Gaussian Processes

MLAI Lecture 23

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Sheffield University

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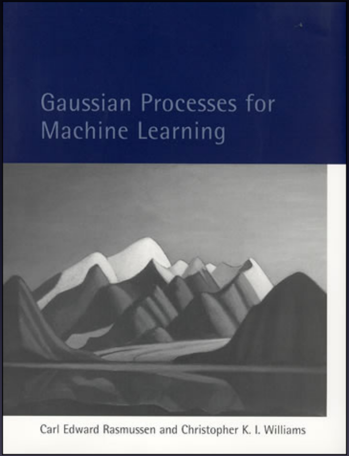
Book



Rasmussen and Williams (2006)

Outline

Distributions over Functions

Covariance from Basis Functions

Basis Function Representations

Constructing Covariance

GP Limitations

Conclusions

Outline

Distributions over Functions

Covariance from Basis Functions

Basis Function Representations

Constructing Covariance

GP Limitations

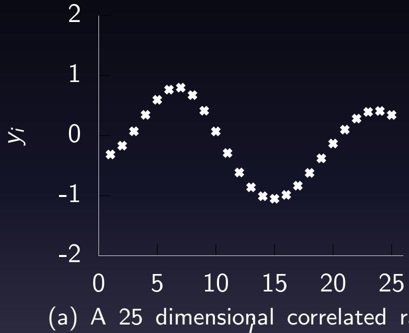
Conclusions

Sampling a Function

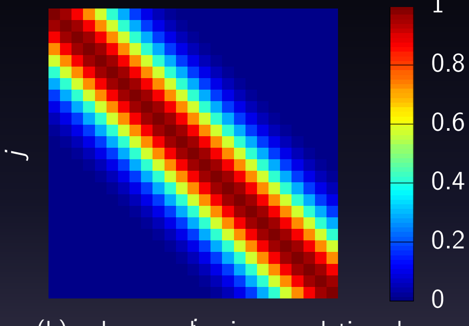
Multi-variate Gaussians

- We will consider a Gaussian with a particular structure of covariance matrix.
- Generate a single sample from this 25 dimensional Gaussian distribution, $\mathbf{y} = [y_1, y_2 \ldots y_{25}]$.
- We will plot these points against their index.

Gaussian Distribution Sample



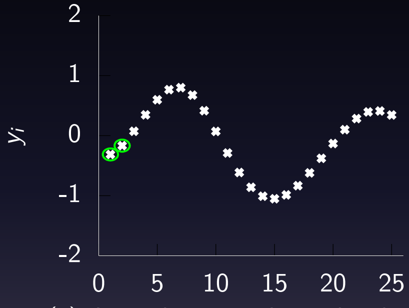
(a) A 25 dimensional correlated random variable (values ploted against index)



(b) colormap showing correlations between dimensions.

Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



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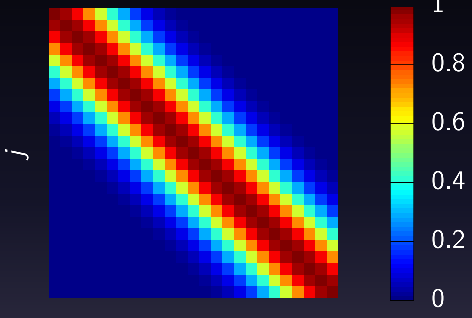

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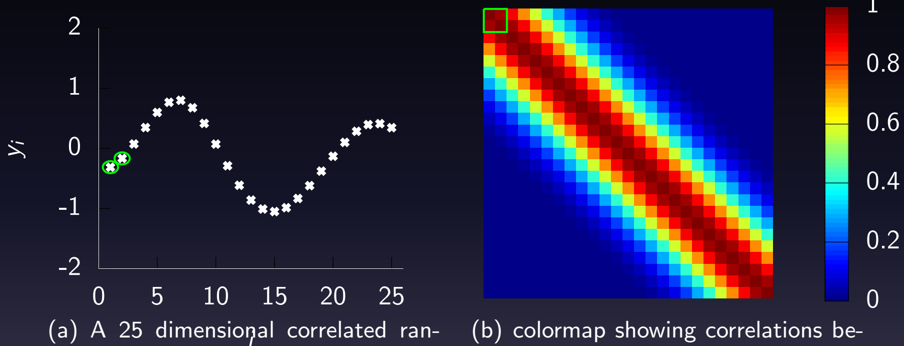

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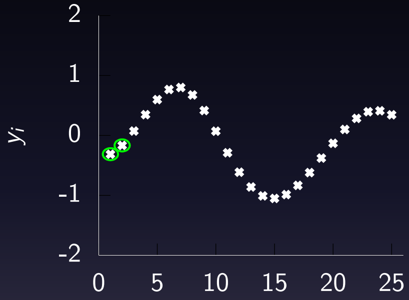

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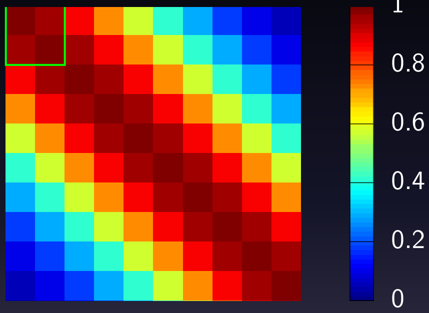

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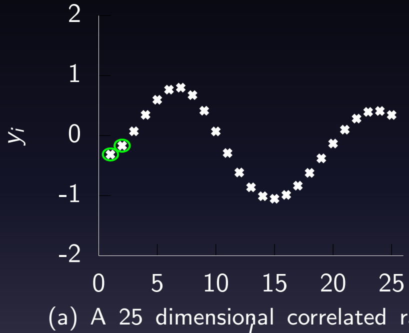

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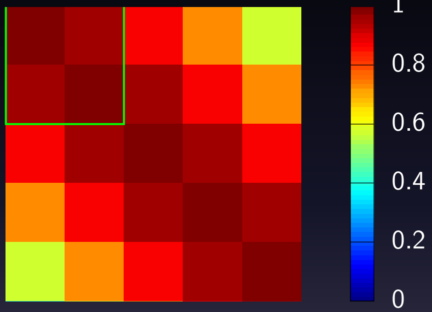

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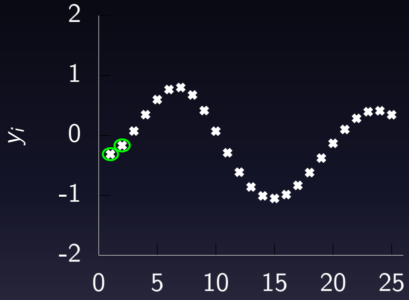
Gaussian Distribution Sample



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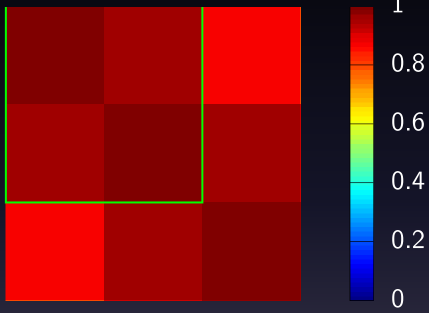

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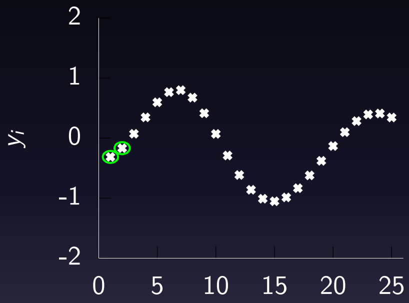
Gaussian Distribution Sample



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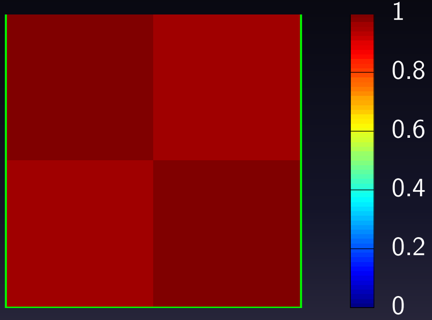

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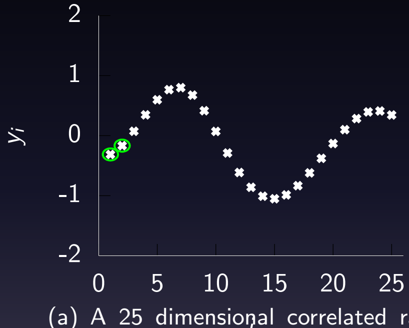
Figure: A sample from a 25 dimensional Gaussian distribution.

Gaussian Distribution Sample



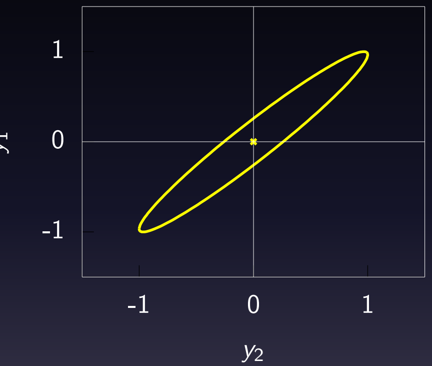
(a) A 25 dimensional correlated random variable (values ploted against index)

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

(b) correlation between y_1 and y_2.

Figure: A sample from a 25 dimensional Gaussian distribution.

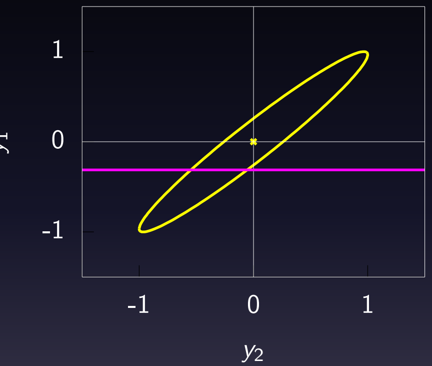
Prediction of y_2 from y_1



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

- The single contour of the Gaussian density represents the joint distribution, $p(y_1, y_2)$.
- We observe that $y_1 = -0.313$.
- Conditional density: $p(y_2|y_1 = -0.313)$.

Prediction of y_2 from y_1



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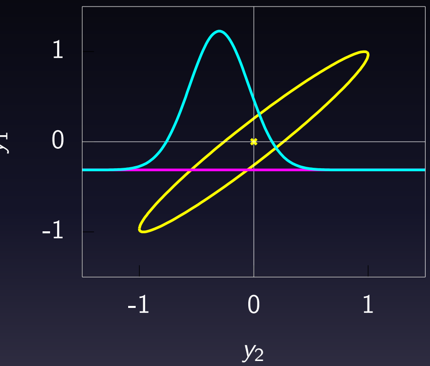

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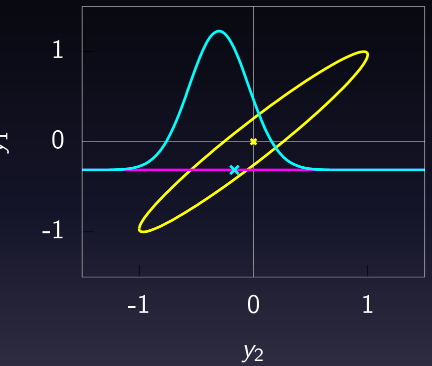

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Prediction with Correlated Gaussians

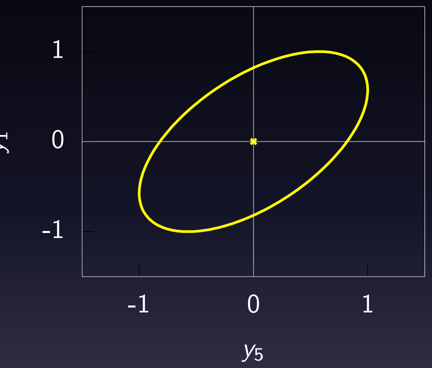
- Prediction of y_2 from y_1 requires *conditional density*.
- Conditional density is *also* Gaussian.

$$p(y_2|y_1) = \mathcal{N}\left(y_2|\frac{k_{1,2}}{k_{1,1}}y_1, k_{2,2} - \frac{k_{1,2}^2}{k_{1,1}}\right)$$

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 y_5 from y_1



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

- The single contour of the Gaussian density represents the joint distribution, $p(y_1, y_5)$.
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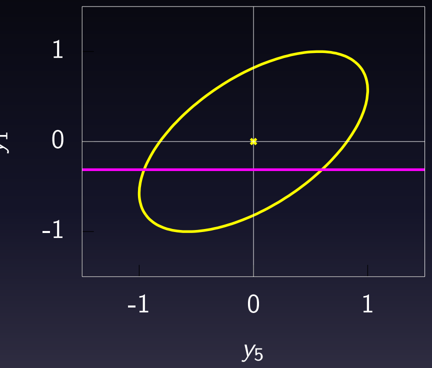
- Conditional density: $p(y_5|y_1 = -0.313)$.

Prediction of y_5 from y_1



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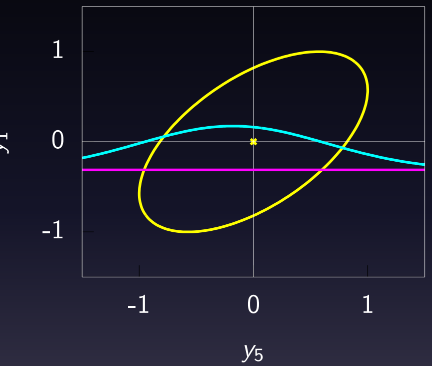
Prediction of y_5 from y_1



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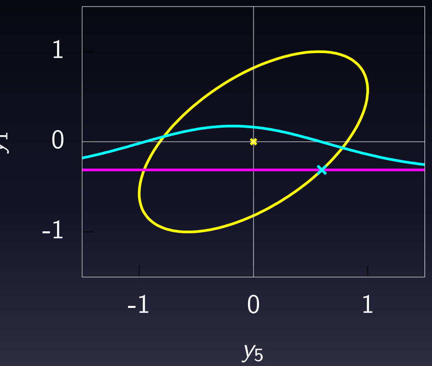
Prediction of y_5 from y_1



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Prediction with Correlated Gaussians

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

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

- Here covariance of joint density is given by

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

Prediction with Correlated Gaussians

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

$$p(\mathbf{y}_*|\mathbf{y}) = \mathcal{N}\left(\mathbf{y}_*|\boldsymbol{\mu}, \Sigma\right)$$

$$\boldsymbol{\mu} = \mathbf{K}_{*,\mathbf{y}}\mathbf{K}_{\mathbf{y},\mathbf{y}}^{-1}\mathbf{y}$$

$$\Sigma = \mathbf{K}_{*,*} - \mathbf{K}_{*,\mathbf{y}}\mathbf{K}_{\mathbf{y},\mathbf{y}}^{-1}\mathbf{K}_{\mathbf{y},*}$$

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

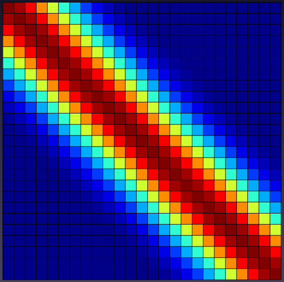
Covariance Functions

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.



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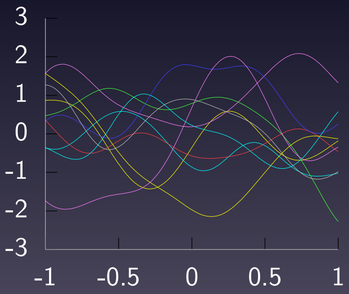

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

Covariance Functions

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

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

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

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

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

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

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Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20$, $x_2 = 1.20$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

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

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

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

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

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

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

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

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

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

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$x_3 = 1.40$, $x_2 = 1.20$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.40$, $x_3 = 1.40$

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

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

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

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Where did this covariance matrix come from?

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

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

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

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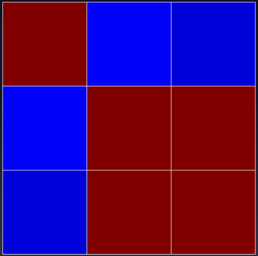
$$k\left(x_i, x_j\right) = \alpha \exp\left(-\frac{||x_i - x_j||^2}{2\ell^2}\right)$$

$x_3 = 1.40$, $x_3 = 1.40$

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



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

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, 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?

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

$x_2 = 1.2$, $x_2 = 1.2$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, 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?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.4$, $x_2 = 1.2$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_3 = 1.4,\ x_2 = 1.2$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, 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?

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

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

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

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

$x_1 = -3$, $x_2 = 1.2$, $x_3 = 1.4$, 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?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_2 = 1.2$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0$, $x_3 = 1.4$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_3 = 1.4$

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

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

$x_1 = -3,\ x_2 = 1.2,\ x_3 = 1.4$, 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?

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

$x_4 = 2.0,\ x_4 = 2.0$

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

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

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

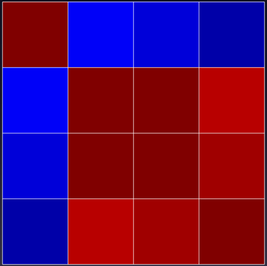
Covariance Functions

Where did this covariance matrix come from?

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

$x_4 = 2.0,\ x_4 = 2.0$

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



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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

$x_2 = 1.20,\ x_1 = -3.0$

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

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

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

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

$x_2 = 1.20,\ x_2 = 1.20$

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

Covariance Functions

Where did this covariance matrix come from?

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

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

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

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

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

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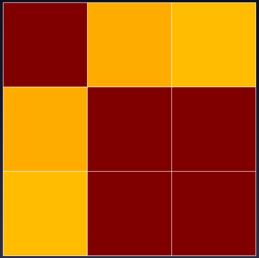

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Outline

Distributions over Functions

Covariance from Basis Functions

Basis Function Representations

Constructing Covariance

GP Limitations

Conclusions

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,

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

- 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:

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

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

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

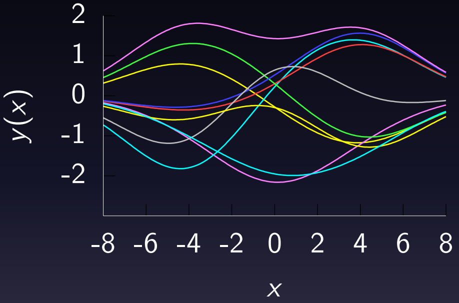

Figure: Functions sampled using the basis set from figure 2. Each line is a separate sample, generated by a weighted sum of the basis set. The weights, $\mathbf{w}$ are sampled from a Gaussian density with variance $\alpha = 1$.

Direct Construction of Covariance Matrix

- Use matrix notation to write function,

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

computed at training data gives a vector

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

- $\mathbf{w}$ and $\mathbf{y}$ are only related by a inner product.
- Φ is fixed and non-stochastic for a given training set.
- $\mathbf{y}$ is Gaussian distributed.
- it is straightforward to compute distribution for $\mathbf{y}$

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Expectations

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

$$\langle \mathbf{y} \rangle = \phi \langle \mathbf{w} \rangle .$$

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

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

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

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

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

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Covariance between Two Points

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

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

or in vector form

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

- For the radial basis used this gives

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

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Selecting Number and Location of Basis

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

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

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Uniform Basis Functions

- Set each center location to

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

- Specify the bases in terms of their indices,

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

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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 $m \to \infty$

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

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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 $b \to \infty$

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

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Infinite Feature Space

- A 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.
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  - this is a special case,
  - in general they are very different
- Similar results can obtained for multi-dimensional input networks Williams (1998); Neal (1996).

Infinite Feature Space

- A 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.
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  - in general they are very different
- Similar results can obtained for multi-dimensional input networks Williams (1998); Neal (1996).

Nonparametric Gaussian Processes

- This work takes us from parametric to non-parametric.
- The limit implies infinite dimensional $\mathbf{w}$.
- Gaussian processes are generally non-parametric: combine data with covariance function to get model.
- This representation *cannot* be summarized by a parameter vector of a fixed size.

The Parametric Bottleneck

- Parametric models have a representation that does not respond to increasing training set size.
- Bayesian posterior distributions over parameters contain the information about the training data.
  - Use Bayes' rule from training data, $p(\mathbf{w}|\mathbf{t}, \mathbf{X})$,
  - Make predictions on test data

$$p(t_*|\mathbf{X}_*, \mathbf{t}, \mathbf{X}) = \int p(t_*|\mathbf{w}, \mathbf{X}_*)\, p(\mathbf{w}|\mathbf{t}, \mathbf{X}) \mathrm{d}\mathbf{w}) \,.$$

- $\mathbf{w}$ becomes a bottleneck for information about the training set to pass to the test set.
- Solution: increase m so that the bottleneck is so large that it no longer presents a problem.
- How big is big enough for m? Non-parametrics says $m \to \infty$.

The Parametric Bottleneck

- Now no longer possible to manipulate the model through the standard parametric form given in (1).
- However, it *is* possible to express *parametric* as GPs:

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

- These are known as degenerate covariance matrices.
- Their rank is at most m, non-parametric models have full rank covariance matrices.
- Most well known is the "linear kernel", $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$.

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Making Predictions

- For non-parametrics prediction at new points $\mathbf{y}_*$ is made by conditioning on $\mathbf{y}$ in the joint distribution.
- In GPs this involves combining the training data with the covariance function and the mean function.
- Parametric is a special case when conditional prediction can be summarized in a *fixed* number of parameters.
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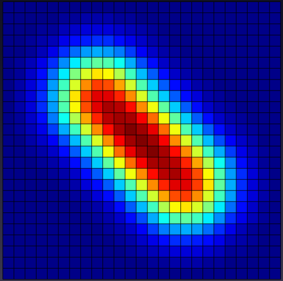
Covariance Functions

RBF Basis Functions

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

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

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



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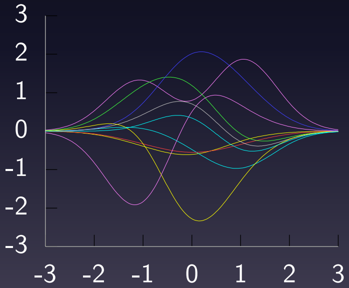

Covariance Functions and Mercer Kernels

- Mercer Kernels and Covariance Functions are similar.
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Outline

Distributions over Functions

Covariance from Basis Functions

Basis Function Representations

Constructing Covariance

GP Limitations

Conclusions

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 $y(\mathbf{x})$ is a Gaussian process.
- $g(\mathbf{x})$ is a deterministic function.
- $h(\mathbf{x}) = y(\mathbf{x})g(\mathbf{x})$
- 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 $y(\cdot)$.

Covariance Functions

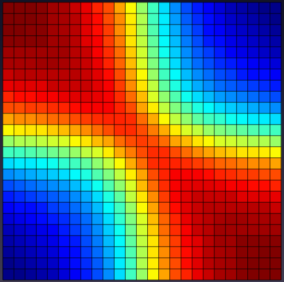
MLP Covariance Function

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

- Based on infinite neural network model.

$$w = 40$$

$$b = 4$$



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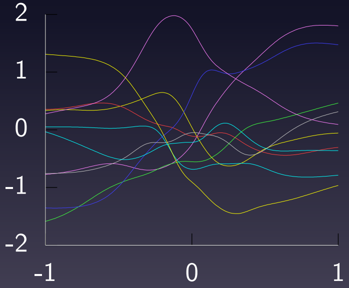


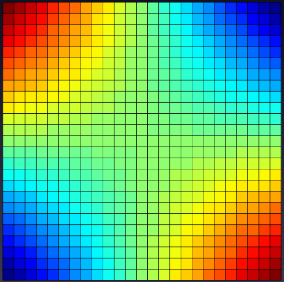
Covariance Functions

Linear Covariance Function

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

- Bayesian linear regression.

$$\alpha = 1$$



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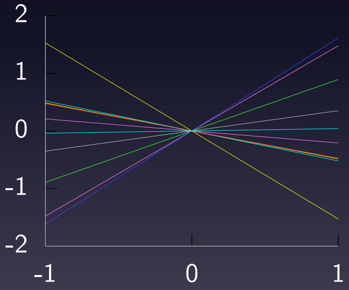

Gaussian Process Interpolation

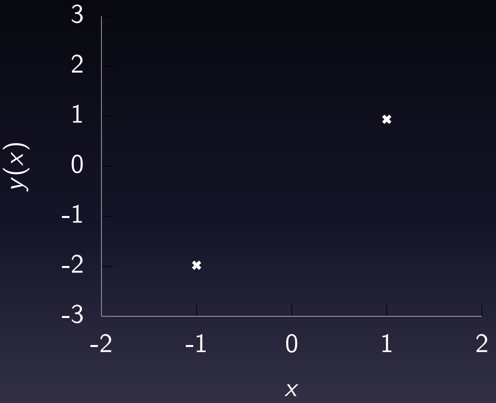

Figure: Real example: BACCO (see *e.g.* (Oakley and O'Hagan, 2002)). Interpolation through outputs from slow computer simulations (*e.g.* atmospheric carbon levels).

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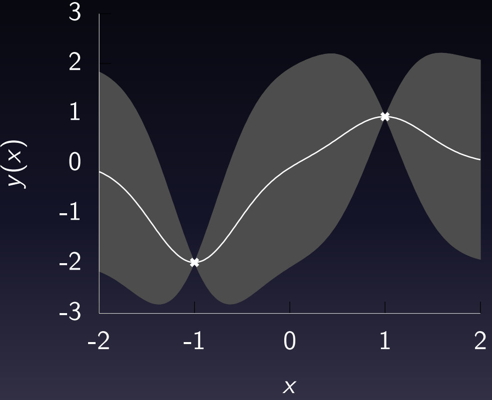

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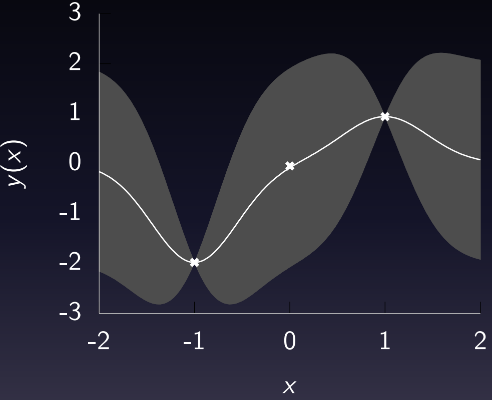

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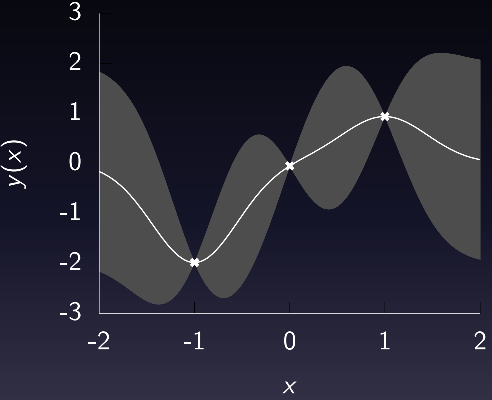

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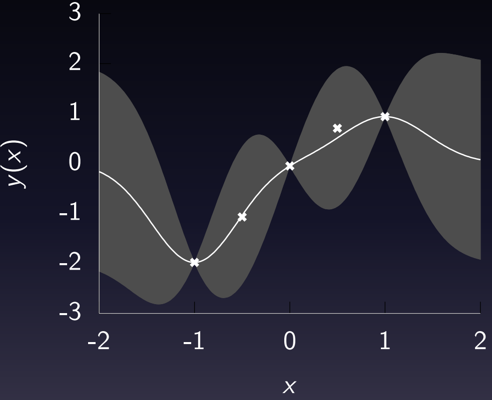

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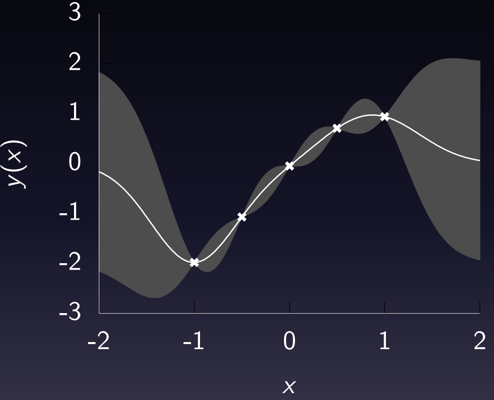

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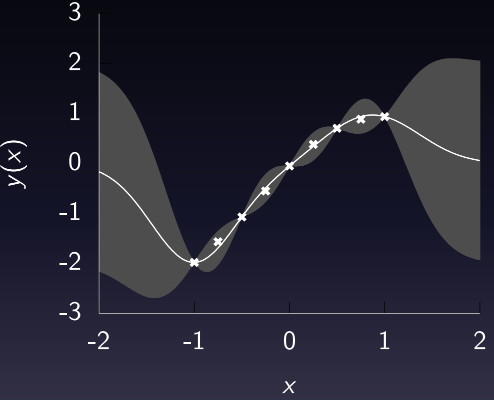

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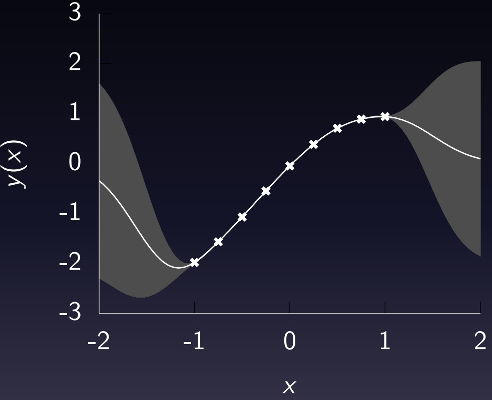

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Gaussian Noise

- Gaussian noise model,

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

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

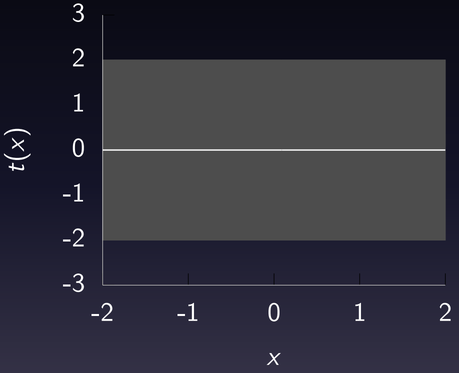

Figure: Examples include WiFi localization, C14 callibration curve.

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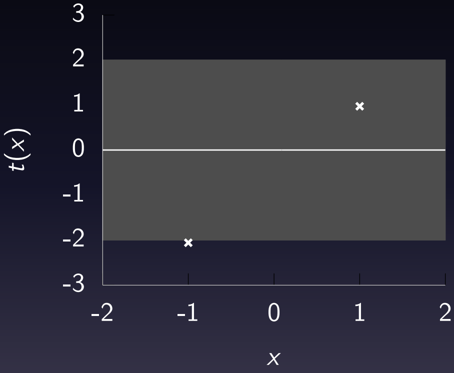

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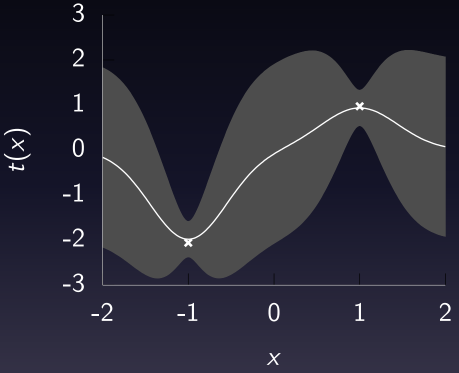

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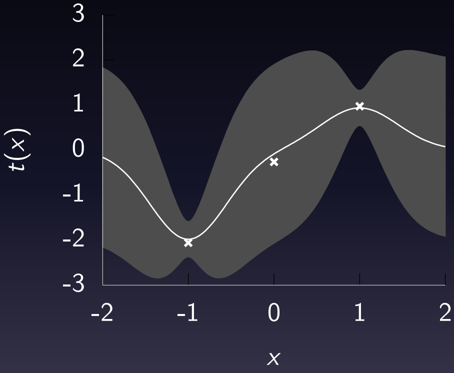

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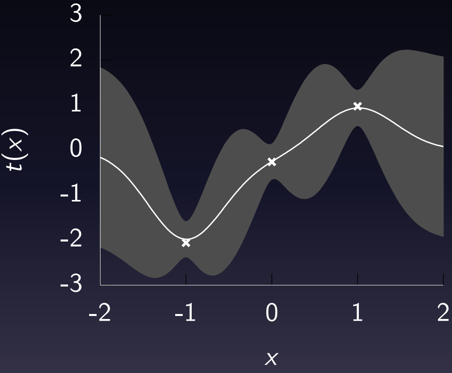

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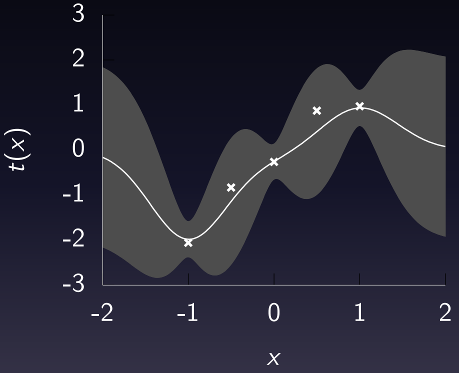

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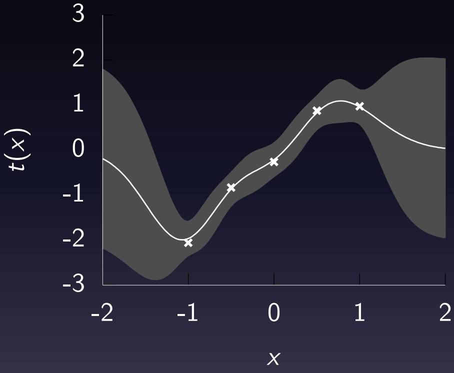

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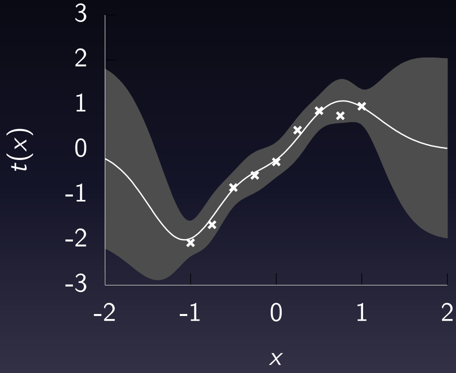

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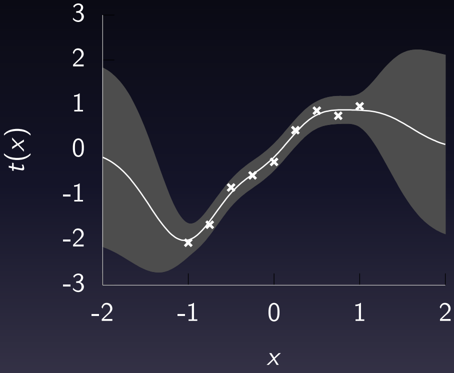

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Learning Covariance Parameters

Can we determine covariance parameters from the data?

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

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

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

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Learning Covariance Parameters

Can we determine covariance parameters from the data?

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

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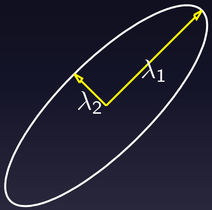
Eigendecomposition of Covariance

A useful decomposition for understanding the objective function.

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



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

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

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

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

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

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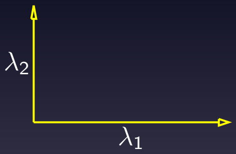

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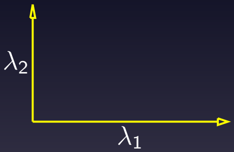

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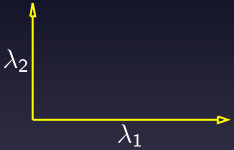

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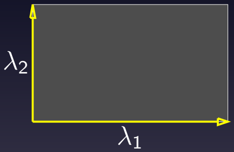

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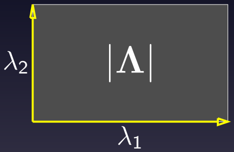

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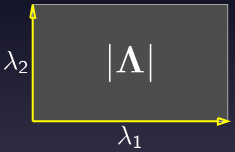

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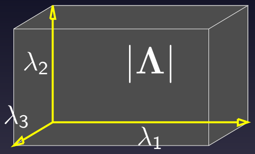

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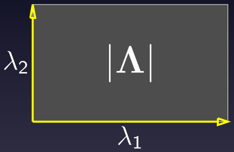

$$|\mathbf{\Lambda}| = \lambda_1 \lambda_2$$

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

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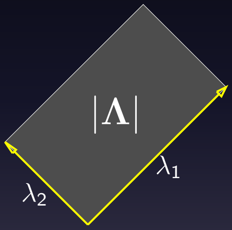

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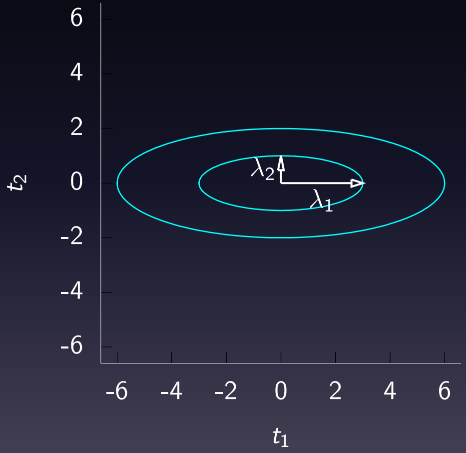
Data Fit: $\frac{\mathbf{t}^{-1}\mathbf{K}^{-1}\mathbf{t}}{2}$



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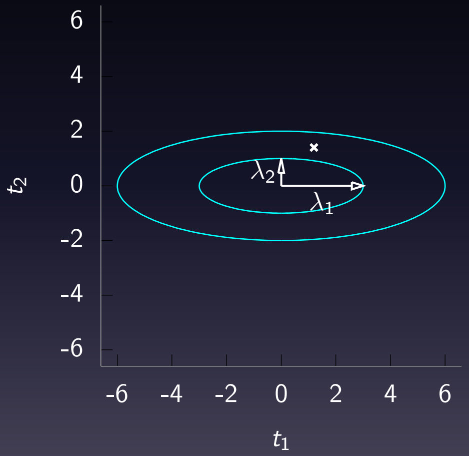

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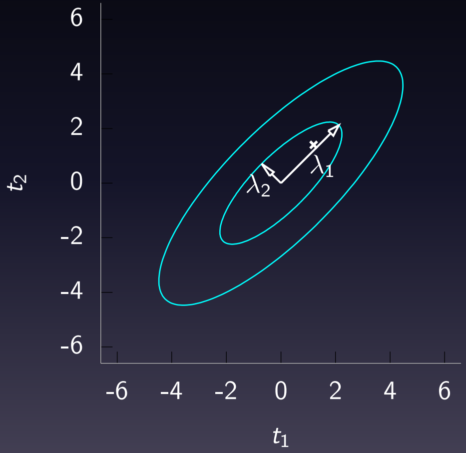
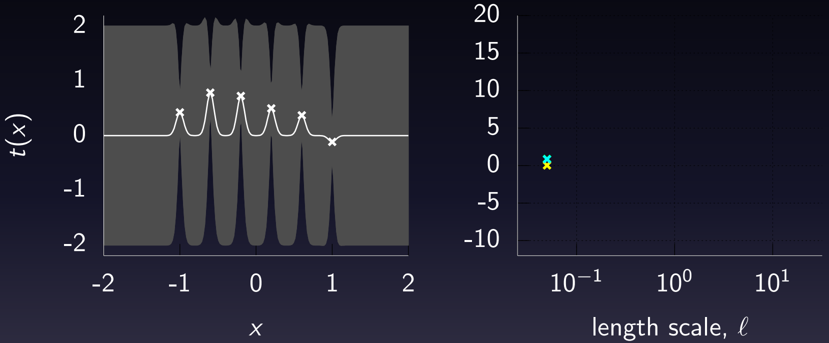


Learning Covariance Parameters

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



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

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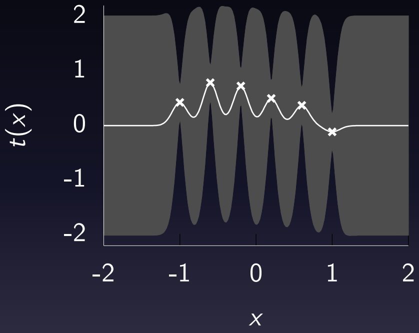

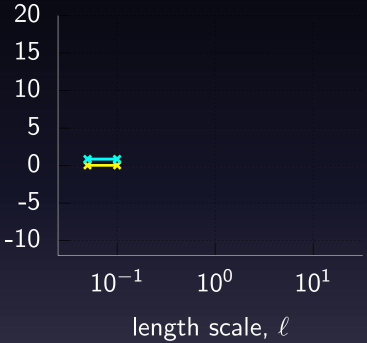

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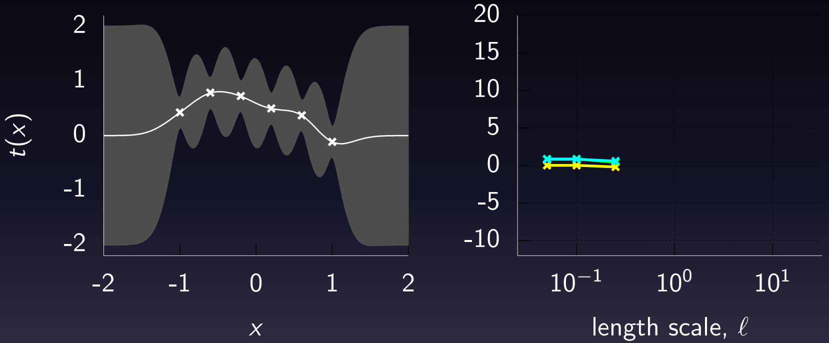

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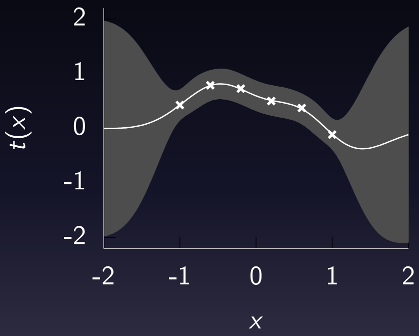

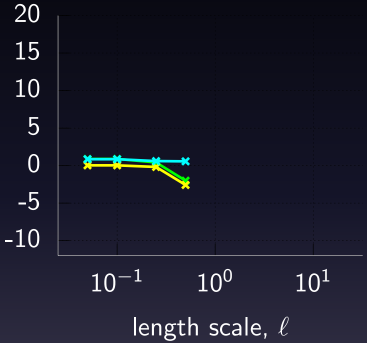

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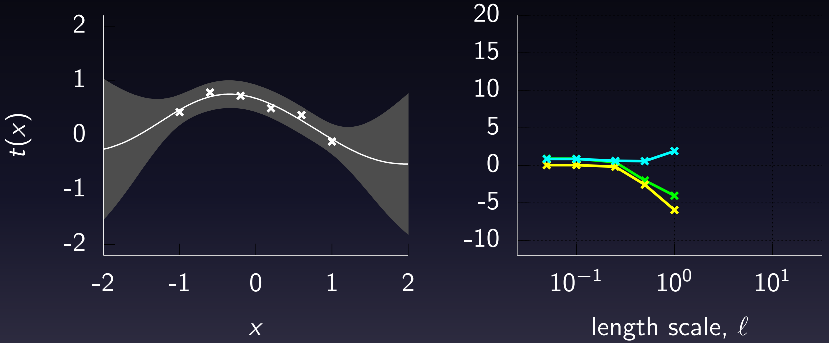

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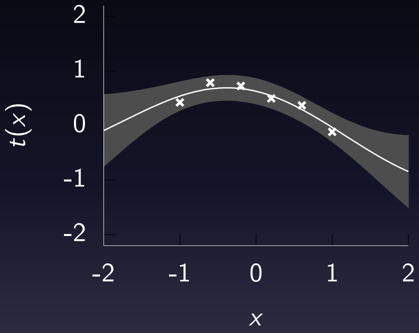

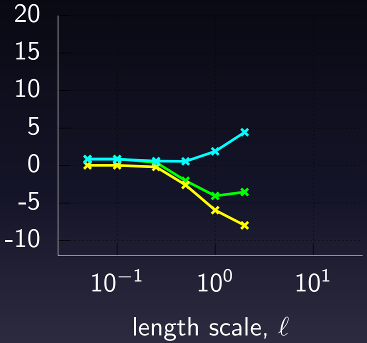

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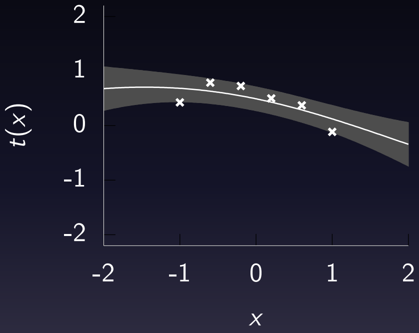

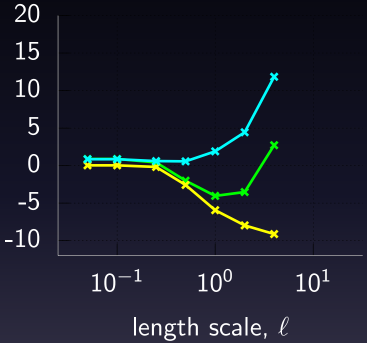

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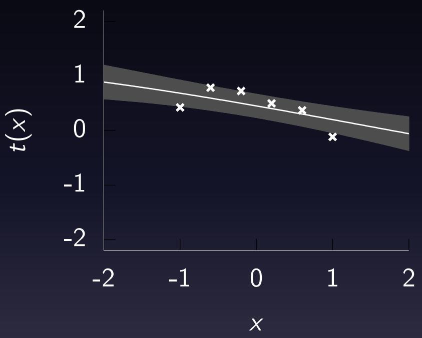

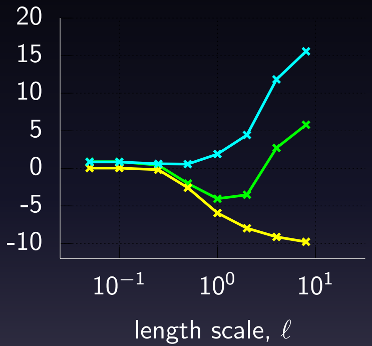

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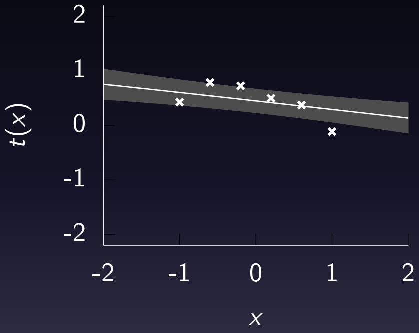

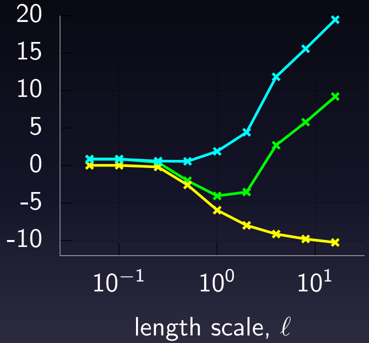

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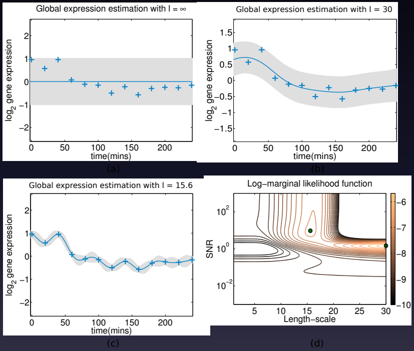
Gene Expression Example



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

Outline

Distributions over Functions

Covariance from Basis Functions

Basis Function Representations

Constructing Covariance

GP Limitations

Conclusions

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.

Reading

- Section 2.3 of Bishop up to top of pg 85 (multivariate Gaussians).
- Section 3.3 of Bishop up to 159 (pg 152–159).

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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].

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