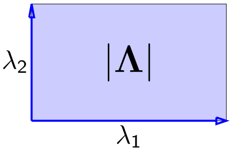
$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$



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

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

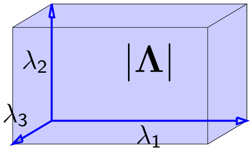
$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$



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

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

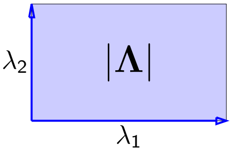
$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$



$$|\mathbf{\Lambda}| = \lambda_1 \lambda_2 \lambda_3$$

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

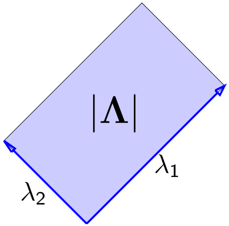
$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$



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

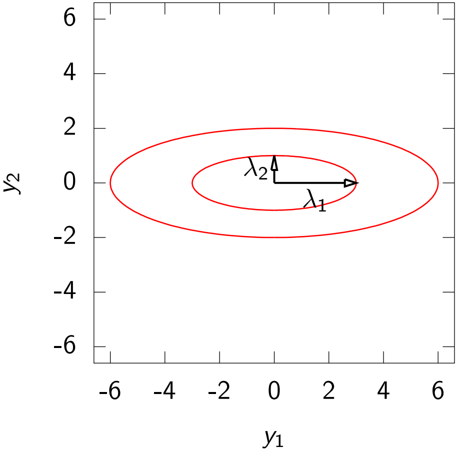
Capacity control: $\log |\mathbf{K}|$

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

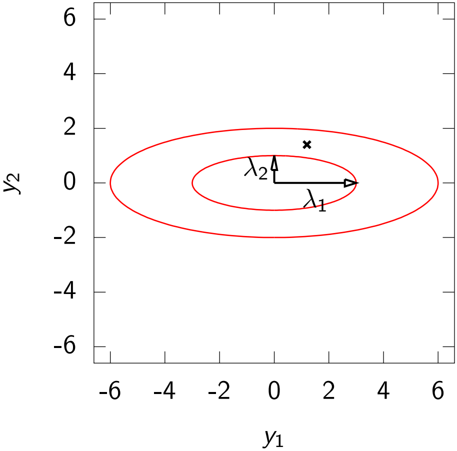


$$|\mathbf{R}\boldsymbol{\Lambda}| = \lambda_1 \lambda_2$$

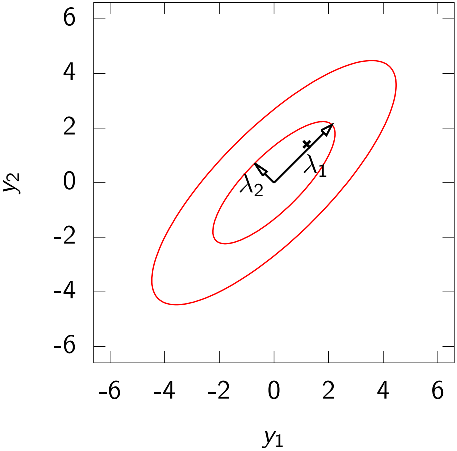
Data Fit: $\frac{\mathbf{y}^{-1}\mathbf{K}^{-1}\mathbf{y}}{2}$



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

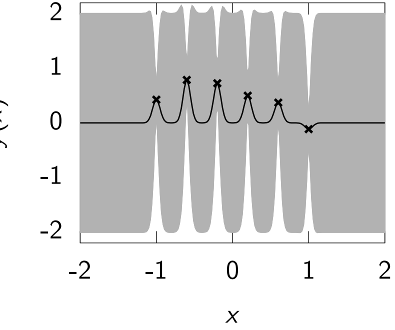


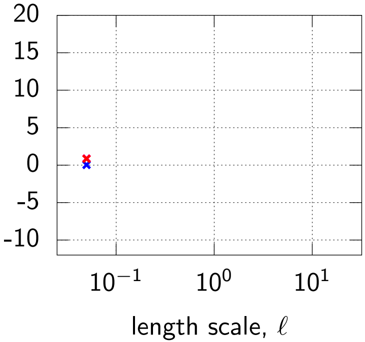
Data Fit: $\frac{\mathbf{y}^{-1}\mathbf{K}^{-1}\mathbf{y}}{2}$



Learning Covariance Parameters

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

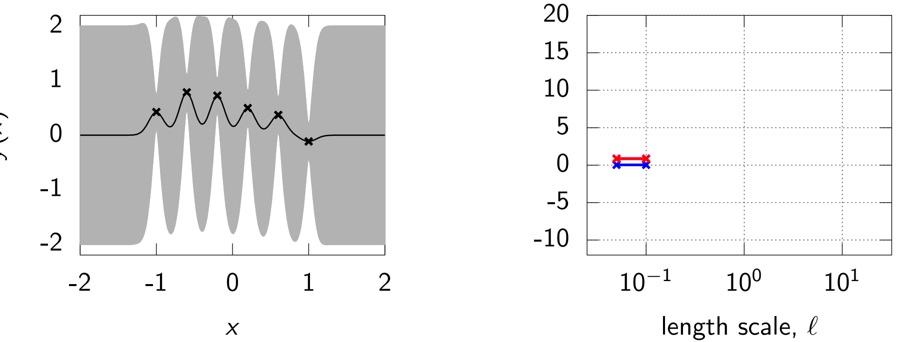




$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

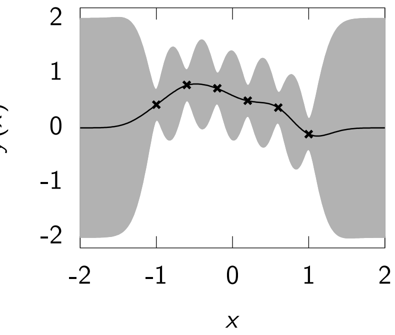
Can we determine length scales and noise levels from the data?

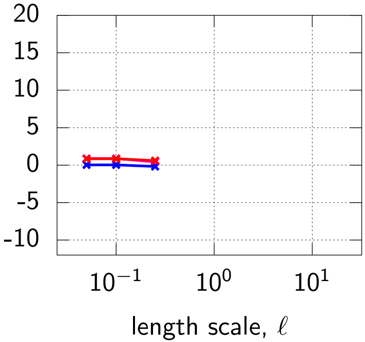


$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

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

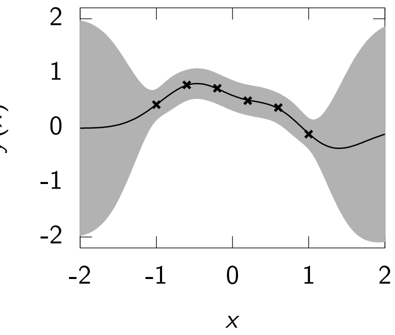


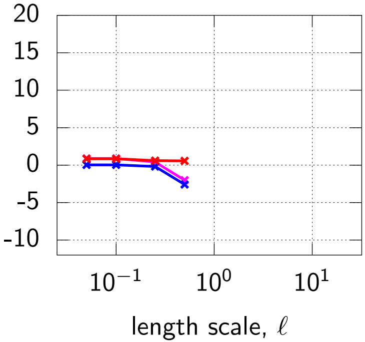


$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^\top\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

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

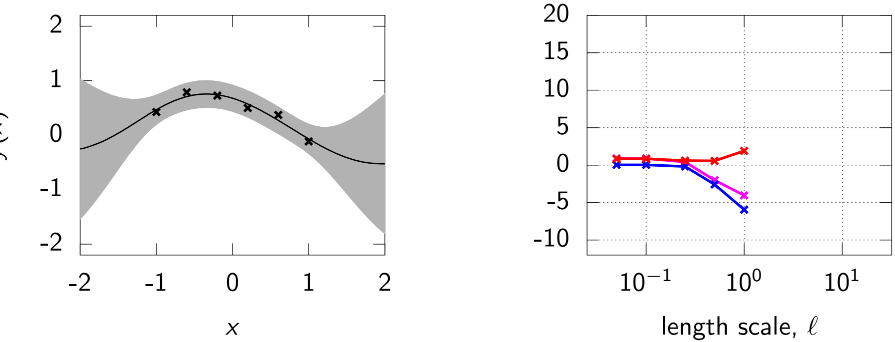




$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

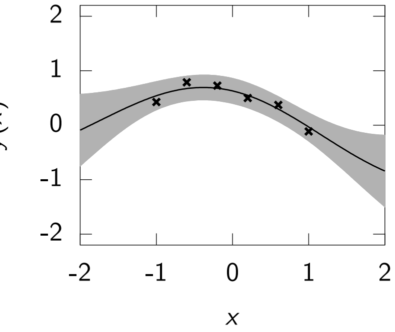
Can we determine length scales and noise levels from the data?

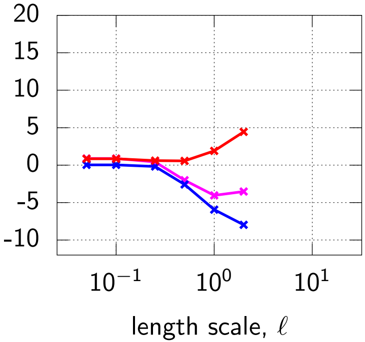


$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

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

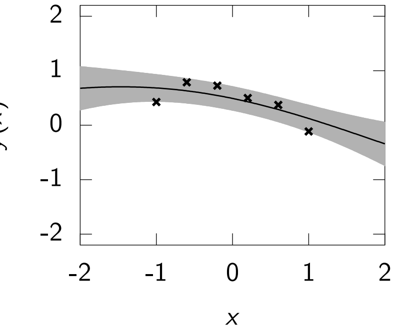


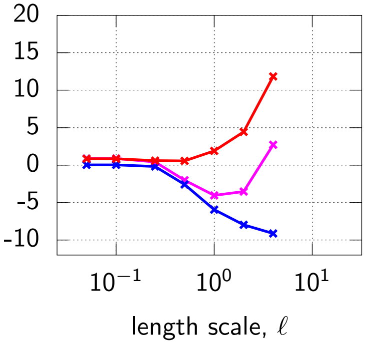


$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

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

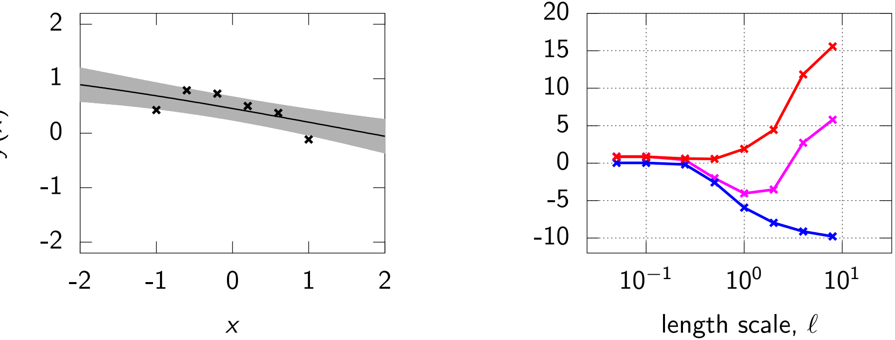




$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^\top \mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

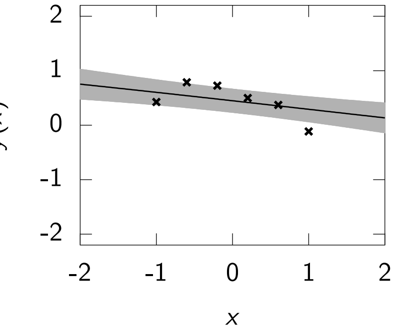
Can we determine length scales and noise levels from the data?

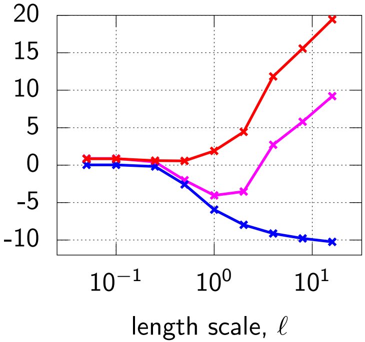


$$E(\boldsymbol{\theta}) = \frac{1}{2}\left|\mathbf{K}\right| + \frac{\mathbf{y}^{\top}\mathbf{K}^{-1}\mathbf{y}}{2}$$

Learning Covariance Parameters

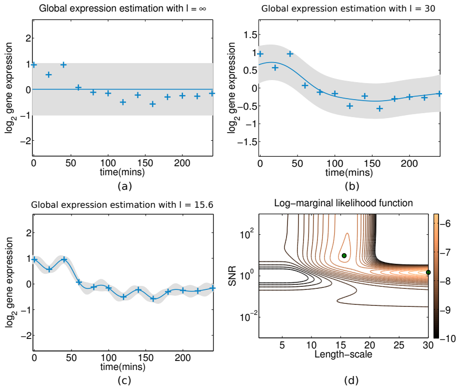
Can we determine length scales and noise levels from the data?





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

Gene Expression Example



Data from Della Gatta et al. (2008). Figure from Kalaitzis and Lawrence (2011).

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!!).

Summary

- Broad introduction to Gaussian processes.
  - Started with Gaussian distribution.
  - Motivated Gaussian processes through the multivariate density.
- Emphasized the role of the covariance (not the mean).
- Performs nonlinear regression with error bars.
- Parameters of the covariance function (kernel) are easily optimized with maximum likelihood.

References I

G. Della Gatta, M. Bansal, A. Ambesi-Impiombato, D. Antonini, C. Missero, and D. di Bernardo. Direct targets of the trp63 transcription factor revealed by a combination of gene expression profiling and reverse engineering. *Genome Research*, 18(6): 939–948, Jun 2008. [URL]. [DOI].

A. A. Kalaitzis and N. D. Lawrence. A simple approach to ranking differentially expressed gene expression time courses through Gaussian process regression. *BMC Bioinformatics*, 12(180), 2011. [DOI].

J. Oakley and A. O'Hagan. Bayesian inference for the uncertainty distribution of computer model outputs. *Biometrika*, 89(4): 769–784, 2002.

C. E. Rasmussen and C. K. I. Williams. *Gaussian Processes for Machine Learning*. MIT Press, Cambridge, MA, 2006. [Google Books] .