

Access Code: **413868**

CMP9794M

Advanced Artificial Intelligence

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Last Week: Gaussian Bayes Nets (GBNs) via Linear Gaussians

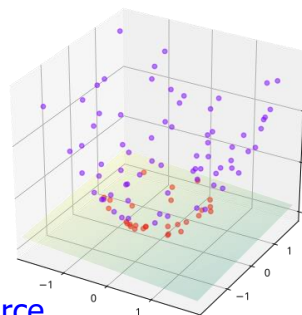
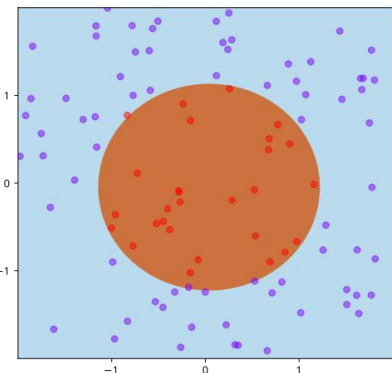
- Let Y be a continuous random variable with continuous parents X_1, \dots, X_k . A linear Gaussian can be defined as

$$P(Y|pa(Y)) = N(\underbrace{\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_k X_k}_{\text{Beta coefficients estimated via linear (such as Ridge, Lasso) or non-linear regression (e.g., KernelRidge)}}; \sigma^2)$$

Beta coefficients estimated via linear (such as Ridge, Lasso) or non-linear regression (e.g., KernelRidge).

Note: The latter (KernelRidge) can be considered as **non-linear in the original feature space** and **linear in the transformed feature space** (via the Kernel trick).

Original feature space



Transformed feature space

[Source](#)

Univariate Gaussian Distribution

A Gaussian (a.k.a. normal distribution) is a **PDF** defined as

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Mean
Standard deviation

$e = 2.71828 \dots$
 $\pi = 3.14159 \dots$

Equivalent to:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Variance

Also written as:

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

or

$$f(x) = \mathcal{N}(\mu, \sigma)$$

Univariate Gaussians

```
import numpy as np

mean = 4.86
stdev = 0.94
var = stdev**2

def get_gaussian_probability_density_v1(x, mean, stdev):
    e_val = -0.5*np.power((x-mean)/stdev, 2)
    return (1/(stdev*np.sqrt(2*np.pi))) * np.exp(e_val)

def get_gaussian_probability_density_v2(x, mean, var):
    e_val = -np.power((x-mean), 2)/(2*var)
    return (1/(np.sqrt(2*np.pi*var))) * np.exp(e_val)

for x in range(0, 10):
    fx_v1 = get_gaussian_probability_density_v1(x, mean, stdev)
    fx_v2 = get_gaussian_probability_density_v2(x, mean, var)
    print("x=%s f(x)_v1=%s f(x)_v2=%s" % (x, fx_v1, fx_v2))
```

```
x=0 f(x)_v1=6.655759025999826e-07 f(x)_v2=6.655759025999814e-07
x=1 f(x)_v1=9.250445860603243e-05 f(x)_v2=9.250445860603242e-05
x=2 f(x)_v1=0.004145930239828833 f(x)_v2=0.004145930239828836
x=3 f(x)_v1=0.059920518610605704 f(x)_v2=0.05992051861060571
x=4 f(x)_v1=0.27926942148327283 f(x)_v2=0.2792694214832728
x=5 f(x)_v1=0.41972559734224435 f(x)_v2=0.4197255973422443
x=6 f(x)_v1=0.20342380572419555 f(x)_v2=0.20342380572419552
x=7 f(x)_v1=0.0317930609592363 f(x)_v2=0.03179306095923628
x=8 f(x)_v1=0.0016023491678576664 f(x)_v2=0.0016023491678576677
x=9 f(x)_v1=2.6042113310168373e-05 f(x)_v2=2.6042113310168322e-05
```

Example GBN: Revisited

Univariate Gaussians

$$E \sim N(50, 10^2)$$

$$G \sim N(50, 10^2)$$

Environmental
Potential (E)

Genetic
Potential (G)

Vegetative
Organs (V)

Linear Gaussians

$$V \mid G, E \sim N(-10.35534 + 0.5G + 0.7711E, 5^2)$$

Number of
Seeds (N)

Seeds Mean
Weight (W)

$$N \mid V \sim N(45 + 0.1V, 9.949874^2)$$

$$W \mid V \sim N(15 + 0.7V, 7.141428^2)$$

Crop (C)

$$C \mid N, W \sim N(0.3N + 0.3W, 6.25^2)$$

Today

- Preliminaries
 - **Overview of linear algebra**
 - Multivariate Gaussian distributions
 - The kernel trick revisited
- Gaussian processes for regression (GPR)
- Gaussian processes for classification (GPC)

Notation of Linear Algebra

Symbol	Description
\mathbf{y}^T	The transpose of vector \mathbf{y}
\mathbf{y}^{-1}	The inverse of vector \mathbf{y}
$\mathbf{y}\mathbf{y}^{-1} = \mathbf{I}$	The identity matrix
\backslash	$\mathbf{a}\backslash\mathbf{b}$ is the vector \mathbf{x} solving $\mathbf{A}\mathbf{x} = \mathbf{b}$
$\mathbf{0}$ or $\mathbf{0}_n$	The vector of all zeros of length n
$ \mathbf{A} $	The determinant of matrix \mathbf{A}
$\text{diag}(\mathbf{y})$	Diagonal matrix containing the elements of \mathbf{y}
$\text{cholesky}(\mathbf{A})$	\mathbf{L} is a lower diagonal matrix such that $\mathbf{L}\mathbf{L}^T = \mathbf{A}$

Note: We will use libraries like [numpy](#) or [scipy](#) to carry out such operations.

Linear Algebra: Transpose

The transpose of vector $y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$ is $y^T = (y_1, y_2, y_3)$

Consider vector $A = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$

In A^T the rows become columns, giving us

$$A^T = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}^T = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

Linear Algebra: Identity Matrix

Consider vector $A = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$

The identify of A is $AA^{-1} = I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Linear Algebra: Determinant

Consider vector $A = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$

$$\det(A) = 4 \cdot \begin{vmatrix} 5 & -5 \\ -5 & 8 \end{vmatrix} - 2 \cdot \begin{vmatrix} 2 & -5 \\ -2 & 8 \end{vmatrix} + (-2) \cdot \begin{vmatrix} 2 & 5 \\ -2 & -5 \end{vmatrix}$$

$$\begin{vmatrix} 5 & -5 \\ -5 & 8 \end{vmatrix} = (5 \cdot 8) - (-5 \cdot -5) = 40 - 25 = 15$$

$$\begin{vmatrix} 2 & -5 \\ -2 & 8 \end{vmatrix} = (2 \cdot 8) - (-5 \cdot -2) = 16 - 10 = 6$$


$$\begin{vmatrix} 2 & 5 \\ -2 & -5 \end{vmatrix} = (2 \cdot -5) - (5 \cdot -2) = 10 - 10 = 0$$

The determinant of A is $|A| = 4 \cdot 15 - 2 \cdot 6 + (-2) \cdot 0 = 48$

Linear Algebra: Inverse

Consider vector $A = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$

$$A^{-1} = \frac{1}{\det(A)} \text{Adj}(A) = \frac{1}{48} \text{Adj}(A)$$

Adjugate 

$$\text{Adj}(A) = \text{Cofactor}(A)^T = \begin{pmatrix} 15 & -6 & 0 \\ -6 & 28 & 16 \\ 0 & 16 & 16 \end{pmatrix}^T = \begin{pmatrix} 15 & -6 & 0 \\ -6 & 28 & 16 \\ 0 & 16 & 16 \end{pmatrix}$$

The inverse of A is $A^{-1} = \begin{pmatrix} 0.3125 & -0.125 & 0 \\ -0.125 & 0.5833 & 0.3333 \\ 0 & 0.3333 & 0.3333 \end{pmatrix}$

Linear Algebra: $a \setminus b$ ($Ax = b$)

Consider vector $b = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

$$x = A^{-1}b = \begin{pmatrix} 0.3125 & -0.125 & 0 \\ -0.125 & 0.5833 & 0.3333 \\ 0 & 0.3333 & 0.3333 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.1875 \\ 0.7917 \\ 0.6667 \end{pmatrix}$$

Linear Algebra: Zero Vector

The zero vector of 3 elements is $O_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$

The zero matrix of 2×3 elements is $O_{2 \times 3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Linear Algebra: Diagonal Matrix

Consider vector $y = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$

The diagonal of y is $\text{diag}(y) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}$

Linear Algebra: Cholesky Decomposition

Consider vector $A = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$ such that $A = LL^T$

The Cholesky decomposition for A gives $L = \begin{pmatrix} 2 & 0 & 0 \\ 1 & 2 & 0 \\ -1 & -2 & \sqrt{3} \end{pmatrix}$

Thus,

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 1 & 2 & 0 \\ -1 & -2 & \sqrt{3} \end{pmatrix} \begin{pmatrix} 2 & 1 & -1 \\ 0 & 2 & -2 \\ 0 & 0 & \sqrt{3} \end{pmatrix} = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

Notation of Linear Algebra: Numpy

Symbol	Description	Numpy Function
\mathbf{y}^T	The transpose of vector \mathbf{y}	<code>y.T</code>
\mathbf{y}^{-1}	The inverse of vector \mathbf{y}	<code>np.linalg.inv(y)</code>
$\mathbf{y}\mathbf{y}^{-1} = \mathbf{I}$	The identity matrix	<code>np.identity(y)</code>
\backslash	$\mathbf{a}\backslash\mathbf{b}$ is the vector \mathbf{x} solving $\mathbf{A}\mathbf{x} = \mathbf{b}$	<code>np.linalg.solve(a, b)</code>
$\mathbf{0}$ or $\mathbf{0}_n$	The vector of all zeros of length n	<code>np.zeros()</code>
$ \mathbf{A} $	The determinant of matrix \mathbf{A}	<code>np.linalg.det(A)</code>
$\text{diag}(\mathbf{y})$	Dialogonal matrix of \mathbf{y}	<code>np.diag(y)</code>
$\text{cholesky}(\mathbf{A})$	For lower diagonal matrix \mathbf{L} , $\mathbf{L}\mathbf{L}^T = \mathbf{A}$	<code>np.linalg.cholesky(A)</code>

Assumption: the above numpy functions receive numpy arrays as inputs. 16

Today

- Preliminaries
 - Overview of linear algebra
 - **Multivariate Gaussian distributions**
 - The kernel trick revisited
- Gaussian processes for regression (GPR)
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Multivariate Gaussian Distribution

A multivariate Gaussian is a generalisation of the 1D Gaussian to multiple continuous random variables, defined as

$$\mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2}|\Sigma|^{1/2}} \exp \left[-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu) \right]$$

Notation:

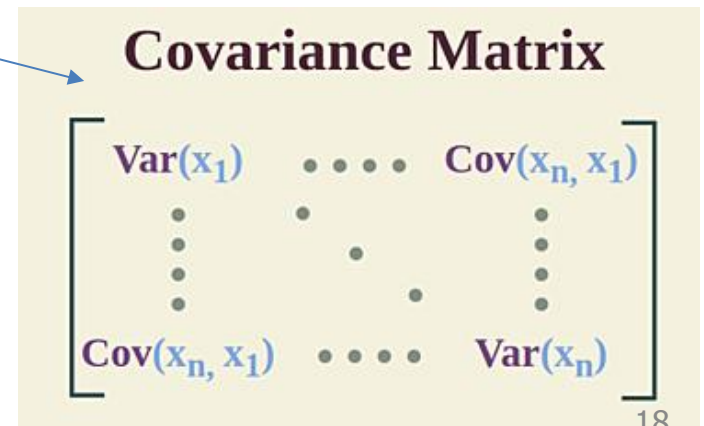
D = dimensionality (number of random variables)

μ = mean vector (D real numbers)

Σ = covariance matrix ($D \times D$),

where $\Sigma_{ij} = \text{cov}(x_i, x_j)$

Covariance=how to random variables differ
+ cov: variables head in same direction
- cov: variables head in opposite direction
0 cov: no relationship between variables



$$\mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]$$



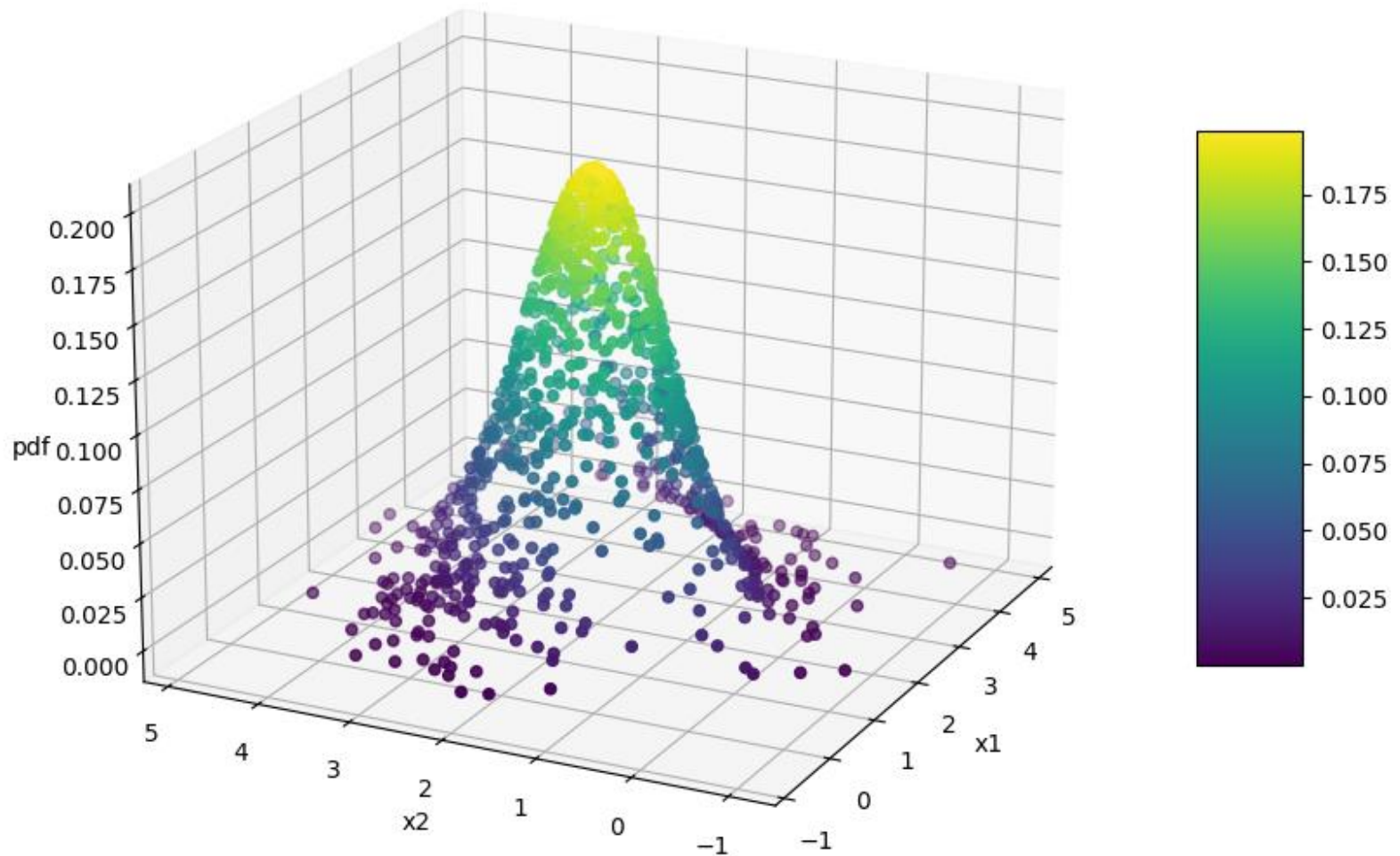
```
import numpy as np
import matplotlib.pyplot as plt

def sample_gaussian(mu, sigma):
    U1 = np.random.uniform(0, 1)
    U2 = np.random.uniform(0, 1)
    Z0 = np.sqrt(-2 * np.log(U1)) * np.cos(2 * np.pi * U2)
    return mu + sigma * Z0

def multivariate_gaussian_pdf(x, mean, covariance):
    D = len(mean)
    cov_det = np.linalg.det(covariance)
    cov_inv = np.linalg.inv(covariance)
    x_no_mean = np.array(x) - np.array(mean)
    exponent = -0.5 * np.dot(x_no_mean.T, np.dot(cov_inv, x_no_mean))
    normalisation_factor = 1 / ((2*np.pi) ** (D/2) * (cov_det ** (1/2)))
    pdf_value = normalisation_factor * np.exp(exponent)
    return pdf_value

mean = [2, 2]
covariance = [[1, 0.6], [0.6, 1]]
data = {'num_samples':1000, 'x1':[], 'x2':[], 'pdfs':[]}
for i in range(0, data['num_samples']):
    x1 = sample_gaussian(mean[0], np.sqrt(covariance[0][0]))
    x2 = sample_gaussian(mean[1], np.sqrt(covariance[1][1]))
    pdf_value = multivariate_gaussian_pdf([x1,x2], mean, covariance)
    print("i=%s x=%s sample=%s" % (i, [x1,x2], pdf_value))
    data['x1'].append(x1)
    data['x2'].append(x2)
    data['pdfs'].append(pdf_value)
```

Output of Previous Implementation



Multivariate Gaussian Distribution: Marginals and Conditionals

Consider a Gaussian with the following mean and covariance

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

Marginals:

$$P(x_1) = \mathcal{N}(x_1 | \mu_1, \Sigma_{11})$$

$$P(x_2) = \mathcal{N}(x_2 | \mu_2, \Sigma_{22})$$

Conditional:

$$P(x_1 | x_2) = \mathcal{N}(x_1 | \mu_{1|2}, \Sigma_{1|2})$$

$$\mu_{1|2} = \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2)$$

$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$$

For further information on marginals and conditionals of multivariate Gaussians, see Bishop. C. Pattern Recognition and Machine Learning. 2006 – sections 2.3.1 and 2.3.2.

Multivariate Gaussian Distribution: Example of Marginals and Conditionals

Consider $x_1 = 2.8$, $x_2 = 3.5$, and mean and covariance

$$\mu = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix}$$

Marginals:

$$P(x_1) = \mathcal{N}(x_1 | \mu_1, \Sigma_{11}) = \mathcal{N}(2.8; 2, 4) = 0.18413$$

$$P(x_2) = \mathcal{N}(x_2 | \mu_2, \Sigma_{22}) = \mathcal{N}(3.5; 3, 5) = 0.17400$$

Conditional:

$$P(x_1 | x_2) = \mathcal{N}(x_1 | \mu_{1|2}, \Sigma_{1|2}) = \mathcal{N}(2.8; 2.2, 3.2) = 0.21081$$

$$\mu_{1|2} = \mu_1 + \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2) = 2 + 2 \times \frac{1}{5} \times (3.5 - 3) = 2.2$$

$$\Sigma_{1|2} = \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} = 4 - 2 \times \frac{1}{5} \times 2 = 3.2$$

Multivariate Gaussian Distribution: Marginals and Conditionals

Consider a Gaussian with the following mean and covariance

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

Marginals:

$$P(x_1) = \mathcal{N}(x_1 | \mu_1, \Sigma_{11})$$

$$P(x_2) = \mathcal{N}(x_2 | \mu_2, \Sigma_{22})$$

Conditional:

$$P(x_2 | x_1) = \mathcal{N}(x_2 | \mu_{2|1}, \Sigma_{2|1})$$

$$\mu_{2|1} = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (x_1 - \mu_1)$$

$$\Sigma_{2|1} = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$$

Note: Vectors and matrices can use bold or non-bold fonts in the literature.

Multivariate Gaussian Distribution: Example of Marginals and Conditionals

Consider $x_1 = 2.8$, $x_2 = 3.5$, and mean and covariance

$$\mu = \begin{pmatrix} 2 \\ 3 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix}$$

Marginals:

$$P(x_1) = \mathcal{N}(x_1 | \mu_1, \Sigma_{11}) = \mathcal{N}(2.8; 2, 4) = 0.18413$$

$$P(x_2) = \mathcal{N}(x_2 | \mu_2, \Sigma_{22}) = \mathcal{N}(3.5; 3, 5) = 0.17400$$

Conditional:

$$P(x_2 | x_1) = \mathcal{N}(x_2 | \mu_{2|1}, \Sigma_{2|1}) = \mathcal{N}(3.5; 3.4, 4.0) = 0.19922$$

$$\mu_{2|1} = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1} (x_1 - \mu_1) = 3 + 2 \times \frac{1}{4} \times (2.8 - 2) = 3.4$$

$$\Sigma_{2|1} = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} = 5 - 2 \times \frac{1}{4} \times 2 = 4.0$$

Multivariate Gaussians: Conditionals

Consider a Gaussian with the following mean and covariance

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

Partitioning μ and Σ , by separating x_3 , we get

$$\mu = \begin{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \\ \mu_3 \end{pmatrix} = \begin{pmatrix} \mu_{1,2} \\ \mu_3 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{1,2} & \Sigma_{1,2,3} \\ \Sigma_{3,1,2} & \Sigma_{33} \end{pmatrix}$$

Conditional:

$$P(x_3 | x_1, x_2) = \mathcal{N}(x_3 | \mu_{3|1,2}, \Sigma_{3|1,2})$$

$$\mu_{3|1,2} = \mu_3 + \Sigma_{3,1,2} \Sigma_{1,2}^{-1} (x_{1,2} - \mu_{1,2})$$

$$\Sigma_{3|1,2} = \Sigma_{33} - \Sigma_{3,1,2} \Sigma_{1,2}^{-1} \Sigma_{1,2,3}$$

Multivariate Gaussian Distributions: Another Example of Conditionals

Consider the following:

$$x = \begin{pmatrix} x_1 = 1 \\ x_2 = 2 \\ x_3 = 3 \end{pmatrix} \quad \mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

Partitioning μ and Σ , by separating x_3 , we get

$$\mu = \begin{pmatrix} \begin{pmatrix} 1 \\ -3 \end{pmatrix} \\ 4 \end{pmatrix} = \begin{pmatrix} \mu_{1,2} \\ \mu_3 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{1,2} & \Sigma_{1,2,3} \\ \Sigma_{3,1,2} & \Sigma_{33} \end{pmatrix}$$

Conditional:

$$P(x_3 | x_1, x_2) = \mathcal{N}(x_3 | \mu_{3|1,2}, \Sigma_{3|1,2}) = ?$$

$$\mu_{3|1,2} = \mu_3 + \Sigma_{3,1,2} \Sigma_{1,2}^{-1} (x_{1,2} - \mu_{1,2}) = ?$$

$$\Sigma_{3|1,2} = \Sigma_{33} - \Sigma_{3,1,2} \Sigma_{1,2}^{-1} \Sigma_{1,2,3} = ?$$

Multivariate Gaussians: Conditionals

Consider a Gaussian with the following mean and covariance

$$\mu = \begin{pmatrix} \mu_1 \\ \dots \\ \mu_5 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \dots & \Sigma_{15} \\ \Sigma_{21} & \Sigma_{22} & \dots & \Sigma_{25} \\ \dots & \dots & \dots & \dots \\ \Sigma_{51} & \Sigma_{52} & \dots & \Sigma_{55} \end{pmatrix}$$

Partitioning μ and Σ , by separating x_4 and x_5 , we get

$$\mu = \begin{pmatrix} \mu_{1:3} \\ \mu_{4:5} \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{1:3,1:3} & \Sigma_{1:3,4:5} \\ \Sigma_{4:5,1:3} & \Sigma_{4:5,4:5} \end{pmatrix}$$

Conditional:

$$P(x_4, x_5 | x_1, x_2, x_3) = \mathcal{N}(x_4, x_5 | \mu_{4:5|1:3}, \Sigma_{4:5|1:3})$$

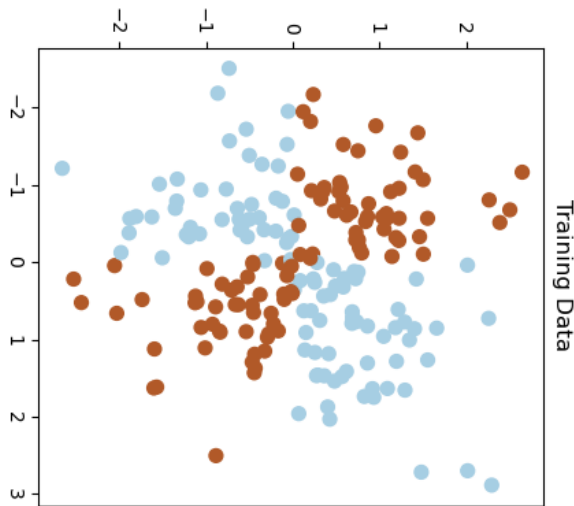
$$\mu_{4:5|1:3} = \mu_{4:5} + \Sigma_{4:5,1:3} \Sigma_{1:3,1:3}^{-1} (x_{1:3} - \mu_{1:3})$$

$$\Sigma_{4:5|1:3} = \Sigma_{4:5,4:5} - \Sigma_{4:5,1:3} \Sigma_{1:3,1:3}^{-1} \Sigma_{1:3,4:5}$$

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 - **The kernel trick revisited**
- Gaussian processes for regression (GPR)
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Revisiting the Kernel Trick



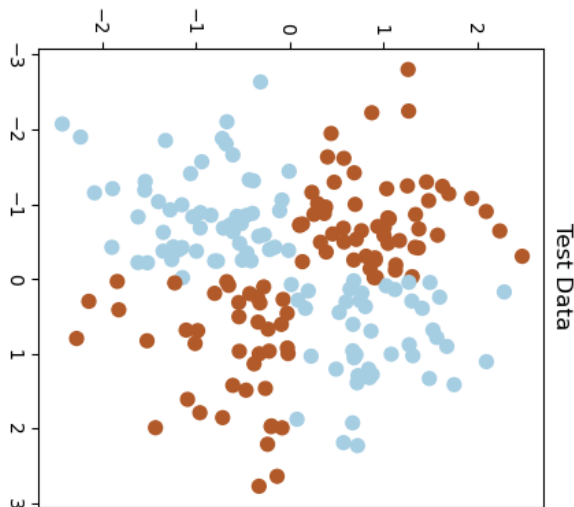
Kernel Function
(RBF, and others)
 $K(X_{train}, X_{train})$



Transformed
Feature Space:
kernel matrix

$$\text{RBF Kernel: } K(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2)$$

Adjusts the similarity
between datapoints



Kernel Function
(RBF, and others)
 $K(x_{test}, X_{train})$



Transformed
Feature Space:
kernel vector per
datapoint

The Kernel Trick: Example

Implementation on Toy Data

```
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

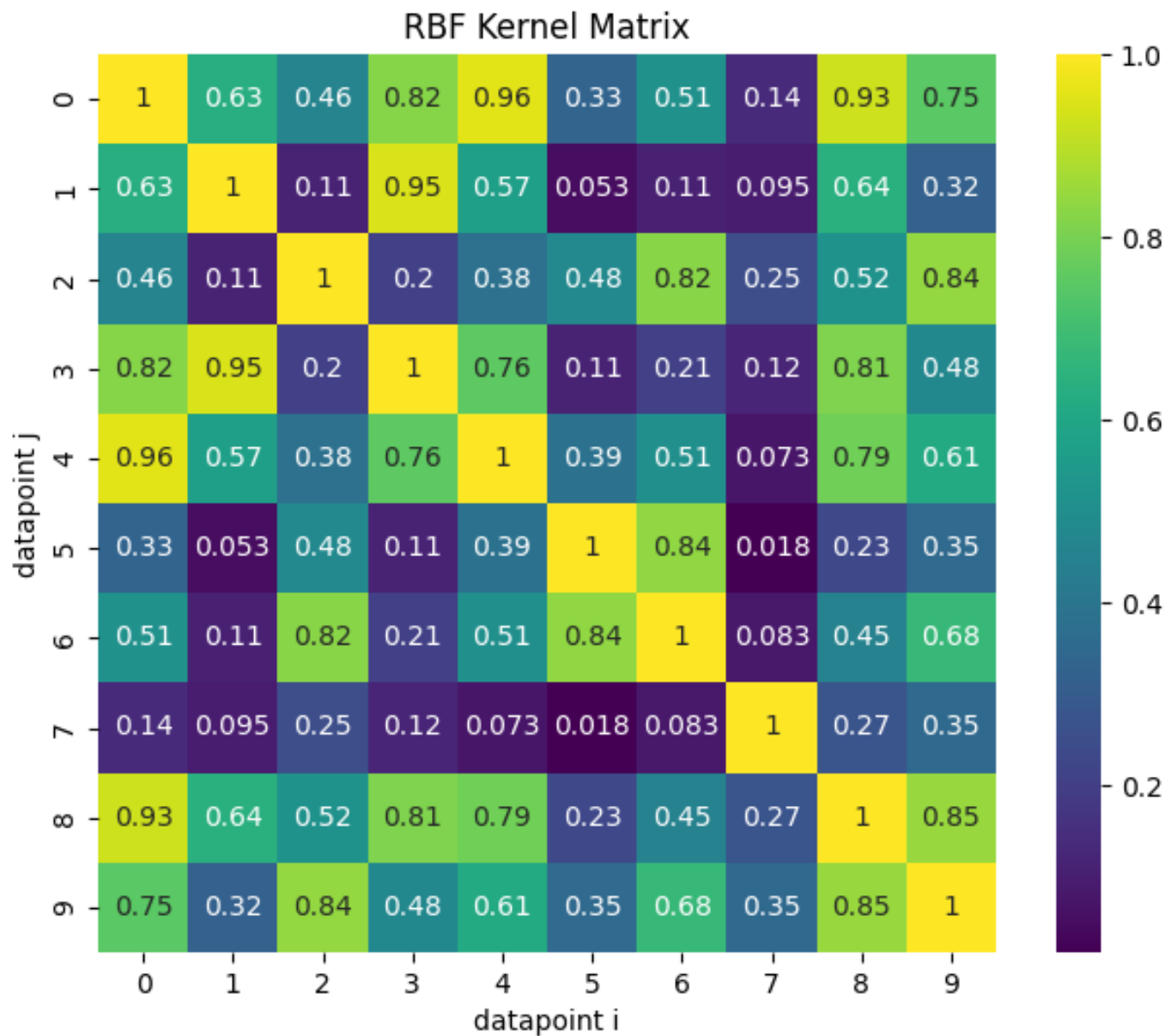
data = np.array([
    [0.630812147, 0.111274637], [1.481231638, 0.550879774],
    [0.085389312, -1.004405455], [1.185220936, 0.397592252],
    [0.44031619, 0.339426538], [-0.824500559, -0.207795318],
    [-0.326158756, -0.538912165], [1.629093681, -1.615757864],
    [0.88984675, -0.1831107], [0.551957891, -0.642928154]
])
gamma = 0.8

def rbf_kernel(X, gamma):
    n = X.shape[0]
    kernel_matrix = np.zeros((n, n))
    for i in range(n):
        for j in range(n):
            distance_squared = np.sum((X[i] - X[j]) ** 2)
            kernel_matrix[i, j] = np.exp(-gamma * distance_squared)
    return kernel_matrix

rbf_kernel_matrix = rbf_kernel(data, gamma)
print("RBF Kernel Matrix:", rbf_kernel_matrix)

plt.figure(figsize=(8, 6))
sns.heatmap(rbf_kernel_matrix, annot=True, cmap='viridis', square=True, cbar=True)
plt.title("RBF Kernel Matrix")
plt.xlabel("datapoint i")
plt.ylabel("datapoint j")
plt.show()
```

The Kernel Trick: Output of Implementation on Toy Data



The Kernel Trick: Example

Implementation on Test Data

```
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

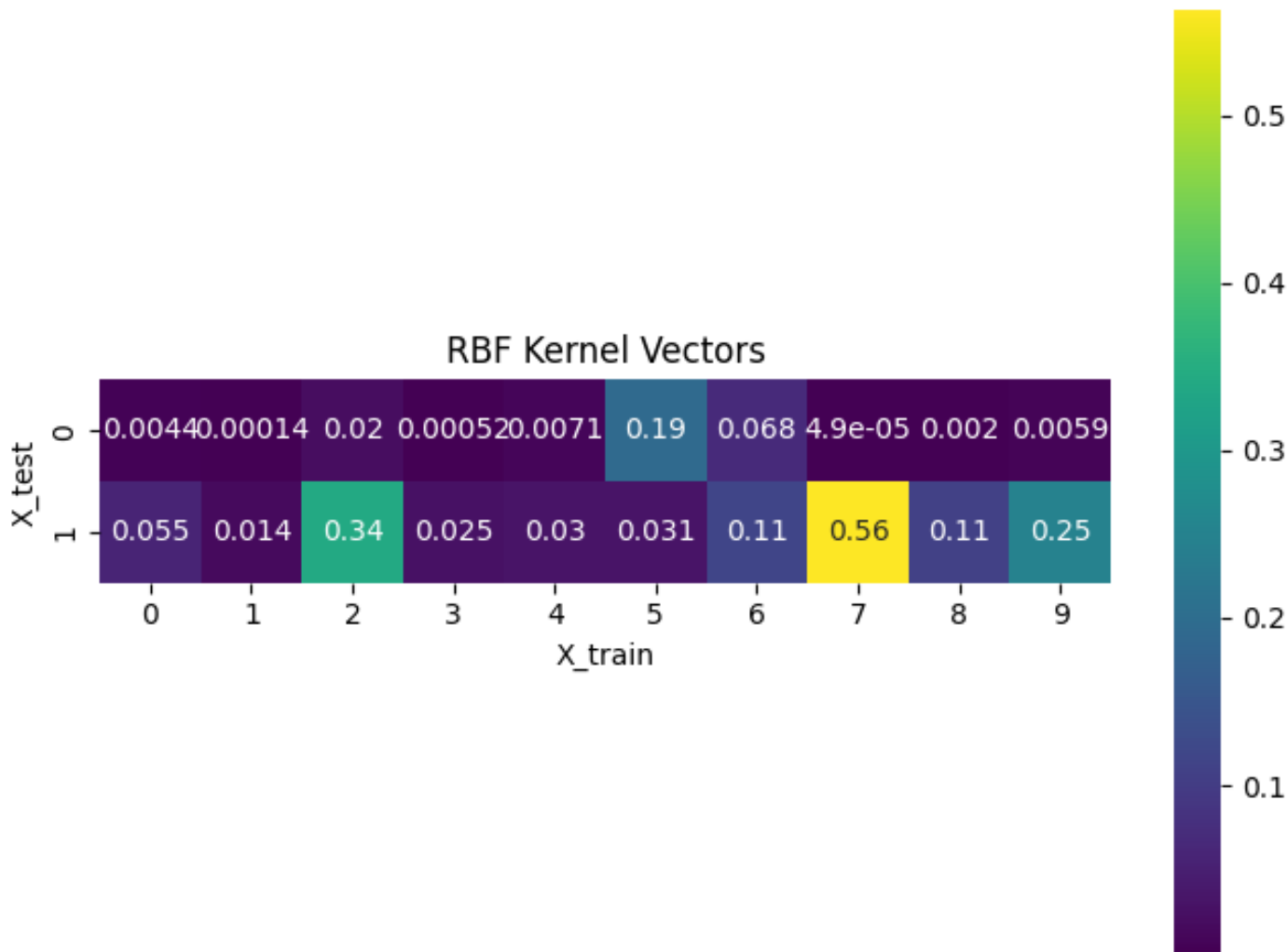
X_train = np.array([
    [0.630812147, 0.111274637], [1.481231638, 0.550879774],
    [0.085389312, -1.004405455], [1.185220936, 0.397592252],
    [0.44031619, 0.339426538], [-0.824500559, -0.207795318],
    [-0.326158756, -0.538912165], [1.629093681, -1.615757864],
    [0.88984675, -0.1831107], [0.551957891, -0.642928154]
])
X_test = np.array([[ -2.63426953, -0.327913873], [0.796193449, -2.289942402]])
gamma = 0.5

def rbf_kernel_vector(x_test, X_train, gamma):
    kernel_vector = np.array([
        np.exp(-gamma * np.sum((x_test - x_train) ** 2))
        for x_train in X_train
    ])
    return kernel_vector

kernel_vectors = []
for x_test in X_test:
    kernel_vector = rbf_kernel_vector(x_test, X_train, gamma)
    print(f"RBF kernel vector for {x_test}:", kernel_vector)
    kernel_vectors.append(kernel_vector)

plt.figure(figsize=(8, 6))
sns.heatmap(kernel_vectors, annot=True, cmap='viridis', square=True, cbar=True)
plt.title("RBF Kernel Vectors")
plt.xlabel("X_train")
plt.ylabel("X_test")
plt.show()
```

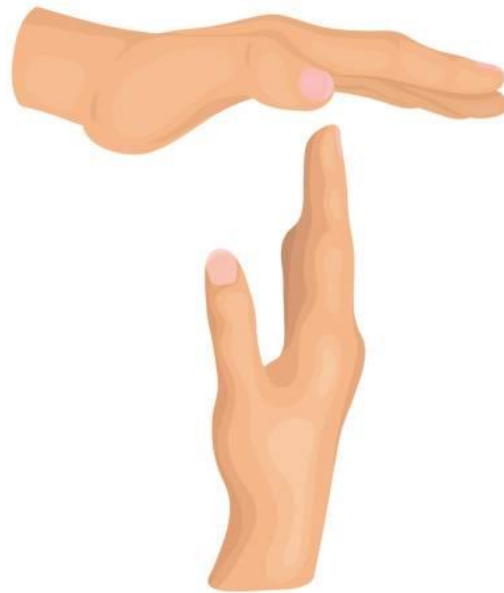

The Kernel Trick: Output of Implementation on Test Data



Linear Regression with Kernelised Data

- A kernel function is needed (such as RBF)
- Training consists of computing the kernel matrix $K(X_{train}, X_{train})$ and applying a loss function to learn coefficients (weights) β as discussed last week.
- Testing consists of computing the kernel vector $K(x_{test}, X_{train})$ and calculating an output value according to $\hat{y} = K(x_{test}, X_{train})^T \beta$

Break



Today

- Preliminaries
 - Overview of linear algebra
 - Multivariate Gaussian distributions
 - The kernel trick revisited
- **Gaussian processes for regression (GPR)**
- Gaussian processes for classification (GPC)

Gaussian Processes for Regression

Consider dataset $\{(\mathbf{x}_i, y_i) | i = 1, \dots, n\}$, where $\mathbf{x}_i \in \mathbb{R}^d$ denotes data point i and $y_i \in \mathbb{R}$ denotes its corresponding target value.

A Gaussian Process (GP) is a collection of random variables, any finite number of which have a joint Gaussian $p(f(\mathbf{x}_1), \dots, f(\mathbf{x}_n))$

$$p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \mathbf{K}) \quad \text{or} \quad \mathbf{f} = \mathcal{GP}(\boldsymbol{\mu}, \mathbf{K})$$

with

- mean vector $\boldsymbol{\mu} = (\mu(\mathbf{x}_1), \dots, \mu(\mathbf{x}_n))$
- covariance matrix (derived from a kernel function) $\mathbf{K}_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$
- function values \mathbf{f} (define the underlying function being modelled)
- data inputs \mathbf{X}
- \mathbf{y} can be seen as $\mathbf{y} = \mathbf{f} + \epsilon$, where ϵ is Gaussian noise.

Gaussian Processes for Regression

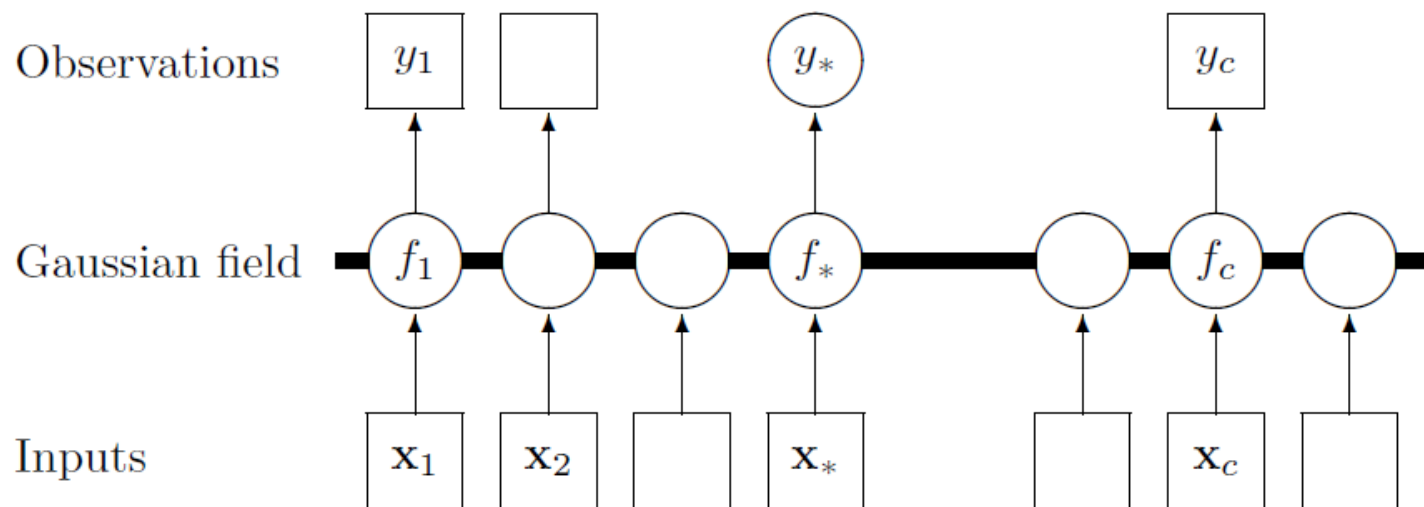


Figure 2.3: Graphical model (chain graph) for a GP for regression. Squares represent observed variables and circles represent unknowns. The thick horizontal bar represents a set of fully connected nodes. Note that an observation y_i is conditionally independent of all other nodes given the corresponding latent variable, f_i . Because of the marginalization property of GPs addition of further inputs, \mathbf{x} , latent variables, f , and *unobserved* targets, y_* , does not change the distribution of any other variables.

Gaussian Processes for Regression

GP prior $p(\mathbf{f}|\mathbf{X})$ can be converted into GP posterior $p(\mathbf{f}_*|\mathbf{X}_*, \mathbf{X}, \mathbf{f})$, where \mathbf{f}_* are the latent predictions of test data \mathbf{X}_* .

The joint distribution of observed values \mathbf{f} and predictions \mathbf{f}_* is a Gaussian represented as

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right)$$

with N training data points and M test data points

$\mathbf{0}$ mean vector (e.g., by removing the means from the data)

$\mathbf{K} = \kappa(\mathbf{X}, \mathbf{X})$ is an $N \times N$ matrix

$\mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*)$ is an $N \times M$ matrix

$\mathbf{K}_*^T = \kappa(\mathbf{X}_*, \mathbf{X})$ is an $M \times N$ matrix

$\mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*)$ is an $M \times M$ matrix

Gaussian Processes for Regression

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{pmatrix}, \begin{pmatrix} \mathbf{K} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right)$$

Can be seen as:

$$\begin{pmatrix} f_1 \\ f_2 \\ \dots \\ f_N \\ f_{*1} \\ f_{*2} \\ \dots \\ f_{*M} \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \mu_1 \\ \mu_2 \\ \dots \\ \mu_N \\ \mu_{*1} \\ \mu_{*2} \\ \dots \\ \mu_{*M} \end{pmatrix}, \begin{pmatrix} \kappa(x, x)_{11} & \dots & \kappa(x, x)_{1N} \\ \kappa(x, x)_{21} & \dots & \kappa(x, x)_{2N} \\ \dots & \dots & \dots \\ \kappa(x, x)_{N1} & \dots & \kappa(x, x)_{NN} \\ \kappa(x_*, x)_{11} & \dots & \kappa(x_*, x)_{1N} \\ \kappa(x_*, x)_{21} & \dots & \kappa(x_*, x)_{2N} \\ \dots & \dots & \dots \\ \kappa(x_*, x)_{M1} & \dots & \kappa(x_*, x)_{MN} \end{pmatrix} \begin{pmatrix} \kappa(x, x_*)_{11} & \dots & \kappa(x, x_*)_{1M} \\ \kappa(x, x_*)_{21} & \dots & \kappa(x, x_*)_{2M} \\ \dots & \dots & \dots \\ \kappa(x, x_*)_{N1} & \dots & \kappa(x, x_*)_{NM} \\ \kappa(x_*, x_*)_{11} & \dots & \kappa(x_*, x_*)_{1M} \\ \kappa(x_*, x_*)_{21} & \dots & \kappa(x_*, x_*)_{2M} \\ \dots & \dots & \dots \\ \kappa(x_*, x_*)_{M1} & \dots & \kappa(x_*, x_*)_{MM} \end{pmatrix} \right)$$

Gaussian Processes for Regression

The predicted distribution (noise-free) is defined as

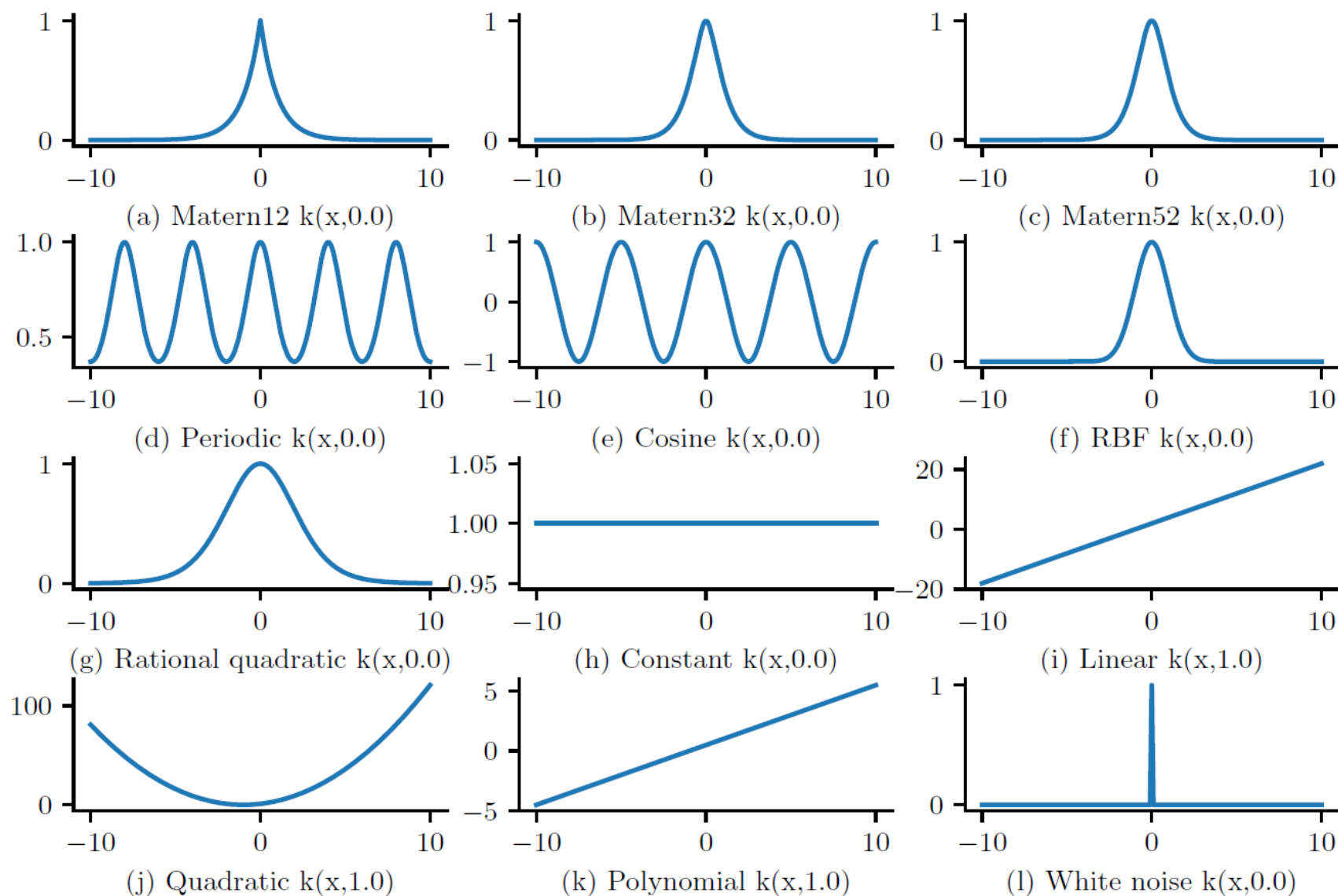
$$\begin{aligned} p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{f}) &= \mathcal{N}(\mathbf{f}_* | \boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \\ \boldsymbol{\mu}_* &= \mathbf{K}^T \mathbf{K}^{-1} \mathbf{f} = \mathbf{K}^T \mathbf{K}^{-1} \mathbf{y} \\ \boldsymbol{\Sigma}_* &= \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}^{-1} \mathbf{K}_* \end{aligned}$$

By adding noise to the function values $\mathbf{y} = \mathbf{f} + \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$, the term \mathbf{K}^{-1} above is rewritten as $(\mathbf{K} + \sigma^2 \mathbf{I})^{-1}$ and illustrated as

$$\begin{pmatrix} \mathbf{f} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{pmatrix} \mathbf{K} + \sigma^2 \mathbf{I} & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right)$$

where \mathbf{I} is the identity matrix.

Gaussian Process Kernels



Radial Basis Function (RBF) Kernel

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp\left(\frac{1}{2l^2} (\mathbf{x}_i - \mathbf{x}_j)^T (\mathbf{x}_i - \mathbf{x}_j)\right)$$

Parameters:

- σ_f controls the vertical variation
- l controls the smoothness of the function

a.k.a. Gaussian kernel,
Squared Exponential kernel

Other kernels not only include Exponential, Matern32, Matern52, Periodic, Cosine, Brownian, Linear, but also their combinations.

A kernel is a positive definite matrix ($\mathbf{x}^T \mathbf{K} \mathbf{x} > 0$):

```
numpy.all(np.linalg.eigvals(K)>0)
```

GPR: Algorithm

```
input:  $X$  (inputs),  $\mathbf{y}$  (targets),  $k$  (covariance function),  $\sigma_n^2$  (noise level),  

 $\mathbf{x}_*$  (test input)  

2:  $L := \text{cholesky}(K + \sigma_n^2 I)$   

 $\alpha := L^\top \backslash (L \backslash \mathbf{y})$  } predictive mean eq. (2.25)  

4:  $\bar{f}_* := \mathbf{k}_*^\top \alpha$   

 $\mathbf{v} := L \backslash \mathbf{k}_*$  } predictive variance eq. (2.26)  

6:  $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$   

 $\log p(\mathbf{y}|X) := -\frac{1}{2} \mathbf{y}^\top \alpha - \sum_i \log L_{ii} - \frac{n}{2} \log 2\pi$  eq. (2.30)  

8: return:  $\bar{f}_*$  (mean),  $\mathbb{V}[f_*]$  (variance),  $\log p(\mathbf{y}|X)$  (log marginal likelihood)
```

Algorithm 2.1: Predictions and log marginal likelihood for Gaussian process regression. The implementation addresses the matrix inversion required by eq. (2.25) and (2.26) using Cholesky factorization, see section A.4. For multiple test cases lines 4-6 are repeated. The log determinant required in eq. (2.30) is computed from the Cholesky factor (for large n it may not be possible to represent the determinant itself). The computational complexity is $n^3/6$ for the Cholesky decomposition in line 2, and $n^2/2$ for solving triangular systems in line 3 and (for each test case) in line 5.

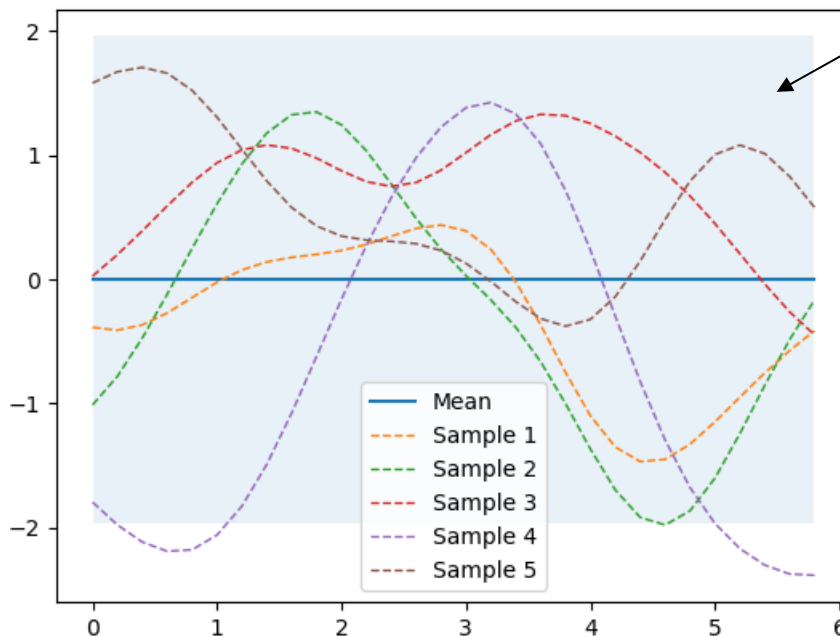
Sampling from a Prior

```
import numpy as np
import matplotlib.pyplot as plt
from gaussian_processes_util import plot_gp

def kernel(X1, X2, l=1.0, sigma_f=1.0):
    sqdist = np.sum(X1**2, 1).reshape(-1, 1) + np.sum(X2**2, 1) - 2 * np.dot(X1, X2.T)
    return sigma_f**2 * np.exp(-0.5 / l**2 * sqdist)

X = np.arange(0, 6, 0.2).reshape(-1, 1)
mu = np.zeros(X.shape)
cov = kernel(X, X)

samples = np.random.multivariate_normal(mu.ravel(), cov, 5)
plot_gp(mu, cov, X, samples=samples)
plt.show()
```



Uncertainty
in blue
(95%
confidence
interval)

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Sampling from a Posterior

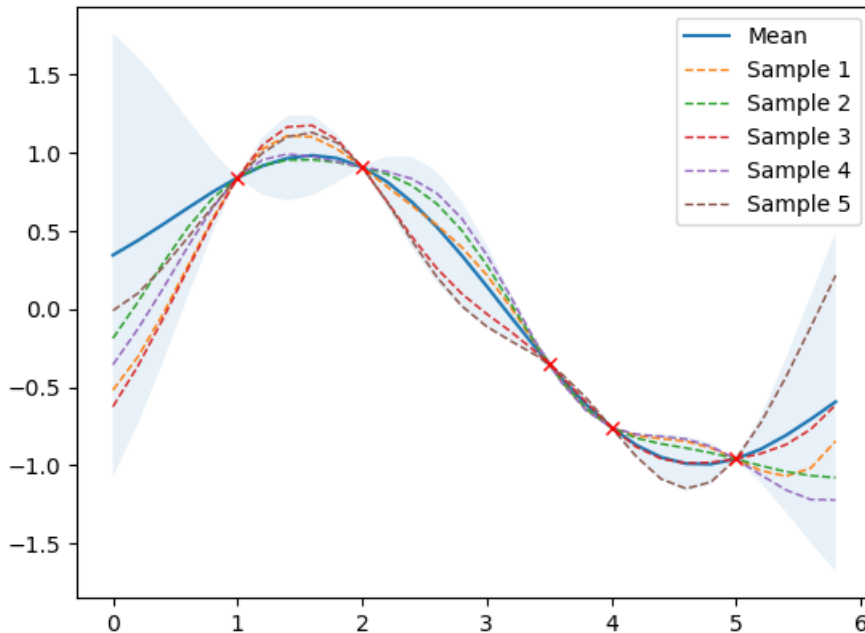
```
import numpy as np
import matplotlib.pyplot as plt
from gaussian_processes_util import plot_gp

def kernel(X1, X2, l=1.0, sigma_f=1.0):

def posterior(X_s, X_train, Y_train, l=1.0, sigma_f=1.0, sigma_y=1e-8):

X = np.arange(0, 6, 0.2).reshape(-1, 1)
X_train = np.array([1, 2, 3.5, 4, 5]).reshape(-1, 1)
Y_train = np.sin(X_train)
mu_s, cov_s = posterior(X, X_train, Y_train) ← Implements equations
                                                of slide 41 (noise-free)

samples = np.random.multivariate_normal(mu_s.ravel(), cov_s, 5)
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train, samples=samples)
plt.show()
```



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Sampling from a Posterior

```
import numpy as np
import matplotlib.pyplot as plt
from gaussian_processes_util import plot_gp

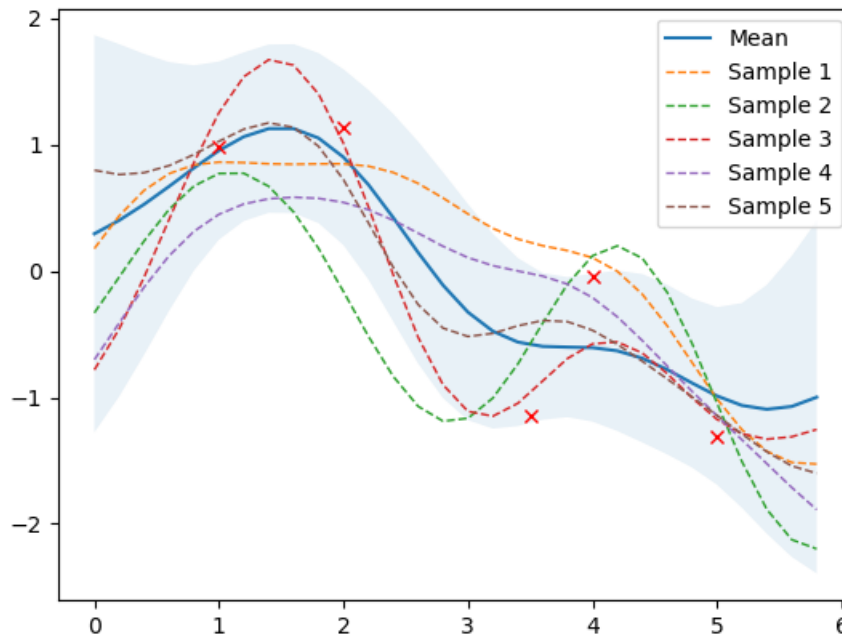
def kernel(X1, X2, l=1.0, sigma_f=1.0):

def posterior(X_s, X_train, Y_train, l=1.0, sigma_f=1.0, sigma_y=1e-8):

noise = 0.4
X = np.arange(0, 6, 0.2).reshape(-1, 1)
X_train = np.array([1, 2, 3.5, 4, 5]).reshape(-1, 1)
Y_train = np.sin(X_train) + noise * np.random.randn(*X_train.shape)
mu_s, cov_s = posterior(X, X_train, Y_train, sigma_y=noise)

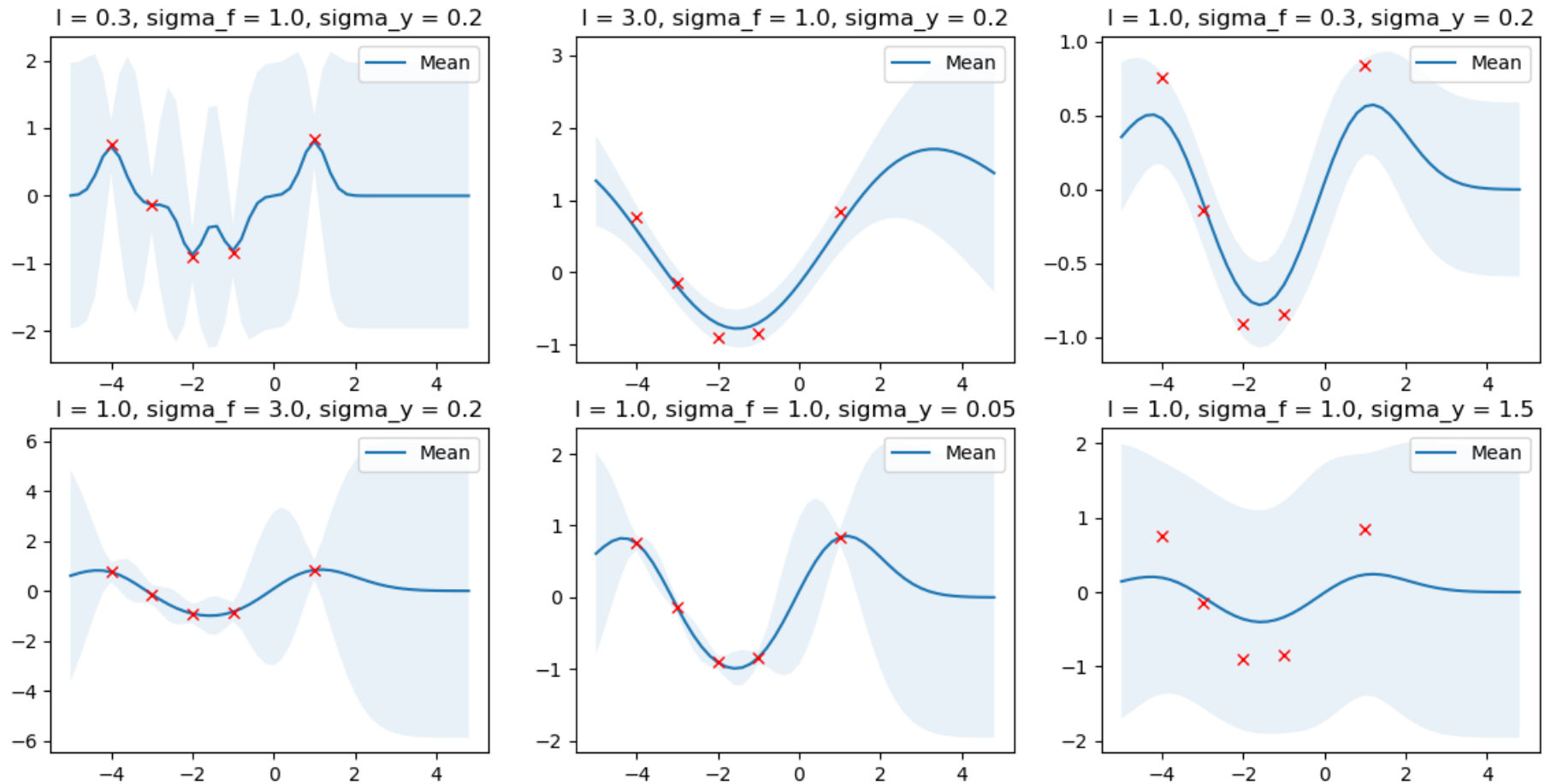
samples = np.random.multivariate_normal(mu_s.ravel(), cov_s, 5)
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train, samples=samples)
plt.show()
```

Noise level to distort the targets
... and increase uncertainty



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from this
[source](#)

Effects of Kernel and Noise Parameters



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Kernel parameters σ_f and l . Noise parameter σ_y .

Optimisation of Kernel Parameters

Optimal values for the kernel parameters can be estimated by maximising the log marginal likelihood

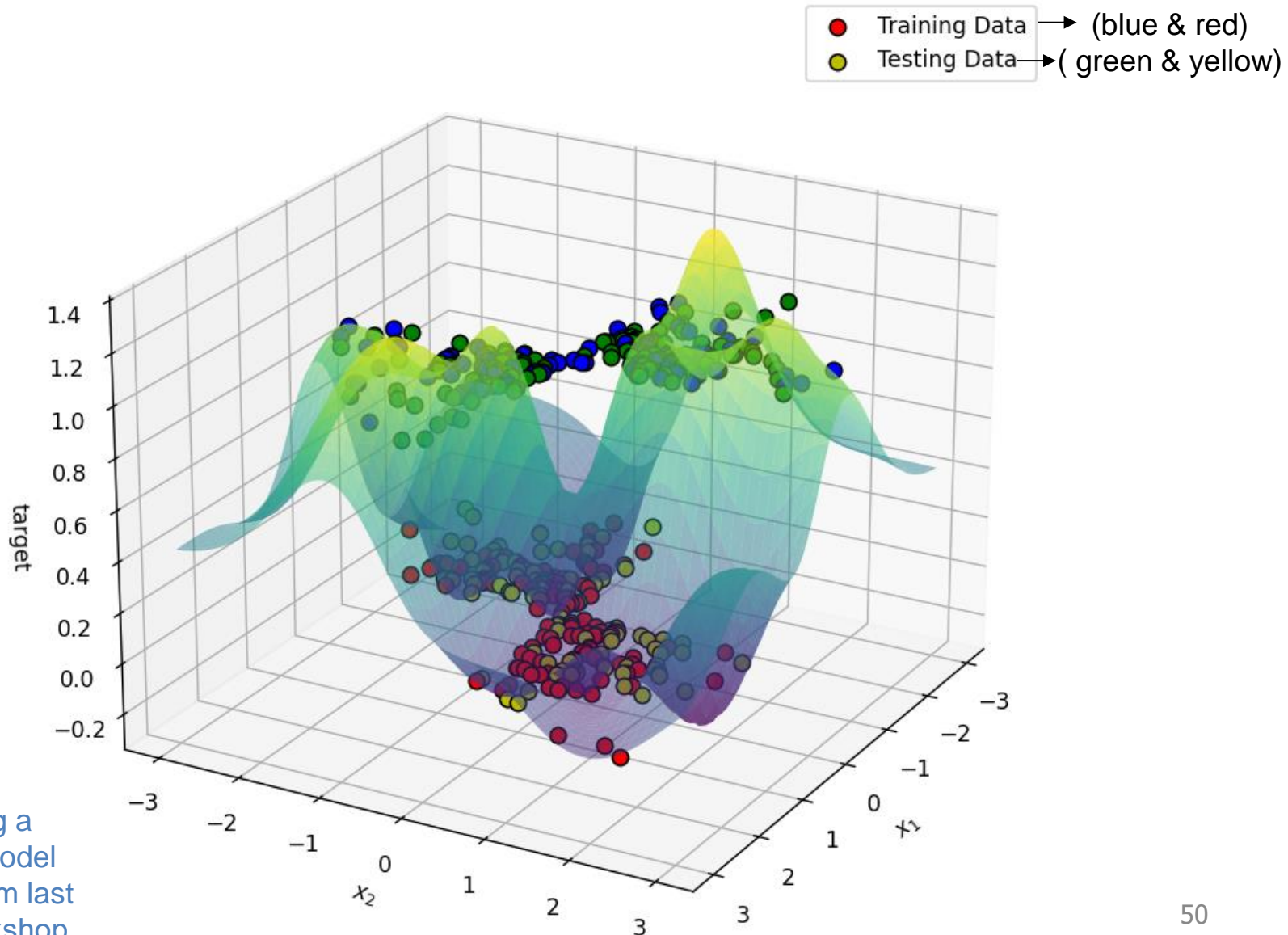
$$\theta^* = \arg \max_{\theta} \log p(\mathbf{y}|\mathbf{X}, \theta)$$

where

$$\begin{aligned} \log p(\mathbf{y}|\mathbf{X}, \theta) &= \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_y) \\ &= -\frac{1}{2} \mathbf{y}^T \mathbf{K}_y^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K}_y| - \frac{N}{2} \log 2\pi \end{aligned}$$

In case of the RBF kernel, the parameters to optimise are l (smoothness of function) and σ_f (vertical variation). Methods to address that include [gradient ascent/descent](#), [L-BFGS](#), etc.

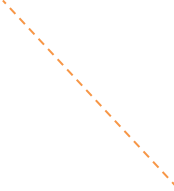
GPR on Non-Linearly Separable Data



Plot using a
gpytorch model
and data from last
week's workshop

Today

- Preliminaries
 - Overview of linear algebra
 - Multivariate Gaussian distributions
 - The kernel trick revisited
- Gaussian processes for regression (GPR)
- **Gaussian processes for classification (GPC)**



With a focus
on binary
classification

How to do classification with GPs?

BASELINE: Treat the task as regression instead of classification, then normalise predicted outputs to produce values $[0 \dots 1]$

This implies training a GPR (as done earlier):

$$p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{f}) = \mathcal{N}(\mathbf{f}_* | \boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*)$$

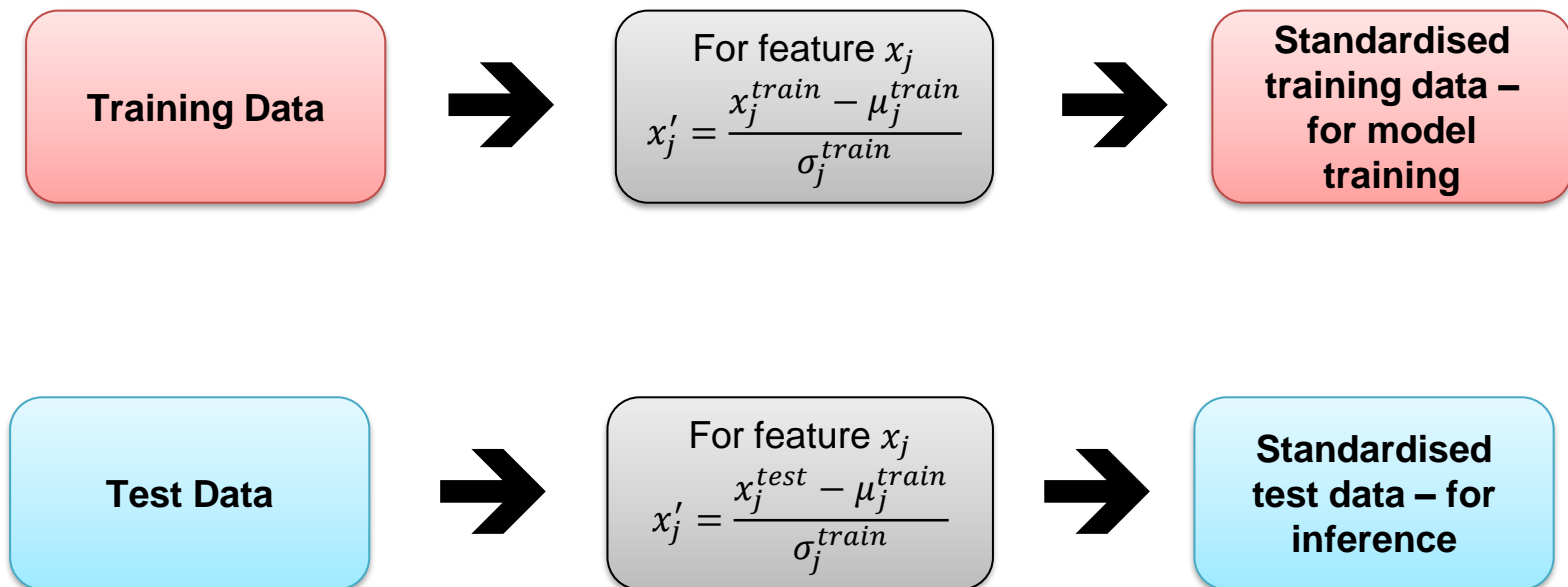
Use the learnt mean vector $\boldsymbol{\mu}_*$ and covariance matrix $\boldsymbol{\Sigma}_*$ to generate predicted outputs for test input x :

$$P(y_* = 1 | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) \approx \frac{\mathcal{N}(1; \mu_{x_*}, \sigma_{x_*})}{\mathcal{N}(1; \mu_{x_*}, \sigma_{x_*}) + \mathcal{N}(0; \mu_{x_*}, \sigma_{x_*})}$$

$$P(y_* = 0 | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) = 1 - P(y_* = 1 | \mathbf{X}, \mathbf{y}, \mathbf{x}_*)$$

Do we Need Data Standardisation?

Not for discrete Bayes Nets or when data is already in a similar scale, but consider it for regression-based models – including Gaussian Processes.



Gaussian Processes for Classification

Consider dataset $\{(\mathbf{x}_i, y_i) | i = 1, \dots, n\}$, where $\mathbf{x}_i \in \mathbb{R}^d$ denotes data point i and $y_i \in \{0, 1\}$ denotes its corresponding target.

Inference in a GP for binary classification follows two steps:

1. Compute the following distribution for the test cases \mathbf{x}_*

$$p(\mathbf{f}_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) = \int p(\mathbf{f}_* | \mathbf{X}, \mathbf{x}_*, \mathbf{f}) p(\mathbf{f} | \mathbf{X}, \mathbf{y}) d\mathbf{f}_*$$

2. Use that distribution to produce probabilistic predictions

$$P(\mathbf{y}_* = 1 | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) = \int \sigma(\mathbf{f}_*) p(\mathbf{f}_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_*) d\mathbf{f}_*$$

Gaussian Processes for Classification

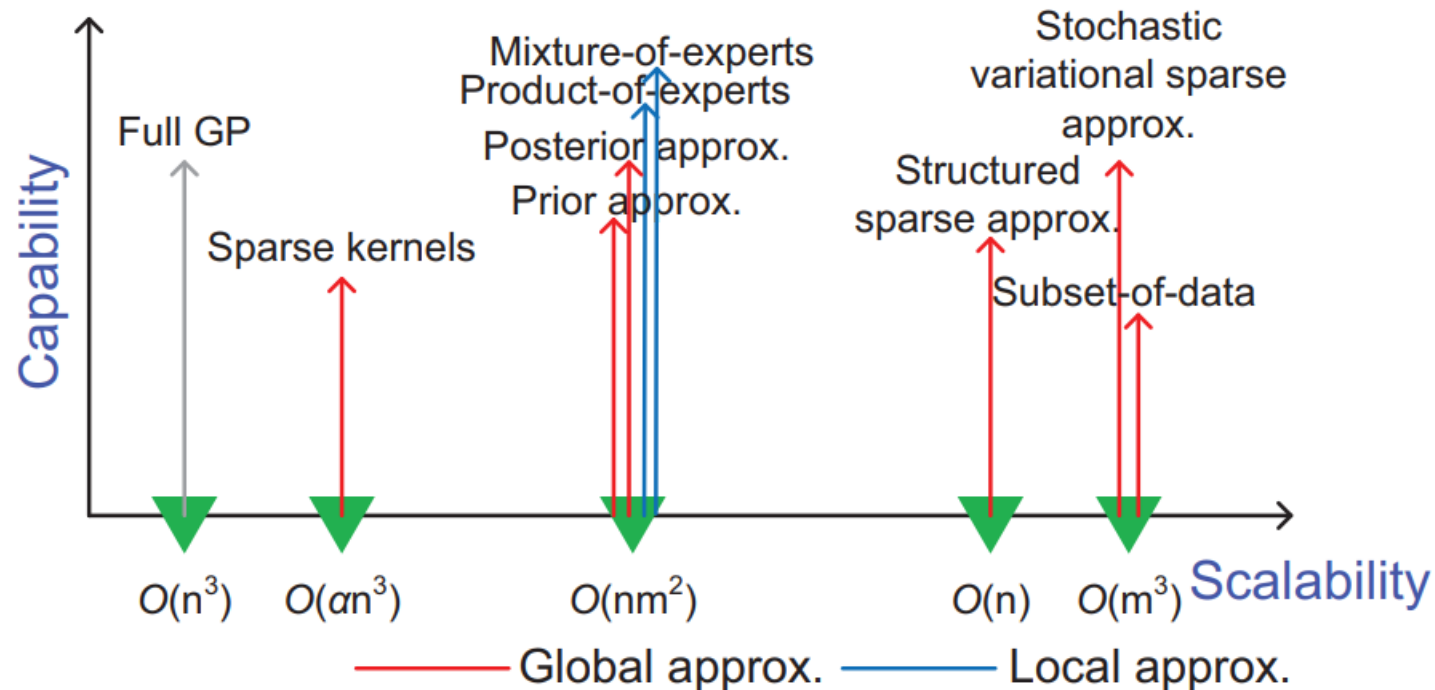
Solutions to $p(\mathbf{f}|\mathbf{X}, \mathbf{y})$ can be approximated via methods such as the following:

- Laplace Approximation
- Expectation Propagation
- Variational Inference

The above are not covered in this module due to extensive implementation details, high computational cost, and not clearly better than the baseline above.

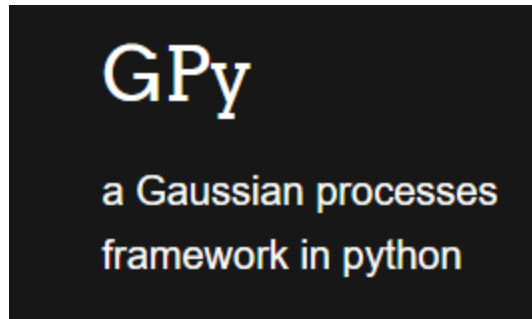
For details, see C.E. Rasmussen & C.K.I. Williams. Gaussian Processes for Machine Learning. MIT Press, 2006 – [chapter 3](#).

GPs: Computational Considerations



Sparse Gaussian Processes summarise data by m instead of n data points, which reduce time complexity from $O(n^3)$ to $O(nm^2)$.

Other Implementations for GPR/GPC



Workshop materials of this week mostly focused on **GPyTorch**

Ideas for your Assignment (optional)

1. Apply Gaussian Processes to continuous data (look for ***gpytorch_GPR.py*** in the workshop materials).
2. Compare and analyse Gaussian Bayesian networks (or any of the previously discussed methods) vs. Gaussian Processes.
3. Compare Gaussian Processes using different kernel functions. Only the RBF kernel is included in the workshop materials.

Today

- Preliminaries of multivariate Gaussians
- Gaussian processes for regression
- Gaussian processes for binary classification

Readings:

- J. Wang. [An intuitive Tutorial to Gaussian Process Regression](#). IEEE, Computing in Science and Engineering, 2024.
- C.E. Rasmussen & C.K.I. Williams. Gaussian Processes for Machine Learning. MIT Press, 2006. [Chapter 2 \(GPR\), 3 \(GPC\)](#)
- K. Murphy. Probabilistic Machine Learning: Advanced Topics, MIT Press, 2023. [Chapter 18](#).

This and Next Week

Workshop (today):

Exercises related to Gaussian conditional probabilities, code for Gaussian Processes, and assignment support.

Lecture (next week):

Probabilistic reasoning over time
(with Riccardo Polvara)

Questions?