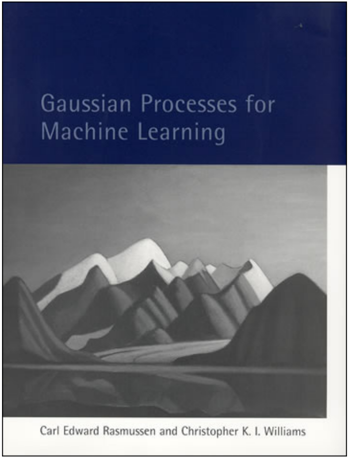
Introduction to Gaussian Processes

Neil D. Lawrence

GPSS
10th June 2013

Book



Rasmussen and Williams (2006)

Outline

Outline

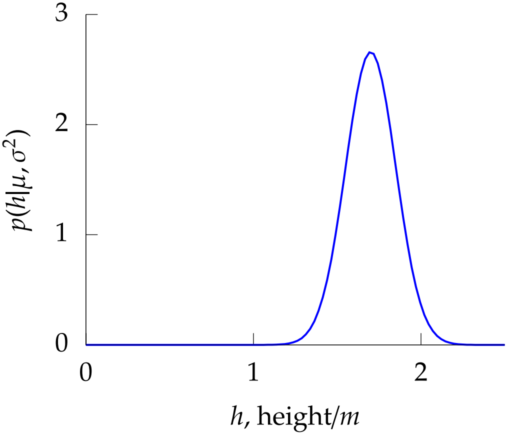
The Gaussian Density

- Perhaps the most common probability density.

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

- 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

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

σ^2 is the variance of the density and μ is the mean.

Two Important Gaussian Properties

Sum of Gaussians

- Sum of Gaussian variables is also Gaussian.

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

Two Important Gaussian Properties

Sum of Gaussians

- Sum of Gaussian variables is also Gaussian.

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

And the sum is distributed as

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

Two Important Gaussian Properties

Sum of Gaussians

- Sum of Gaussian variables is also Gaussian.

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

And the sum is distributed as

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

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

Two Important Gaussian Properties

Sum of Gaussians

- Sum of Gaussian variables is also Gaussian.

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

And the sum is distributed as

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

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

Two Important Gaussian Properties

Scaling a Gaussian

- Scaling a Gaussian leads to a Gaussian.

Two Important Gaussian Properties

Scaling a Gaussian

- Scaling a Gaussian leads to a Gaussian.

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

Two Important Gaussian Properties

Scaling a Gaussian

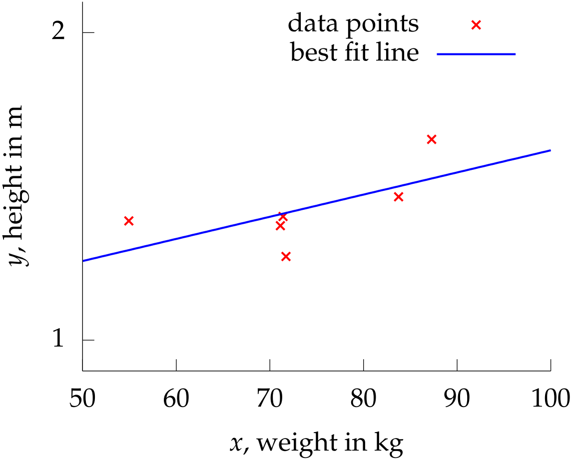
- Scaling a Gaussian leads to a Gaussian.

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

And the scaled density is distributed as

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

Linear Function

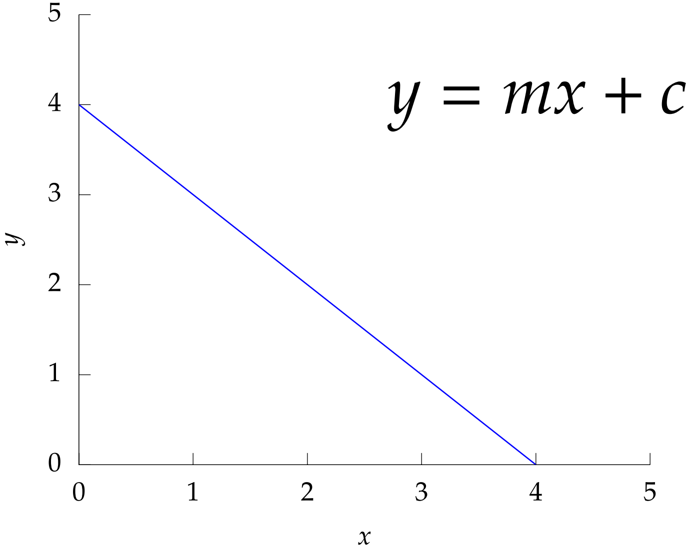


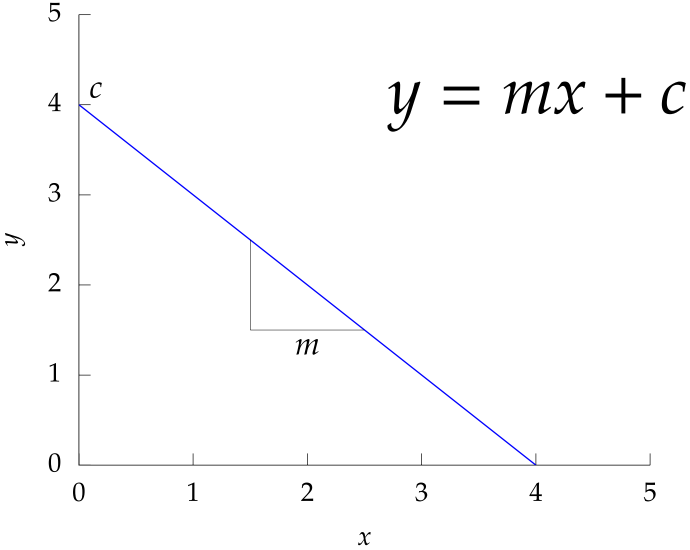
A linear regression between height and weight.

Regression Examples

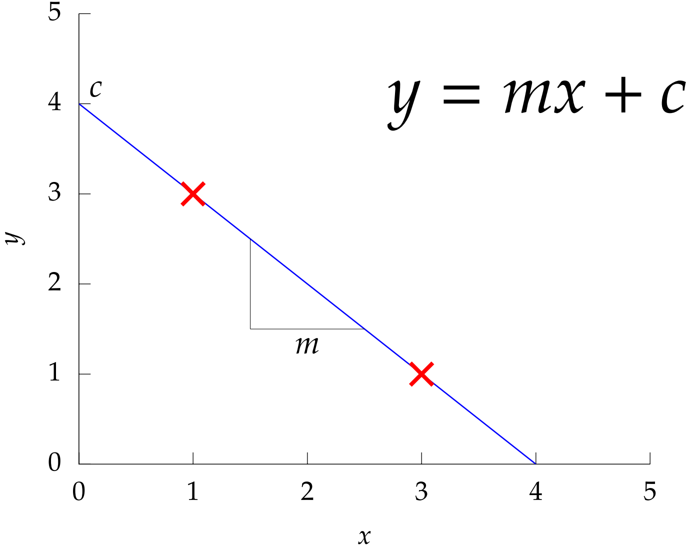
- Predict a real value, y_i given some inputs $\mathbf{x}_i$.
- Predict quality of meat given spectral measurements (Tecator data).
- Radiocarbon dating, the C14 calibration curve: predict age given quantity of C14 isotope.
- Predict quality of different Go or Backgammon moves given expert rated training data.

$$y = mx + c$$

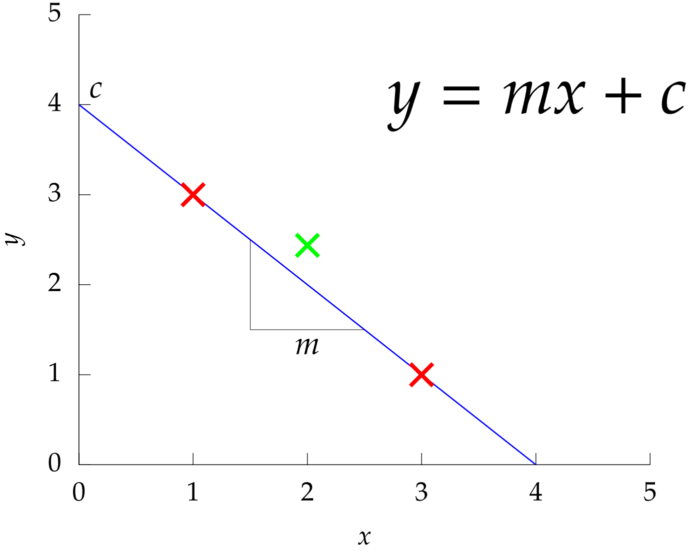

$y = mx + c$
5
4
3
2
1
0
y
0
1
2
3
4
5
x

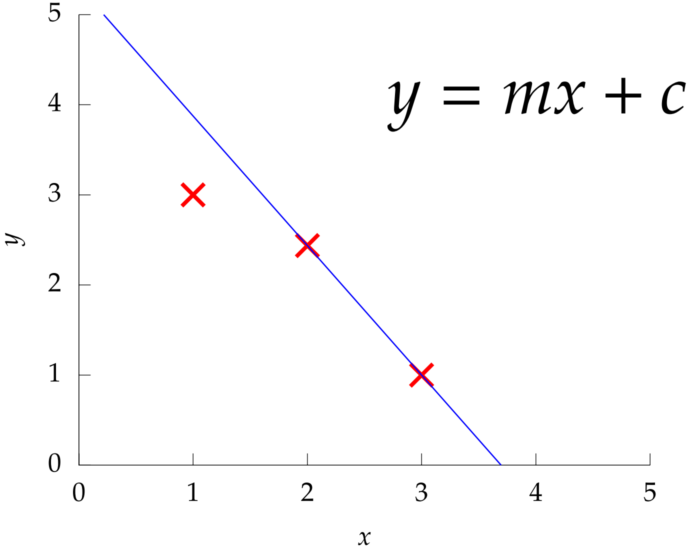


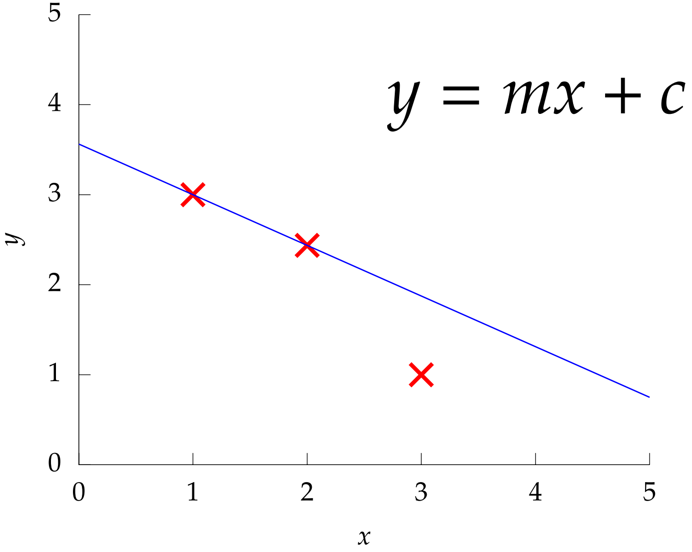
$y = mx + c$
c
m
y
x
0
1
2
3
4
5



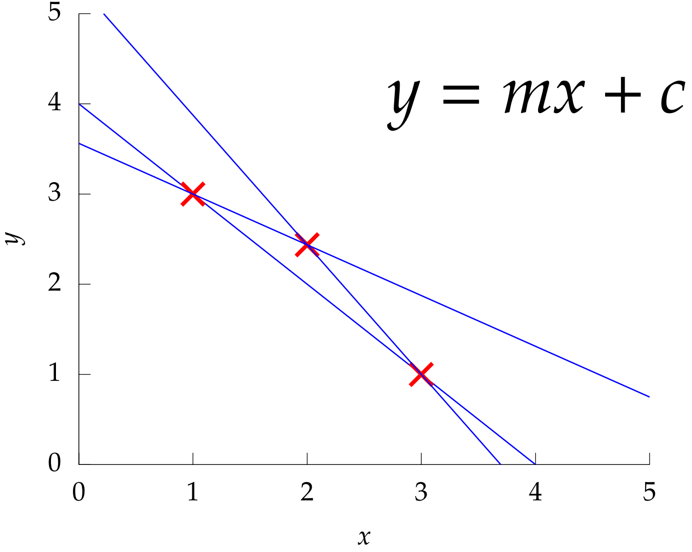
$y = mx + c$
c
m
0
1
2
3
4
5
0
1
2
3
4
5
x
y


$y = mx + c$
c
m
y
x
0
1
2
3
4
5


$y = mx + c$
y
x
0
1
2
3
4
5
0
1
2
3
4
5



$y = mx + c$
0
1
2
3
4
5
0
1
2
3
4
5
x
y


$y = mx + c$
y
x
0
1
2
3
4
5
0
1
2
3
4
5

point 1: $x = 1$, $y = 3$

$$3 = m + c$$

point 2: $x = 3$, $y = 1$

$$1 = 3m + c$$

point 3: $x = 2$, $y = 2.5$

$$2.5 = 2m + c$$

point 1: $x = 1, y = 3$

$$3 = m + c + \epsilon_1$$

point 2: $x = 3, y = 1$

$$1 = 3m + c + \epsilon_2$$

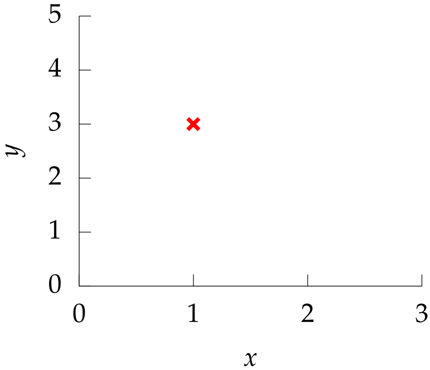
point 3: $x = 2, y = 2.5$

$$2.5 = 2m + c + \epsilon_3$$

Underdetermined System

What about two unknowns and *one* observation?

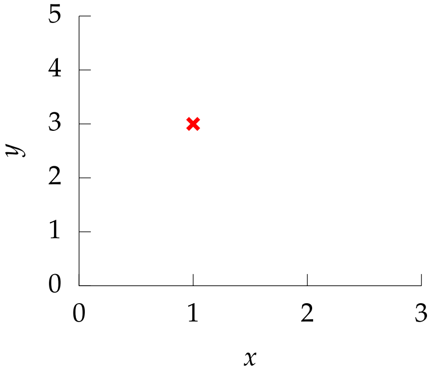
$$y_1 = mx_1 + c$$



Underdetermined System

Can compute m given c.

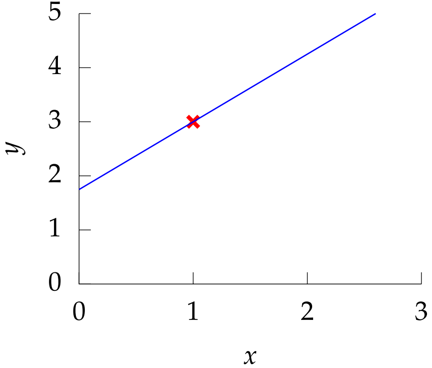
$$m = \frac{y_1 - c}{x}$$



Underdetermined System

Can compute m given c.

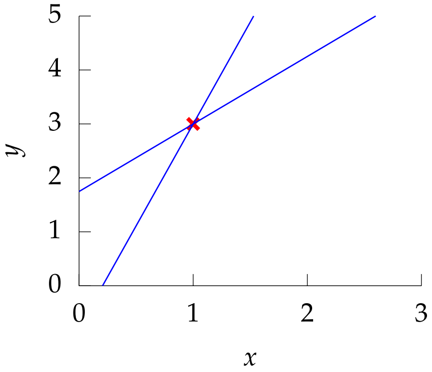
$$c = 1.75 \implies m = 1.25$$



Underdetermined System

Can compute m given c.

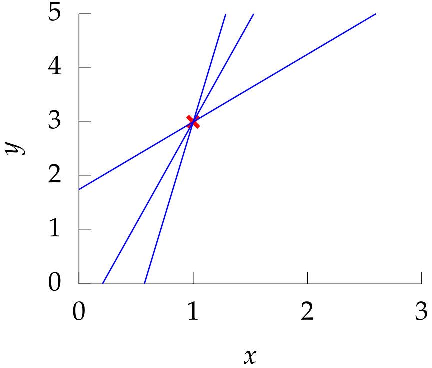
$$c = -0.777 \implies m = 3.78$$



Underdetermined System

Can compute m given c.

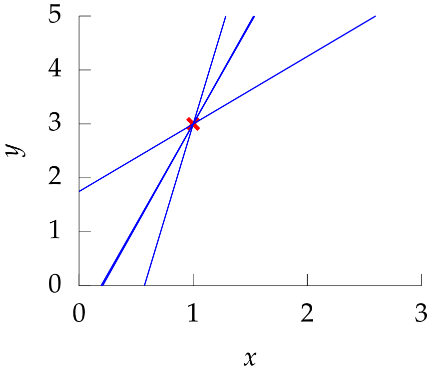
$$c = -4.01 \Longrightarrow m = 7.01$$



Underdetermined System

Can compute m given c.

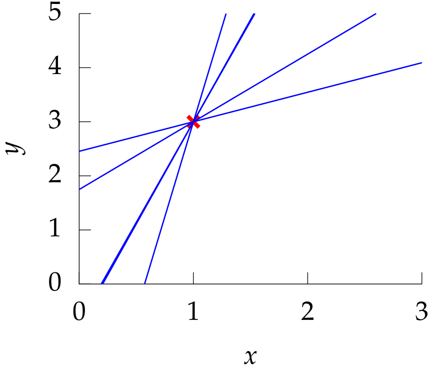
$$c = -0.718 \implies m = 3.72$$



Underdetermined System

Can compute m given c.

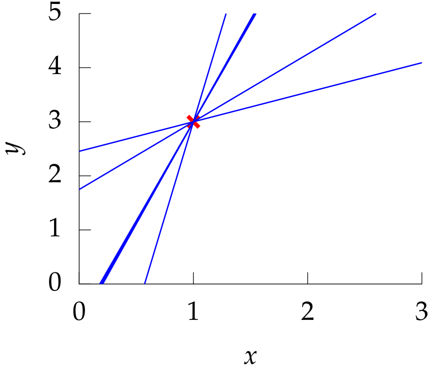
$$c = 2.45 \implies m = 0.545$$



Underdetermined System

Can compute m given c.

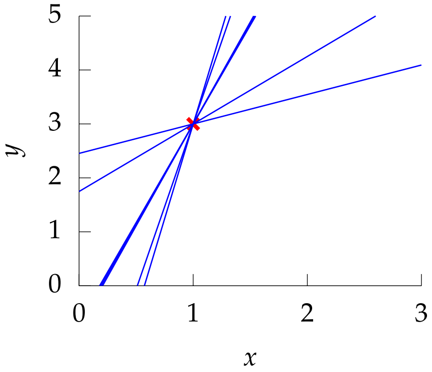
$$c = -0.657 \implies m = 3.66$$



Underdetermined System

Can compute m given c.

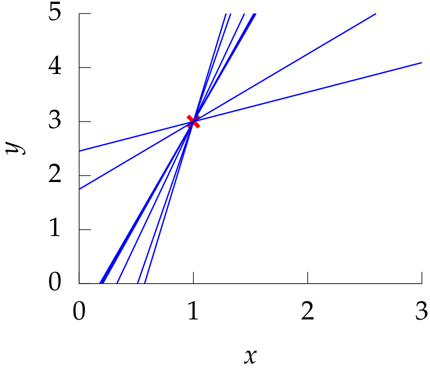
$$c = -3.13 \Longrightarrow m = 6.13$$



Underdetermined System

Can compute m given c.

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

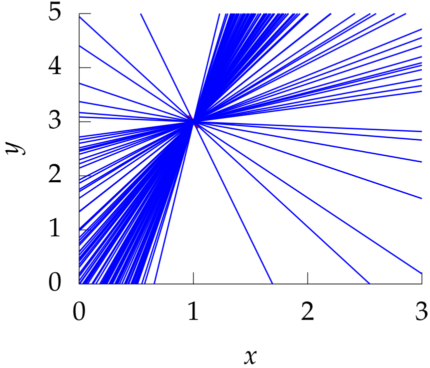


Underdetermined System

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.

Multivariate Prior Distributions

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

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

  (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).

Multivariate Prior Distributions

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

  $$y_i = \mathbf{w}^\top \mathbf{x}_{i,:} + \epsilon_i$$

  (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).

Prior Distribution

- Bayesian inference requires a prior on the parameters.
- The prior represents your belief *before* you see the data of the likely value of the parameters.
- For linear regression, consider a Gaussian prior on the intercept:

$$c \sim \mathcal{N}(0, \alpha_1)$$

Gaussian Noise

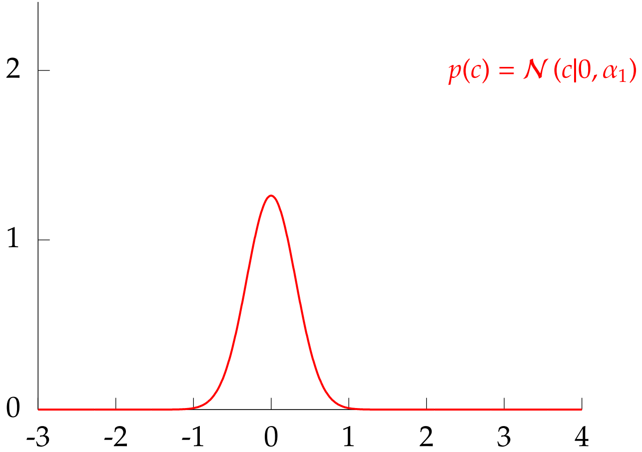


Figure: A Gaussian prior combines with a Gaussian likelihood for a Gaussian posterior.

Gaussian Noise

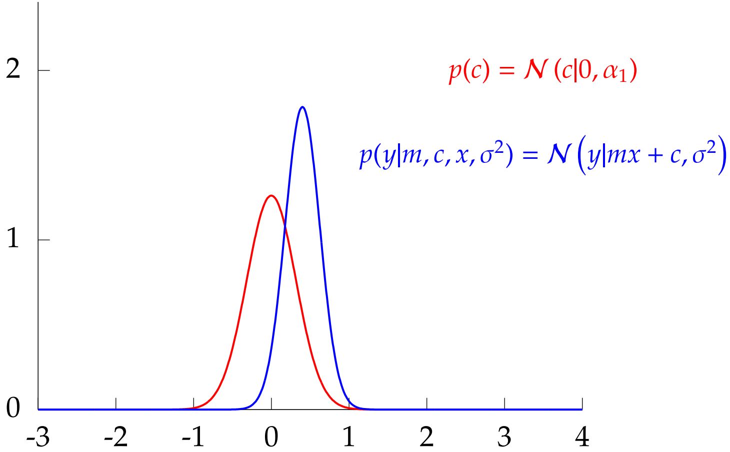


Figure: A Gaussian prior combines with a Gaussian likelihood for a Gaussian posterior.

Gaussian Noise

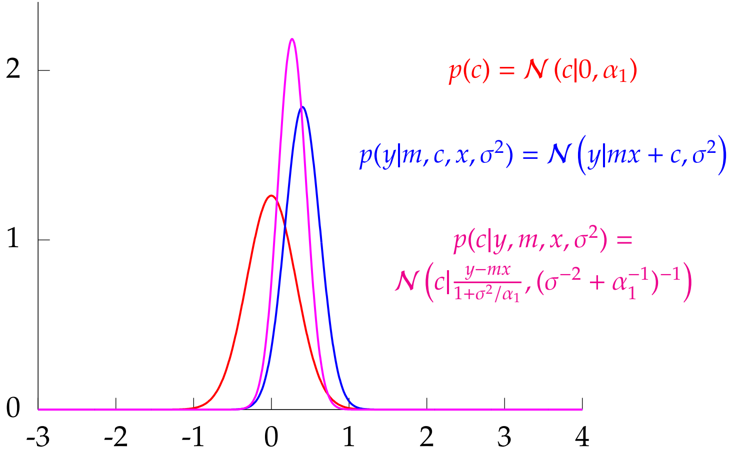


Figure: A Gaussian prior combines with a Gaussian likelihood for a Gaussian posterior.

Stages to Derivation of the Posterior

- Multiply likelihood by prior
  - they are "exponentiated quadratics", the answer is always also an exponentiated quadratic because $\exp(a^2)\exp(b^2) = \exp(a^2 + b^2)$.
- Complete the square to get the resulting density in the form of a Gaussian.
- Recognise the mean and (co)variance of the Gaussian. This is the estimate of the posterior.

Multivariate Regression Likelihood

- Noise corrupted data point

$$y_i = \mathbf{w}^\top \mathbf{x}_{i,:} + \epsilon_i$$

Multivariate Regression Likelihood

- Noise corrupted data point

$$y_i = \mathbf{w}^\top \mathbf{x}_{i,:} + \epsilon_i$$

- Multivariate regression likelihood:

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y_i - \mathbf{w}^\top \mathbf{x}_{i,:}\right)^2\right)$$

Multivariate Regression Likelihood

- Noise corrupted data point

$$y_i = \mathbf{w}^\top \mathbf{x}_{i,:} + \epsilon_i$$

- Multivariate regression likelihood:

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y_i - \mathbf{w}^\top \mathbf{x}_{i,:}\right)^2\right)$$

- Now use a multivariate Gaussian prior:

$$p(\mathbf{w}) = \frac{1}{(2\pi\alpha)^{\frac{p}{2}}} \exp\left(-\frac{1}{2\alpha} \mathbf{w}^\top \mathbf{w}\right)$$

Two Dimensional Gaussian

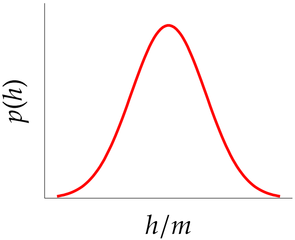
- Consider height, h/m and weight, w/kg.
- Could sample height from a distribution:

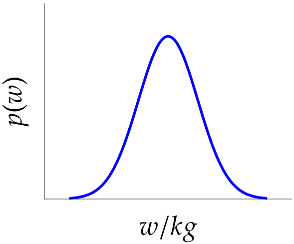
$$p(h) \sim \mathcal{N}(1.7, 0.0225)$$

- And similarly weight:

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

Height and Weight Models

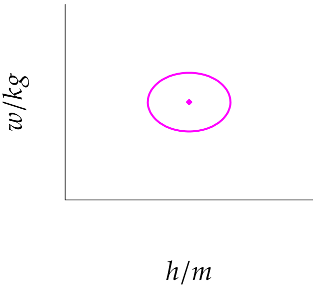




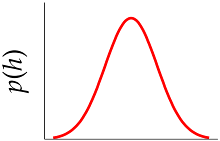
Gaussian distributions for height and weight.

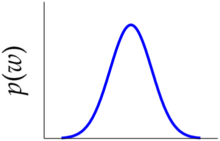
Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions

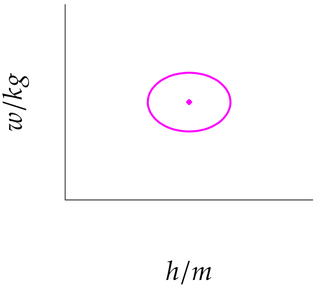




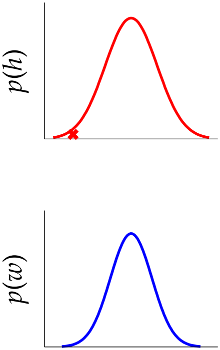
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



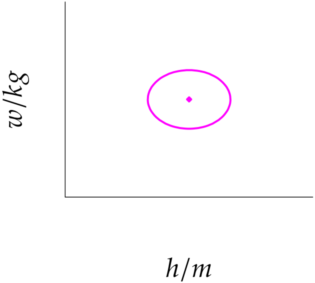
Marginal Distributions



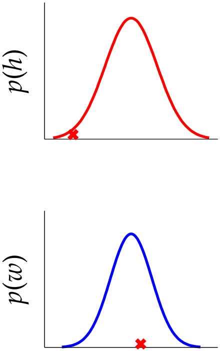
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



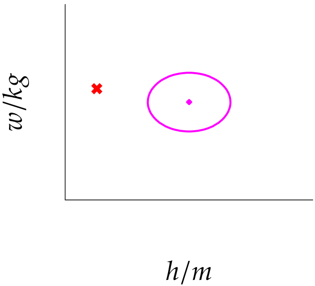
Marginal Distributions



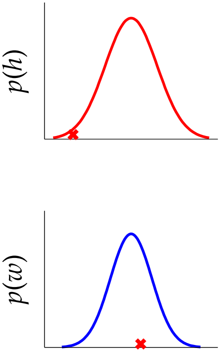
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions

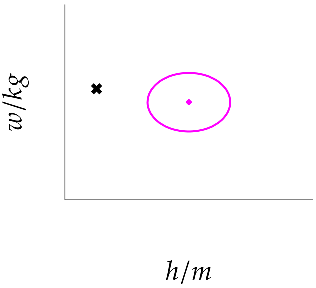


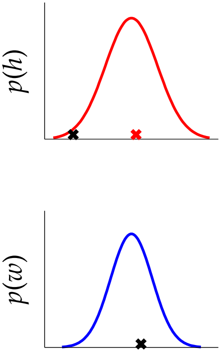
Samples of height and weight

Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution

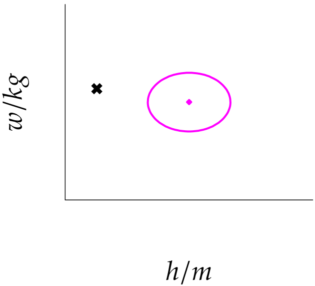




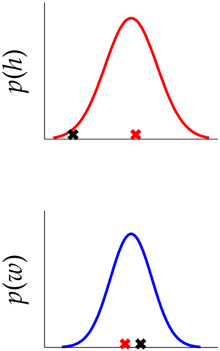
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions

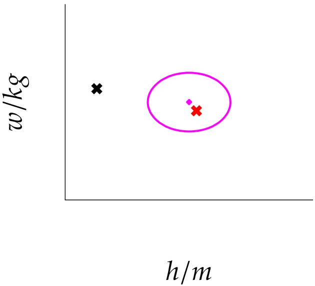


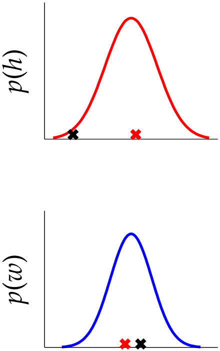
Samples of height and weight

Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution



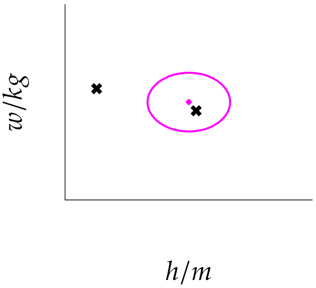


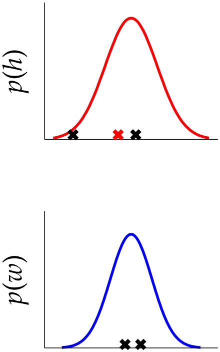
Samples of height and weight

Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution

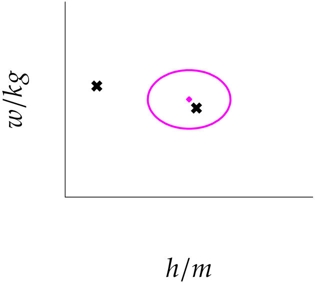




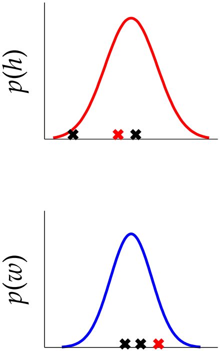
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution

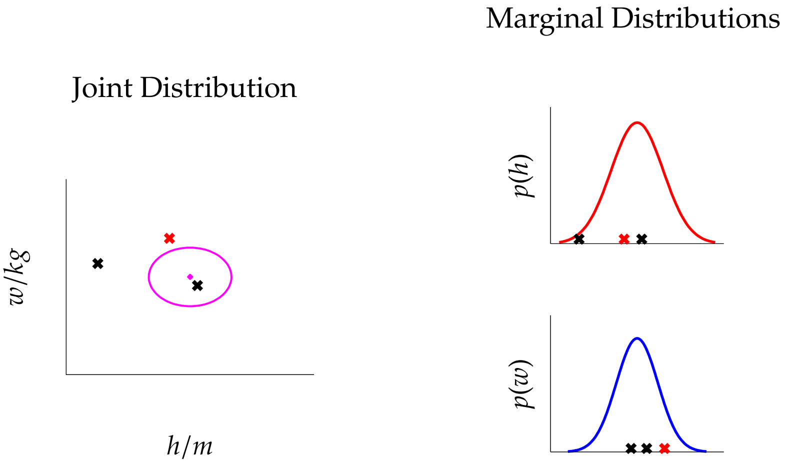


Marginal Distributions



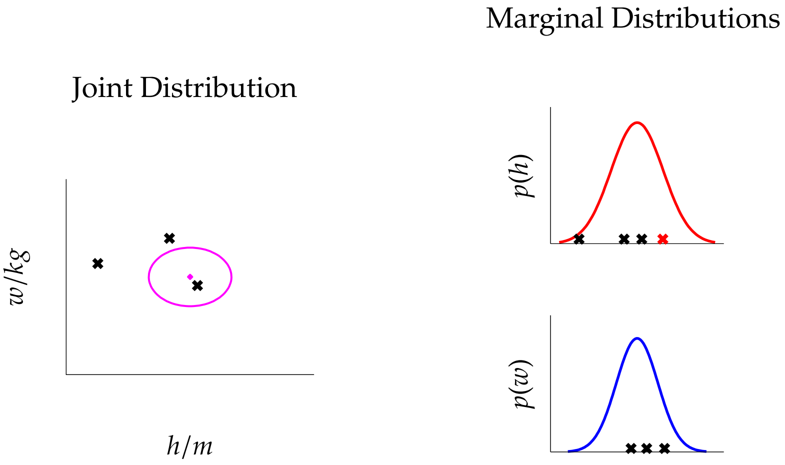
Samples of height and weight

Sampling Two Dimensional Variables



Samples of height and weight

Sampling Two Dimensional Variables

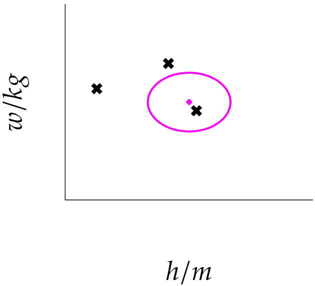


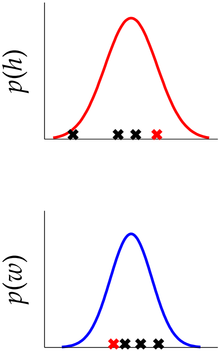
Samples of height and weight

Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution



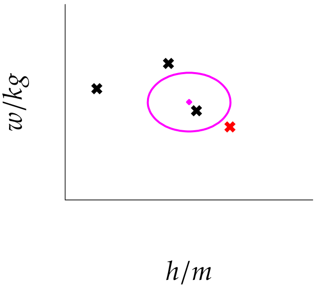


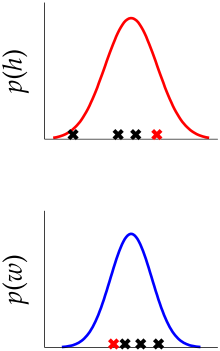
Samples of height and weight

Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution

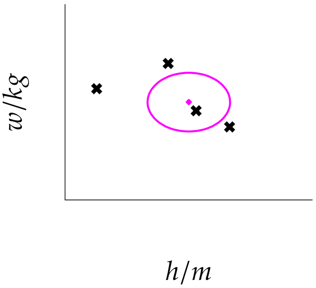




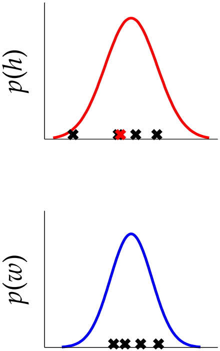
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



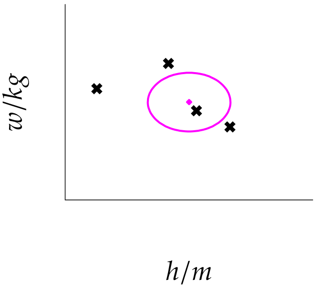
Marginal Distributions



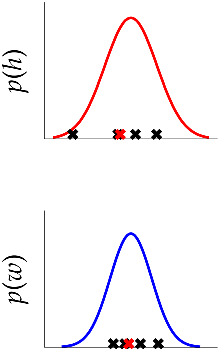
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution

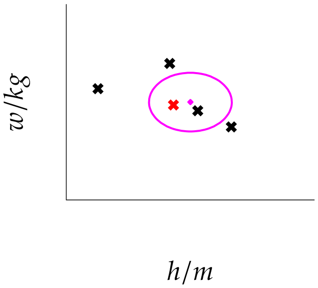


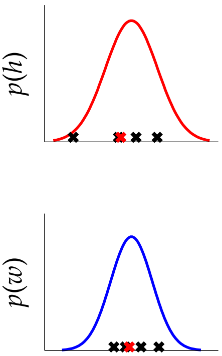
Marginal Distributions



Samples of height and weight

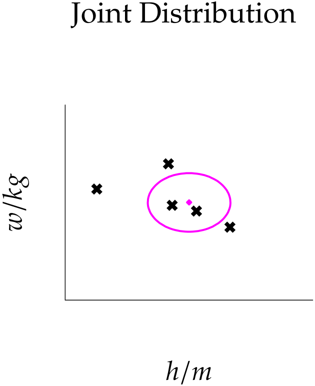
Sampling Two Dimensional Variables

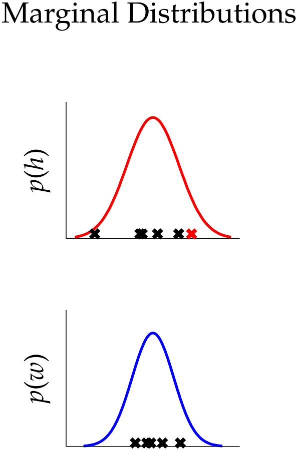




Samples of height and weight

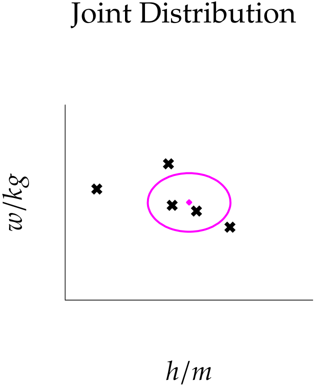
Sampling Two Dimensional Variables

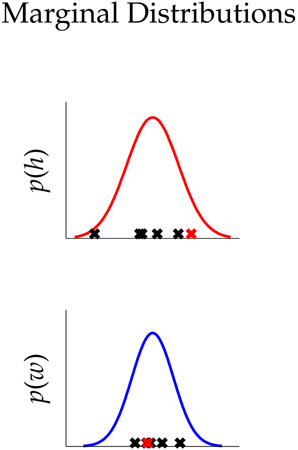




Samples of height and weight

Sampling Two Dimensional Variables

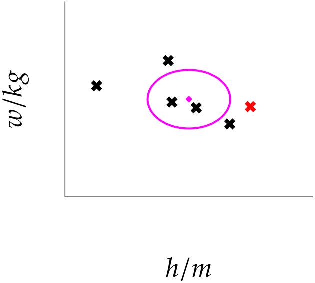




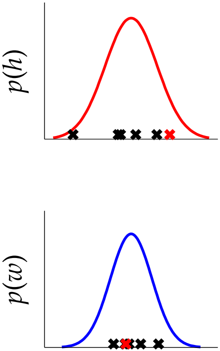
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



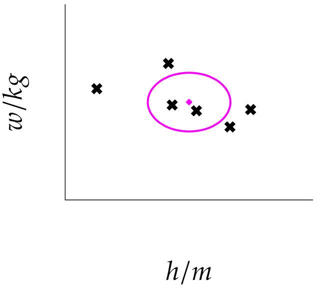
Marginal Distributions



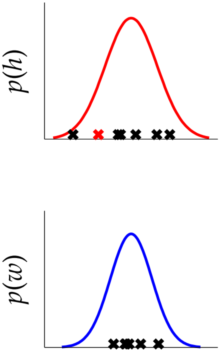
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution

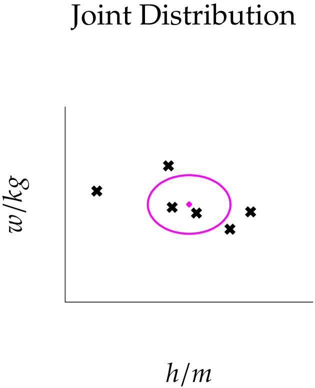


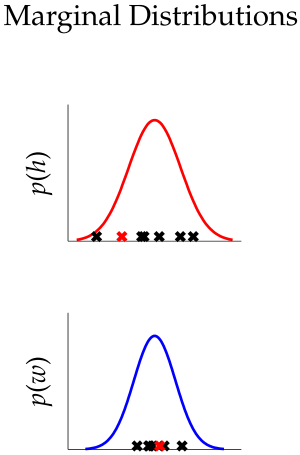
Marginal Distributions



Samples of height and weight

Sampling Two Dimensional Variables

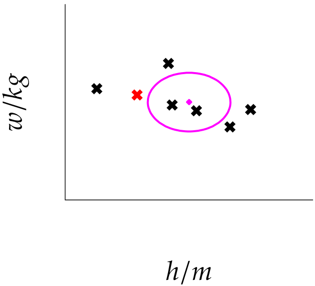




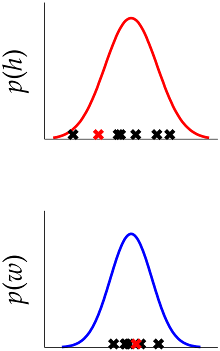
Samples of height and weight

Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions

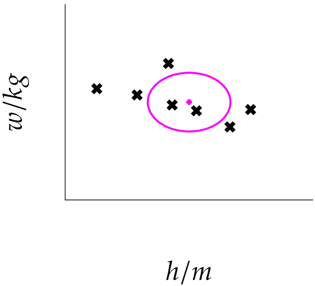


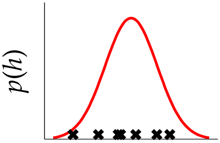
Samples of height and weight

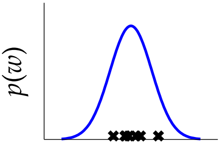
Sampling Two Dimensional Variables

Marginal Distributions

Joint Distribution







Samples of height and weight

Independence Assumption

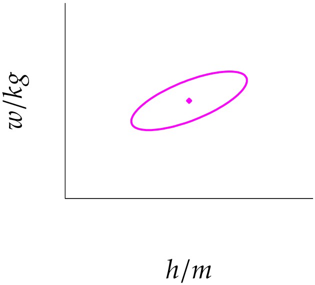
- This assumes height and weight are independent.

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

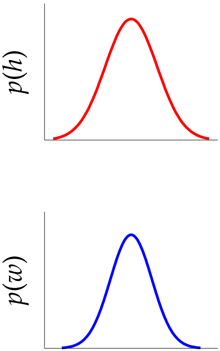
- In reality they are dependent (body mass index) $= \frac{w}{h^2}$.

Sampling Two Dimensional Variables

Joint Distribution



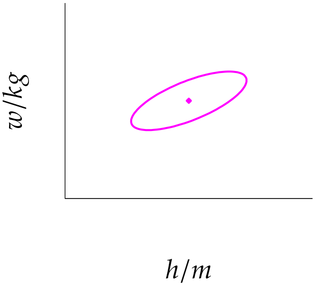
Marginal Distributions

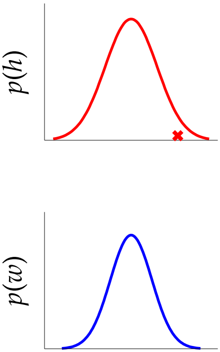


Sampling Two Dimensional Variables

Marginal Distributions

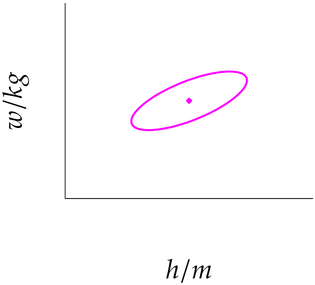
Joint Distribution



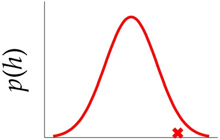


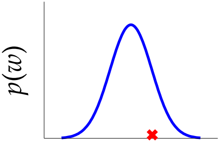
Sampling Two Dimensional Variables

Joint Distribution



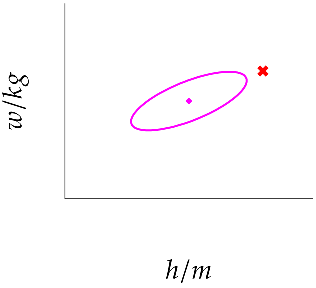
Marginal Distributions



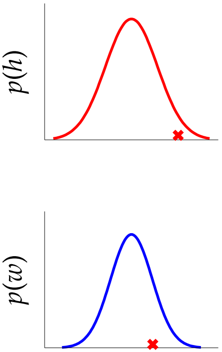


Sampling Two Dimensional Variables

Joint Distribution

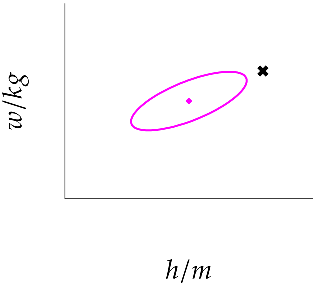


Marginal Distributions

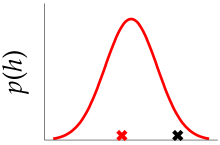


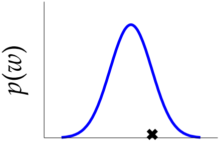
Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions

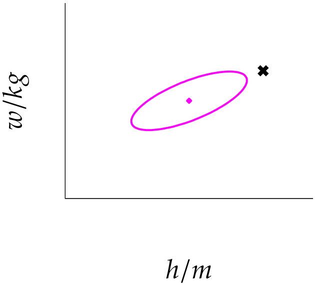


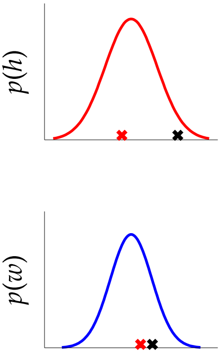


Sampling Two Dimensional Variables

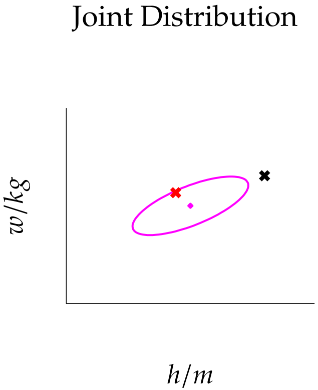
Marginal Distributions

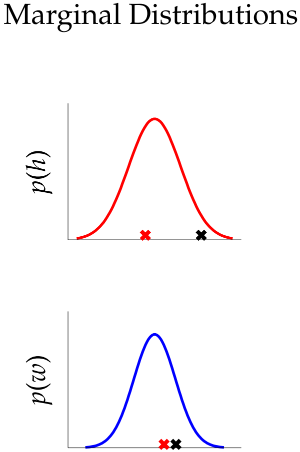
Joint Distribution





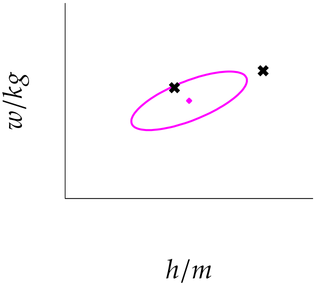
Sampling Two Dimensional Variables



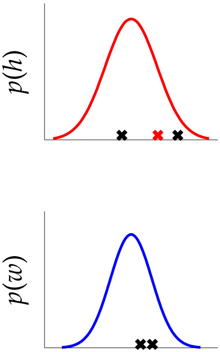


Sampling Two Dimensional Variables

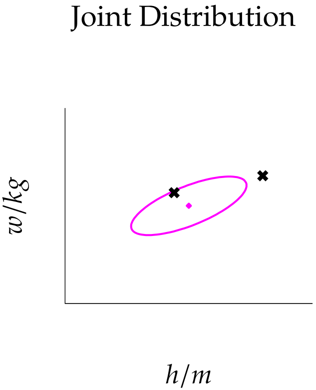
Joint Distribution

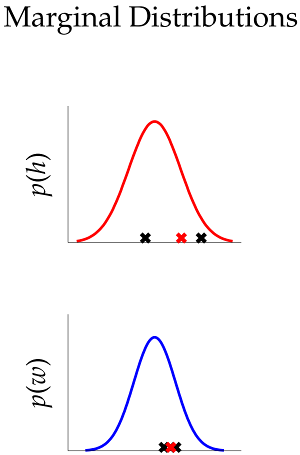


Marginal Distributions

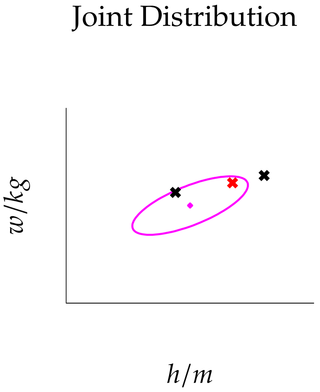


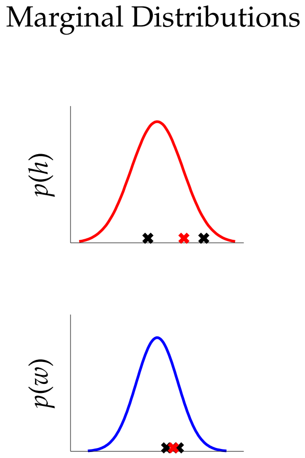
Sampling Two Dimensional Variables



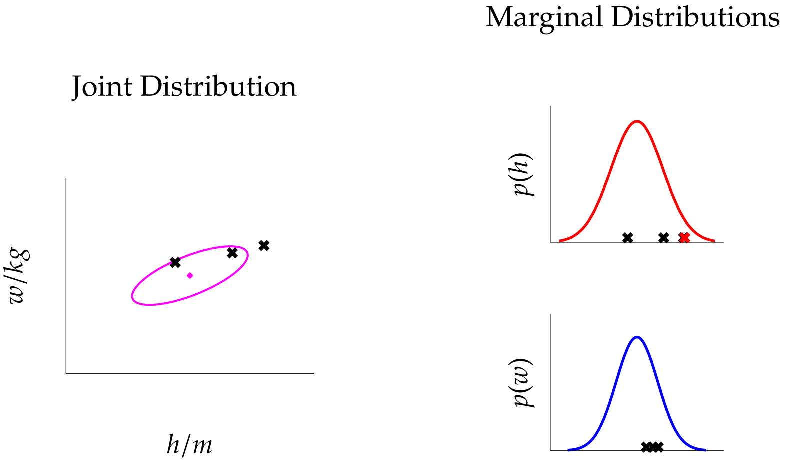


Sampling Two Dimensional Variables





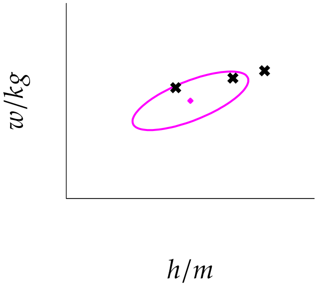
Sampling Two Dimensional Variables

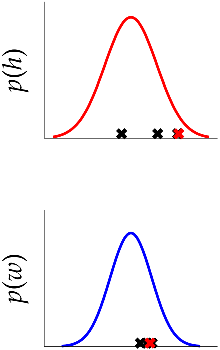


Sampling Two Dimensional Variables

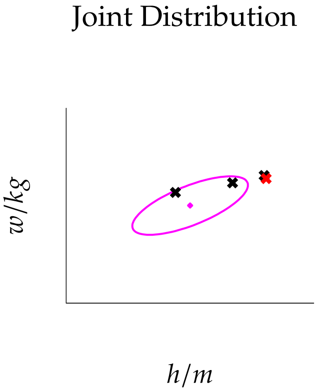
Marginal Distributions

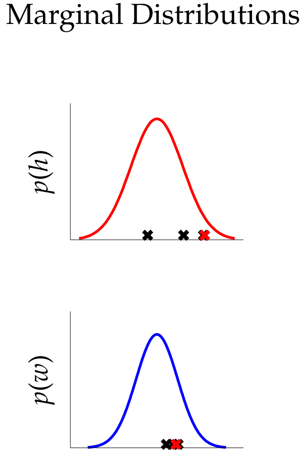
Joint Distribution





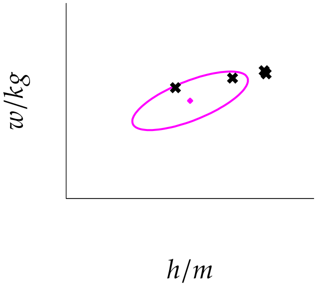
Sampling Two Dimensional Variables



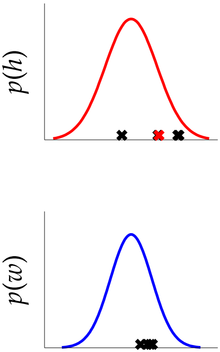


Sampling Two Dimensional Variables

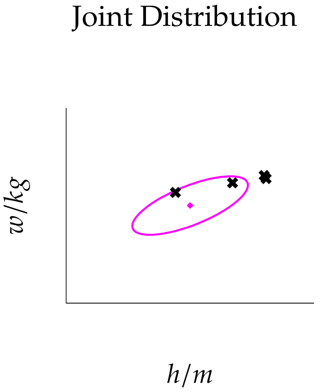
Joint Distribution

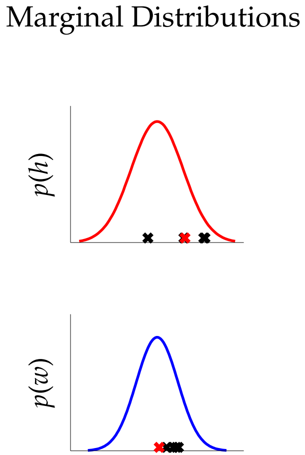


Marginal Distributions



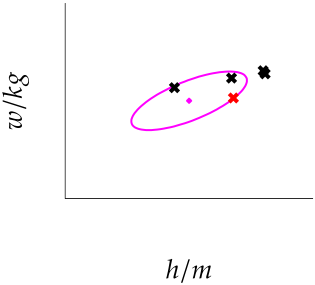
Sampling Two Dimensional Variables



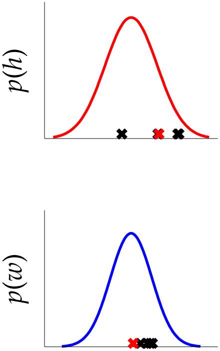


Sampling Two Dimensional Variables

Joint Distribution

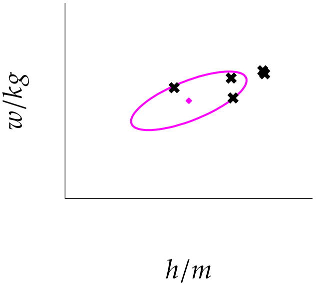


Marginal Distributions

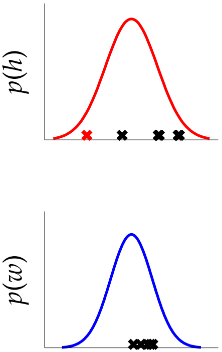


Sampling Two Dimensional Variables

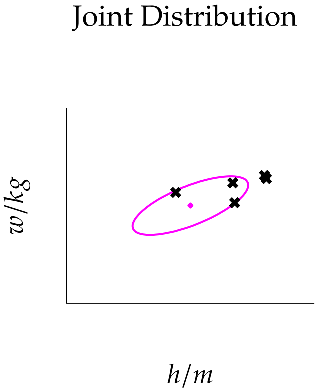
Joint Distribution

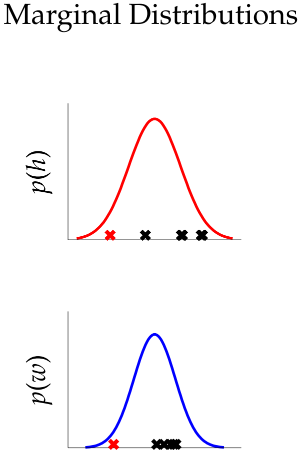


Marginal Distributions



Sampling Two Dimensional Variables

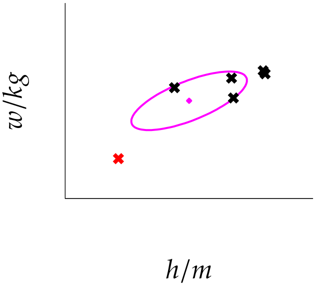


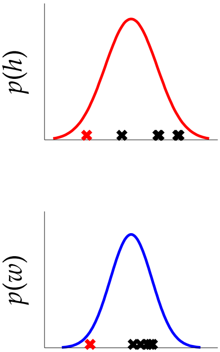


Sampling Two Dimensional Variables

Marginal Distributions

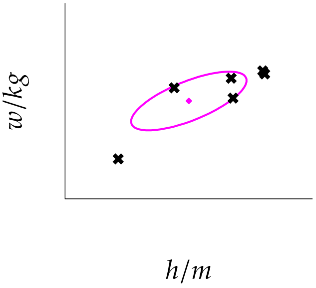
Joint Distribution



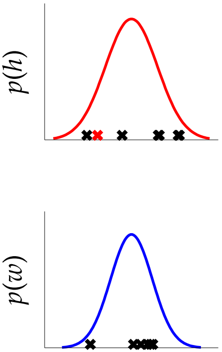


Sampling Two Dimensional Variables

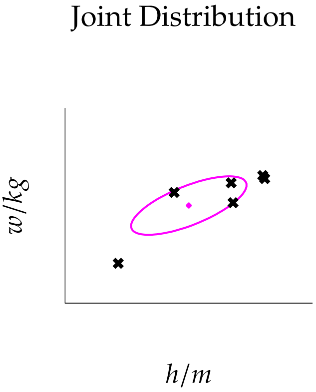
Joint Distribution

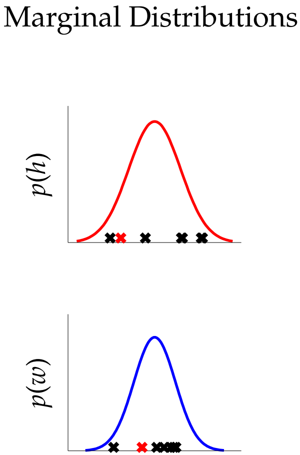


Marginal Distributions



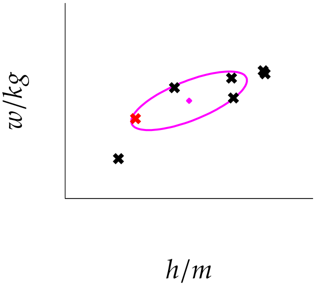
Sampling Two Dimensional Variables



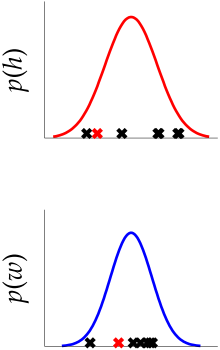


Sampling Two Dimensional Variables

Joint Distribution

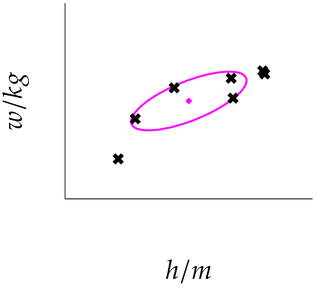


Marginal Distributions

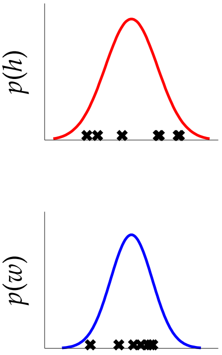


Sampling Two Dimensional Variables

Joint Distribution



Marginal Distributions



Independent Gaussians

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

Independent Gaussians

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

Independent Gaussians

$$p(w,h) = \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2}} \exp\left(-\frac{1}{2}\left(\begin{bmatrix} w \\ h \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right)^\top \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}^{-1} \left(\begin{bmatrix} w \\ h \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right)\right)$$

Independent Gaussians

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

Correlated Gaussian

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

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

Correlated Gaussian

Form correlated from original by rotating the data space using matrix $\mathbf{R}$.

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

Correlated Gaussian

Form correlated from original by rotating the data space using matrix $\mathbf{R}$.

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

this gives a covariance matrix:

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

Correlated Gaussian

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

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

this gives a covariance matrix:

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

Recall Univariate Gaussian Properties

1. Sum of Gaussian variables is also Gaussian.

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

Recall Univariate Gaussian Properties

1. Sum of Gaussian variables is also Gaussian.

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

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

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.

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.

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

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.

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

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

Multivariate Consequence

- If

$$\mathbf{x} \sim \mathcal{N}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$

Multivariate Consequence

- If

$$\mathbf{x} \sim \mathcal{N}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$

- And

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

Multivariate Consequence

- If

$$\mathbf{x} \sim \mathcal{N}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$

- And

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

- Then

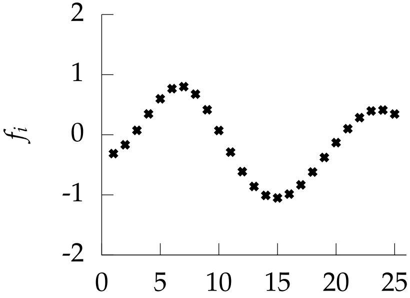
$$\mathbf{y} \sim \mathcal{N}\left(\mathbf{W}\boldsymbol{\mu}, \mathbf{W}\boldsymbol{\Sigma}\mathbf{W}^{\top}\right)$$

Sampling a Function

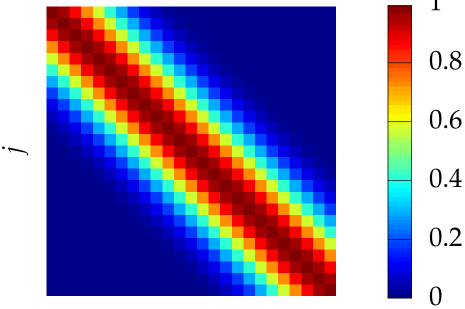
Multi-variate Gaussians

- 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



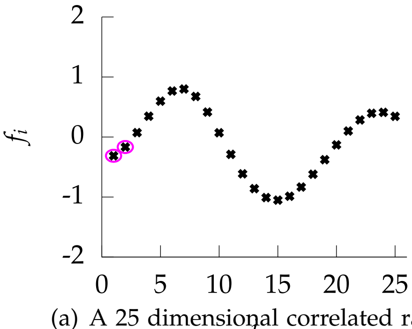
(a) A 25 dimensional correlated random variable (values ploted against index)



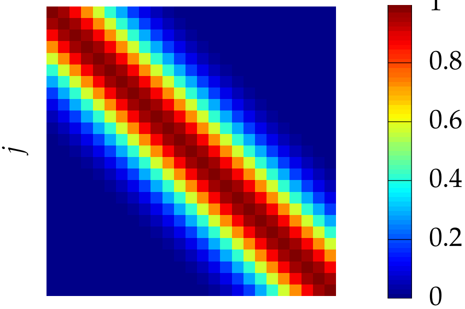
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



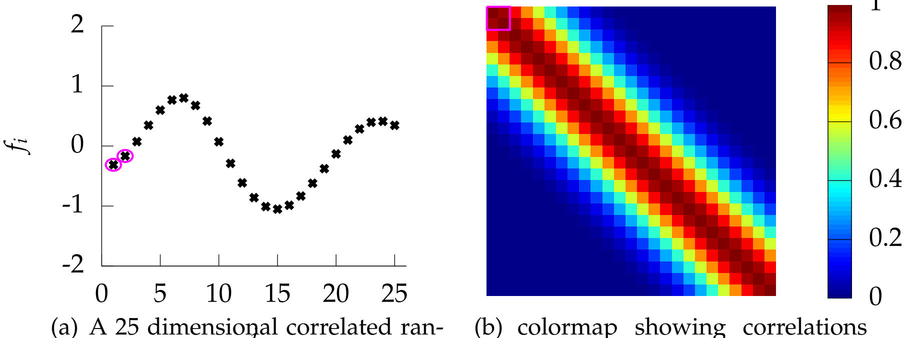
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample

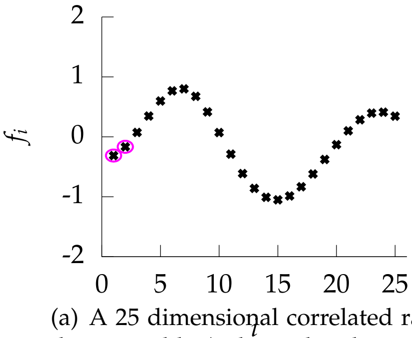


(a) A 25 dimensional correlated random variable (values ploted against index)

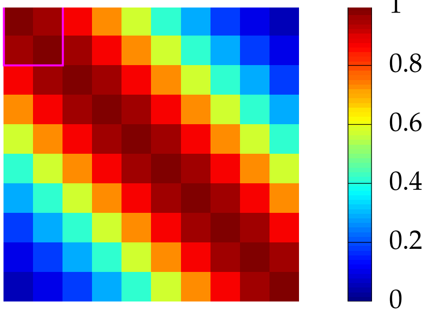
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



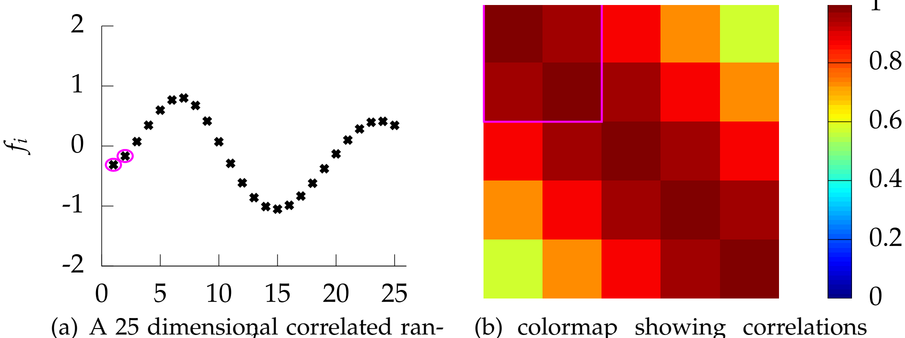
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample

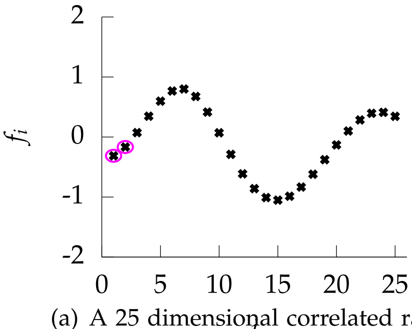


(a) A 25 dimensional correlated random variable (values ploted against index)

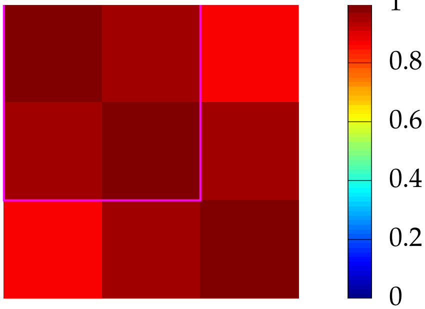
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



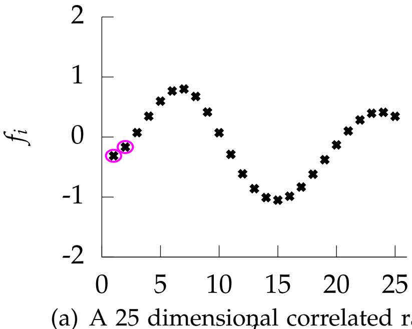
(a) A 25 dimensional correlated random variable (values ploted against index)



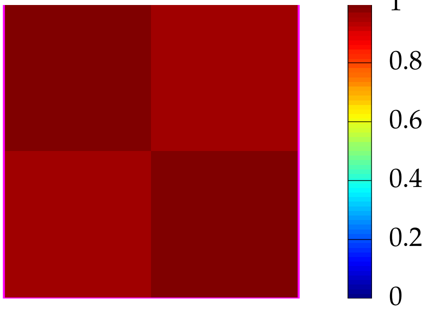
(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



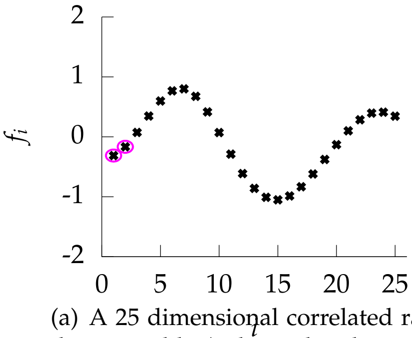
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



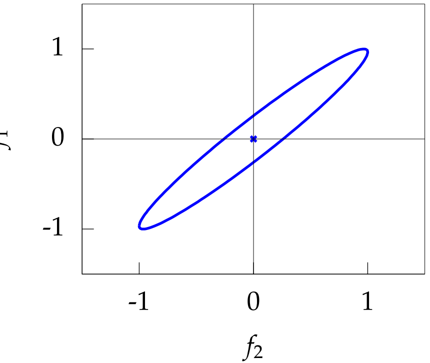
(a) A 25 dimensional correlated random variable (values ploted against index)

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

(b) correlation between f_1 and f_2.

Figure: A sample from a 25 dimensional Gaussian distribution.

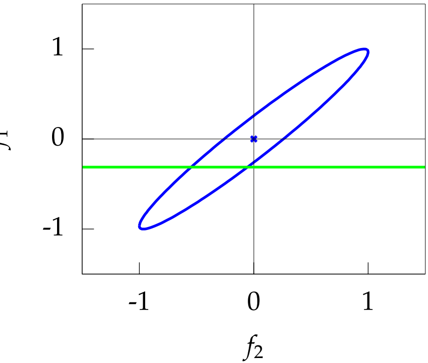
Prediction of f_2 from f_1



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

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_2)$.

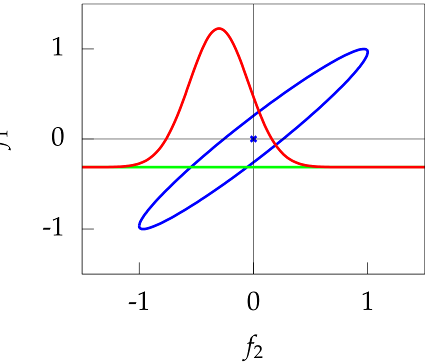
Prediction of f_2 from f_1



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

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

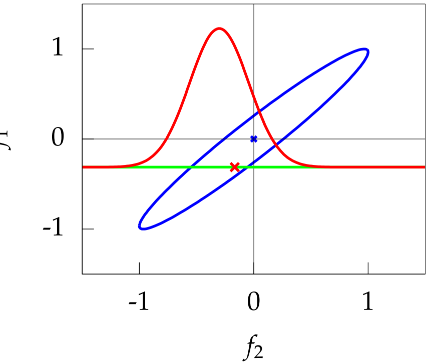
Prediction of f_2 from f_1



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

- 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

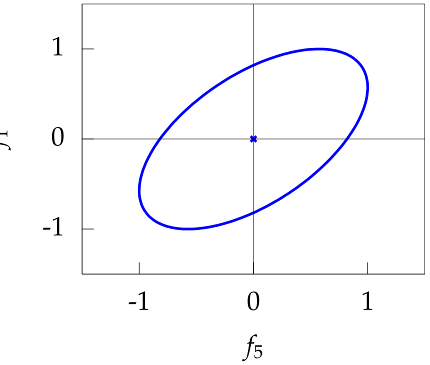
- Prediction of f_2 from f_1 requires *conditional density*.
- Conditional density is *also* Gaussian.

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

where covariance of joint density is given by

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

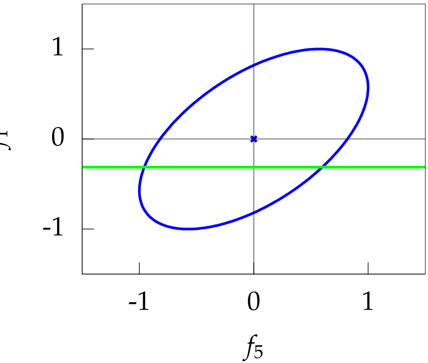
Prediction of f_5 from f_1



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

- The single contour of the Gaussian density represents the joint distribution, $p(f_1, f_5)$.

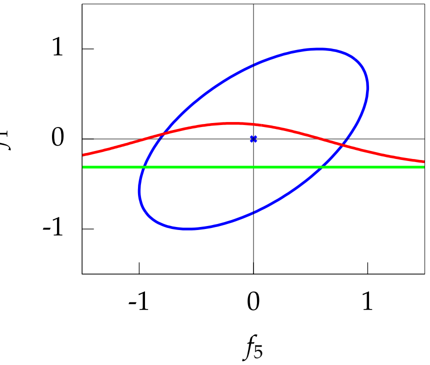
Prediction of f_5 from f_1



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

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

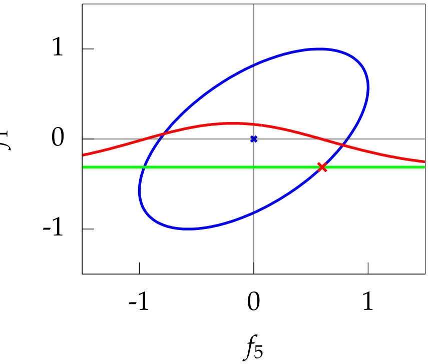
Prediction of f_5 from f_1



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

- 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

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

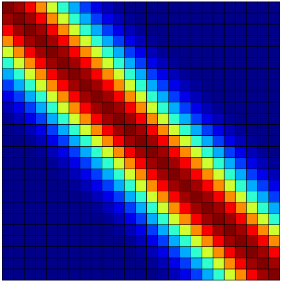
Covariance Functions

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 **x**.
- For the example above it was based on Euclidean distance.
- The covariance function is also know as a kernel.



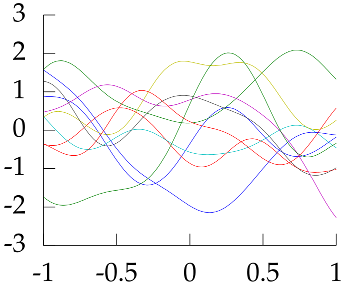
Covariance Functions

Where did this covariance matrix come from?

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

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

- 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?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 1.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40-1.20)^2}{2\times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40-1.20)^2}{2\times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 1.00 \times \exp\left(-\frac{(1.40 - 1.20)^2}{2 \times 2.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

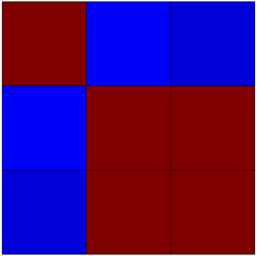
Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40$, $x_3 = 1.40$

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



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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 1.0 \times \exp\left(-\frac{(1.2 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.2$, $x_2 = 1.2$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4, x_2 = 1.2$$

$$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4 - 1.2)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4-1.2)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 1.0 \times \exp\left(-\frac{(1.4-1.2)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4, x_3 = 1.4$$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.4, x_3 = 1.4$$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{4,1} = 1.0 \times \exp\left(-\frac{(2.0 - -3)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-1.2)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_2 = 1.2$$

$$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-1.2)^2}{2 \times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_2 = 1.2$$

$$k_{4,2} = 1.0 \times \exp\left(-\frac{(2.0-1.2)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-1.4)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_3 = 1.4$$

$$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-1.4)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_3 = 1.4$$

$$k_{4,3} = 1.0 \times \exp\left(-\frac{(2.0-1.4)^2}{2\times 2.0^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_4 = 2.0$$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_4 = 2.0$$

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

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

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

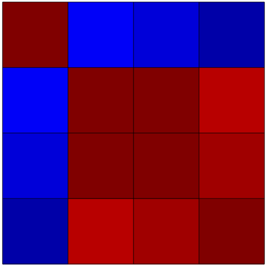
Covariance Functions

Where did this covariance matrix come from?

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

$$x_4 = 2.0, x_4 = 2.0$$

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



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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{2,1} = 4.00 \times \exp\left(-\frac{(1.20 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20$, $x_2 = 1.20$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_2 = 1.20, x_2 = 1.20$$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,1} = 4.00 \times \exp\left(-\frac{(1.40 - -3.0)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40-1.20)^2}{2\times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40 - 1.20)^2}{2 \times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

$$k_{3,2} = 4.00 \times \exp\left(-\frac{(1.40-1.20)^2}{2\times 5.00^2}\right)$$

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$$x_3 = 1.40, x_3 = 1.40$$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

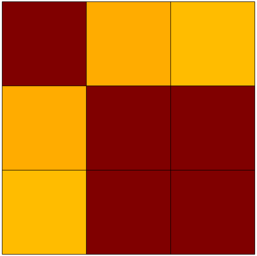
Covariance Functions

Where did this covariance matrix come from?

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

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

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



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

Outline

Basis Function Form

Radial basis functions commonly have the form

$$\phi_k(\mathbf{x}_i) = \exp\left(-\frac{\left|\mathbf{x}_i - \boldsymbol{\mu}_k\right|^2}{2\ell^2}\right).$$

- Basis function maps data into a "feature space" in which a linear sum is a non linear function.

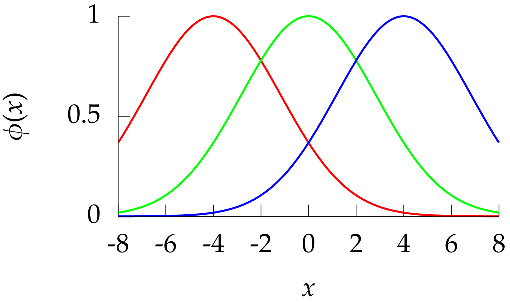


Figure: A set of radial basis functions with width $\ell = 2$ and location parameters $\boldsymbol{\mu} = [-4 \;\; 0 \;\; 4]^\top$.

Basis Function Representations

- Represent a function by a linear sum over a basis,

$$f(\mathbf{x}_{i,:}; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_{i,:}), \tag{1}$$

- Here: m basis functions and $\phi_k(\cdot)$ is kth basis function and

$$\mathbf{w} = [w_1, \ldots, w_m]^\top .$$

- For standard linear model: $\phi_k(\mathbf{x}_{i,:}) = x_{i,k}$.

Random Functions

Functions derived using:

$$f(x) = \sum_{k=1}^{m} w_k \phi_k(x),$$

where $\mathbf{W}$ is sampled from a Gaussian density,

$$w_k \sim \mathcal{N}(0, \alpha).$$

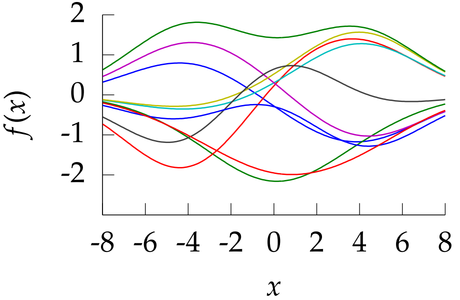


Figure: Functions sampled using the basis set from figure 3. Each line is a separate sample, generated by a weighted sum of the basis set. The weights, $\mathbf{w}$ are sampled from a Gaussian density with variance $\alpha = 1$.

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

computed at training data gives a vector

$$\mathbf{f} = \mathbf{\Phi}\mathbf{w}.$$

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

computed at training data gives a vector

$$\mathbf{f} = \mathbf{\Phi}\mathbf{w}.$$

$\mathbf{w}$ and $\mathbf{f}$ are only related by an *inner product*.

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

computed at training data gives a vector

$$\mathbf{f} = \mathbf{\Phi}\mathbf{w}.$$

$\mathbf{w}$ and $\mathbf{f}$ are only related by an *inner product*.

$\mathbf{\Phi} \in \Re^{n \times p}$ is a *design matrix*

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

computed at training data gives a vector

$$\mathbf{f} = \mathbf{\Phi}\mathbf{w}.$$

$\mathbf{w}$ and $\mathbf{f}$ are only related by an *inner product*.

$\mathbf{\Phi} \in \Re^{n \times p}$ is a *design matrix*

$\mathbf{\Phi}$ is fixed and non-stochastic for a given training set.

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

$$f(\mathbf{x}_i; \mathbf{w}) = \sum_{k=1}^{m} w_k \phi_k(\mathbf{x}_i)$$

computed at training data gives a vector

$$\mathbf{f} = \mathbf{\Phi}\mathbf{w}.$$

$\mathbf{w}$ and $\mathbf{f}$ are only related by an *inner product*.

$\mathbf{\Phi} \in \Re^{n \times p}$ is a *design matrix*

$\mathbf{\Phi}$ is fixed and non-stochastic for a given training set.

$\mathbf{f}$ is Gaussian distributed.

Expectations

- We have
$$\langle \mathbf{f} \rangle = \boldsymbol{\Phi} \langle \mathbf{w} \rangle \,.$$

We use $\langle \cdot \rangle$ to denote expectations under prior distributions.

Expectations

- We have

$$\langle \mathbf{f} \rangle = \mathbf{\Phi} \langle \mathbf{w} \rangle .$$

- Prior mean of $\mathbf{w}$ was zero giving

$$\langle \mathbf{f} \rangle = \mathbf{0}.$$

We use $\langle \cdot \rangle$ to denote expectations under prior distributions.

Expectations

- We have
$$\langle \mathbf{f} \rangle = \mathbf{\Phi} \langle \mathbf{w} \rangle .$$
- Prior mean of $\mathbf{w}$ was zero giving
$$\langle \mathbf{f} \rangle = \mathbf{0}.$$
- Prior covariance of $\mathbf{f}$ is
$$\mathbf{K} = \left\langle \mathbf{f}\mathbf{f}^\top \right\rangle - \langle \mathbf{f} \rangle \langle \mathbf{f} \rangle^\top$$

We use $\langle \cdot \rangle$ to denote expectations under prior distributions.

Expectations

- We have

$$\langle \mathbf{f} \rangle = \mathbf{\Phi} \langle \mathbf{w} \rangle .$$

- Prior mean of $\mathbf{w}$ was zero giving

$$\langle \mathbf{f} \rangle = \mathbf{0}.$$

- Prior covariance of $\mathbf{f}$ is

$$\mathbf{K} = \left\langle \mathbf{f}\mathbf{f}^\top \right\rangle - \langle \mathbf{f} \rangle \langle \mathbf{f} \rangle^\top$$

$$\left\langle \mathbf{f}\mathbf{f}^\top \right\rangle = \mathbf{\Phi} \left\langle \mathbf{w}\mathbf{w}^\top \right\rangle \mathbf{\Phi}^\top,$$

giving

$$\mathbf{K} = \gamma' \mathbf{\Phi}\mathbf{\Phi}^\top.$$

We use $\langle \cdot \rangle$ to denote expectations under prior distributions.

Covariance between Two Points

- The prior covariance between two points $\mathbf{x}_i$ and $\mathbf{x}_j$ is

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \phi_:\left(\mathbf{x}_i\right)^\top \phi_:\left(\mathbf{x}_j\right),$$

Covariance between Two Points

- The prior covariance between two points $\mathbf{x}_i$ and $\mathbf{x}_j$ is

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \phi_:\left(\mathbf{x}_i\right)^\top \phi_:\left(\mathbf{x}_j\right),$$

or in sum notation

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \gamma' \sum_{\ell}^{m} \phi_\ell\left(\mathbf{x}_i\right) \phi_\ell\left(\mathbf{x}_j\right)$$

Covariance between Two Points

- The prior covariance between two points $\mathbf{x}_i$ and $\mathbf{x}_j$ is

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \phi_{:}\left(\mathbf{x}_i\right)^\top \phi_{:}\left(\mathbf{x}_j\right),$$

  or in sum notation

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \gamma' \sum_{\ell}^{m} \phi_{\ell}\left(\mathbf{x}_i\right) \phi_{\ell}\left(\mathbf{x}_j\right)$$

- For the radial basis used this gives

Covariance between Two Points

- The prior covariance between two points $\mathbf{x}_i$ and $\mathbf{x}_j$ is

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \phi_{:}\left(\mathbf{x}_i\right)^\top \phi_{:}\left(\mathbf{x}_j\right),$$

  or in sum notation

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \gamma' \sum_{\ell}^{m} \phi_\ell\left(\mathbf{x}_i\right) \phi_\ell\left(\mathbf{x}_j\right)$$

- For the radial basis used this gives

$$k\left(\mathbf{x}_i, \mathbf{x}_j\right) = \gamma' \sum_{k=1}^{m} \exp\left(-\frac{\left|\mathbf{x}_i - \boldsymbol{\mu}_k\right|^2 + \left|\mathbf{x}_j - \boldsymbol{\mu}_k\right|^2}{2\ell^2}\right).$$

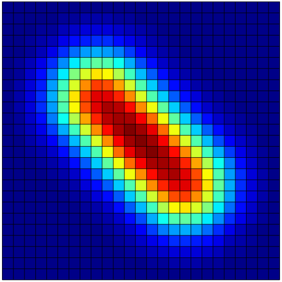
Covariance Functions

RBF Basis Functions

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

$$\phi_i(x) = \exp\left(-\frac{\left\|x - \mu_i\right\|_2^2}{\ell^2}\right)$$

$$\boldsymbol{\mu} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$



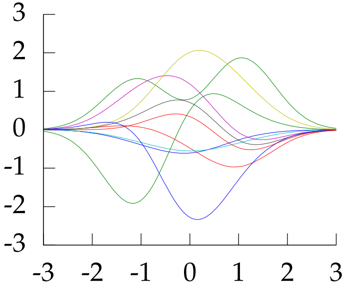
Covariance Functions

RBF Basis Functions

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

$$\phi_i(x) = \exp\left(-\frac{\left\|x - \mu_i\right\|_2^2}{\ell^2}\right)$$

$$\boldsymbol{\mu} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$



Selecting Number and Location of Basis

- Need to choose
  1. location of centers

Selecting Number and Location of Basis

- Need to choose
  1. location of centers
  2. number of basis functions

Selecting Number and Location of Basis

- Need to choose
  1. location of centers
  2. number of basis functions
- Consider uniform spacing over a region:

$$k\left(x_i, x_j\right) = \gamma\Delta\sum_{k=1}^{m}\exp\left(-\frac{x_i^2 + x_j^2 - 2\mu_k\left(x_i + x_j\right) + 2\mu_k^2}{2\ell^2}\right),$$

Restrict analysis to 1-D input, x.

Uniform Basis Functions

- Set each center location to

$$\mu_k = a + \Delta\mu \cdot (k - 1).$$

Uniform Basis Functions

- Set each center location to

$$\mu_k = a + \Delta\mu \cdot (k - 1).$$

- Specify the basis functions in terms of their indices,

$$k\left(x_i, x_j\right) = \gamma\Delta\mu \sum_{k=0}^{m-1} \exp\Bigg(- \frac{x_i^2 + x_j^2}{2\ell^2} - \frac{2\left(a + \Delta\mu \cdot k\right)\left(x_i + x_j\right) + 2\left(a + \Delta\mu \cdot k\right)^2}{2\ell^2}\Bigg).$$

Infinite Basis Functions

- Take $\mu_0 = a$ and $\mu_m = b$ so $b = a + \Delta\mu \cdot (m - 1)$.

Infinite Basis Functions

- Take $\mu_0 = a$ and $\mu_m = b$ so $b = a + \Delta\mu \cdot (m - 1)$.
- Take limit as $\Delta\mu \to 0$ so $m \to \infty$

Infinite Basis Functions

- Take $\mu_0 = a$ and $\mu_m = b$ so $b = a + \Delta\mu \cdot (m - 1)$.
- Take limit as $\Delta\mu \to 0$ so $m \to \infty$

$$
\begin{aligned}
k(x_i, x_j) =& \gamma \int_a^b \exp\Bigg(-\frac{x_i^2 + x_j^2}{2\ell^2} \\
&+ \frac{2\left(\mu - \frac{1}{2}\left(x_i + x_j\right)\right)^2 - \frac{1}{2}\left(x_i + x_j\right)^2}{2\ell^2} \Bigg) \mathrm{d}\mu,
\end{aligned}
$$

where we have used $k \cdot \Delta\mu \to \mu$.

Result

- Performing the integration leads to

$$
\begin{aligned}
k(x_i,x_j) &= \gamma \frac{\sqrt{\pi \ell^2}}{2} \exp\left(-\frac{\left(x_i - x_j\right)^2}{4\ell^2} \right) \\
&\quad \times \left[\operatorname{erf}\left(\frac{\left(b - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell} \right) - \operatorname{erf}\left(\frac{\left(a - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell} \right) \right],
\end{aligned}
$$

Result

- Performing the integration leads to

$$k(x_i,x_j) = \gamma \frac{\sqrt{\pi \ell^2}}{2} \exp\left(-\frac{\left(x_i - x_j\right)^2}{4\ell^2}\right)$$
$$\times \left[\operatorname{erf}\left(\frac{\left(b - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell}\right) - \operatorname{erf}\left(\frac{\left(a - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell}\right)\right],$$

- Now take limit as $a \to -\infty$ and $b \to \infty$

Result

- Performing the integration leads to

$$k(x_i,x_j) = \gamma \frac{\sqrt{\pi \ell^2}}{2} \exp\left(-\frac{\left(x_i - x_j\right)^2}{4\ell^2}\right)$$
$$\times \left[\operatorname{erf}\left(\frac{\left(b - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell}\right) - \operatorname{erf}\left(\frac{\left(a - \frac{1}{2}\left(x_i + x_j\right)\right)}{\ell}\right)\right],$$

- Now take limit as $a \to -\infty$ and $b \to \infty$

$$k\left(x_i, x_j\right) = \alpha \exp\left(-\frac{\left(x_i - x_j\right)^2}{4\ell^2}\right).$$

where $\alpha = \gamma \sqrt{\pi \ell^2}$.

Infinite Feature Space

- An RBF model with infinite basis functions is a Gaussian process.

Infinite Feature Space

- An RBF model with infinite basis functions is a Gaussian process.
- The covariance function is given by the exponentiated quadratic covariance function.

$$k\left(x_i, x_j\right) = \alpha \exp\left(-\frac{\left(x_i - x_j\right)^2}{4\ell^2}\right).$$

where $\alpha = \gamma\sqrt{\pi\ell^2}$.

Infinite Feature Space

- An RBF model with infinite basis functions is a Gaussian process.
- The covariance function is the exponentiated quadratic.
- **Note:** The functional form for the covariance function and basis functions are similar.
    - this is a special case,
    - in general they are very different

Similar results can obtained for multi-dimensional input models Williams (1998); Neal (1996).

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].

R. M. Neal. *Bayesian Learning for Neural Networks*. Springer, 1996. Lecture Notes in Statistics 118.

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] .

C. K. I. Williams. Computation with infinite neural networks. *Neural Computation*, 10(5):1203–1216, 1998.