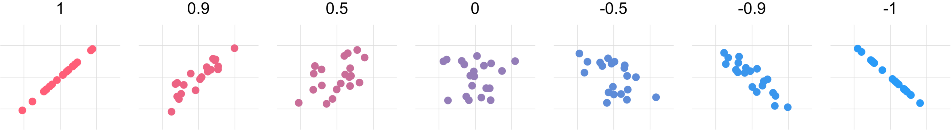
COMS20011 – Data-Driven Computer Science



February 2024

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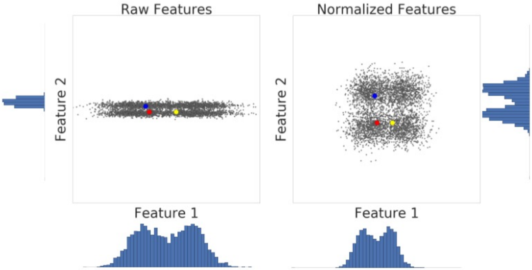
with some slides from Rui Ponte Costa & Dima Damen

Lecture MM-03

This lecture



- ➢ Data acquisition
- ➢ Data characteristics: distance measures
- ➢ **Data characteristics: summary statistics [*reminder*]**
- ➢ **Data normalisation and outliers**

Mean and Variance

For one-dimensional data $\mathbf{x} = \{x_1, .., x_n\}$,

Mean: [average]

$$\mu = \frac{1}{N} \sum_i x_i$$

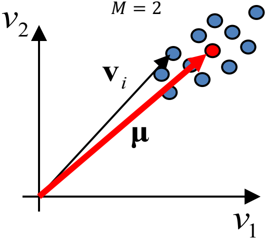
Variance: [spread]

$$\sigma^2 = \frac{1}{N-1} \sum_i (x_i - \mu)^2$$

Standard Deviation:

$$\sigma = \sqrt{\frac{1}{N-1} \sum_i (x_i - \mu)^2}$$

Mean and Covariance



For multi-dimensional data:

e.g. M dimensions with $\{\mathbf{v}_1, \dots, \mathbf{v}_N\}$, i.e there are N vectors/datapoints where each vector has M elements.

Mean vector:

Computed independently for each dimension

$$\boldsymbol{\mu} = \frac{1}{N}\sum_i \mathbf{v}_i$$

Covariance:

Gives both spread and correlation

$$\mathbf{C} = \frac{1}{N-1}\sum_i (\mathbf{v}_i - \boldsymbol{\mu})^2$$

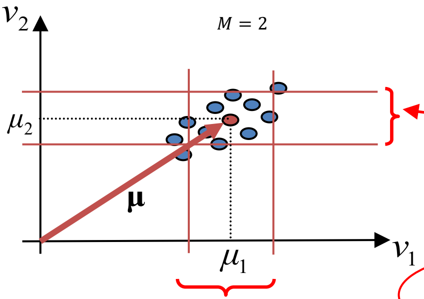
$$\mathbf{C} = \frac{1}{N-1}\sum_i (\mathbf{v}_i - \boldsymbol{\mu})^{\mathrm{T}}(\mathbf{v}_i - \boldsymbol{\mu})$$

$$\mathbf{C} = \frac{1}{N}\sum_i \begin{bmatrix} (v_{i1} - \mu_1)^2 & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ (v_{i1} - \mu_1)(v_{i2} - \mu_2) & (v_{i2} - \mu_2)^2 \end{bmatrix}$$

N when the population mean is known, N-1 when not!

Mean and Covariance

Covariance between components



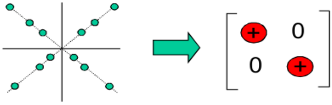
Variance along 1st dimension

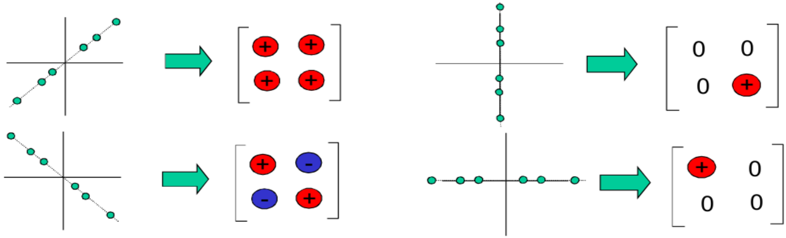
Variance along 2nd dimension

$$\mathbf{C} = \frac{1}{N}\sum_i \begin{bmatrix} \boxed{(v_{i1} - \mu_1)^2} & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ \boxed{(v_{i1} - \mu_1)(v_{i2} - \mu_2)} & \boxed{(v_{i2} - \mu_2)^2} \end{bmatrix}$$

Covariance Matrix

$$\mathbf{C} = \frac{1}{N}\sum_i \begin{bmatrix} (v_{i1} - \mu_1)^2 & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ (v_{i1} - \mu_1)(v_{i2} - \mu_2) & (v_{i2} - \mu_2)^2 \end{bmatrix}$$

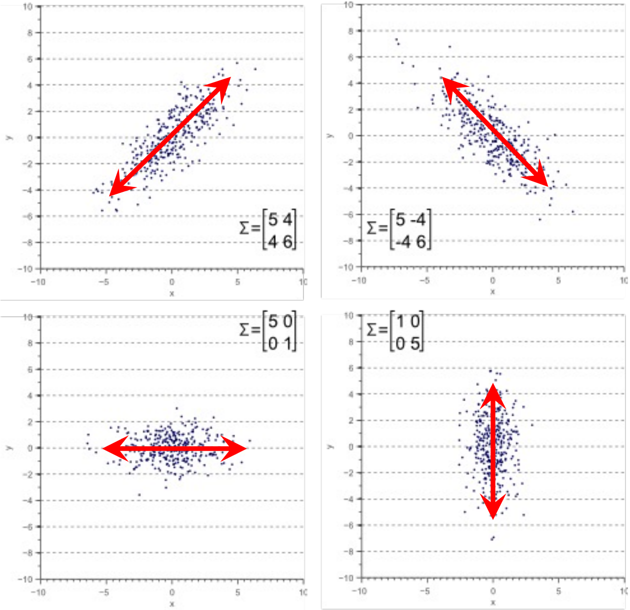




Spread and Covariance

- The shape of the data is defined by the covariance matrix.

- Diagonal spread is captured by the covariance, while axis-aligned spread is captured by the variance.



Covariance Matrix

In three dimensions,

$$\mathbf{C} = \frac{1}{N}\sum_i \begin{bmatrix} (v_{i1}-\mu_1)^2 & (v_{i1}-\mu_1)(v_{i2}-\mu_2) & (v_{i1}-\mu_1)(v_{i3}-\mu_3) \\ (v_{i1}-\mu_1)(v_{i2}-\mu_2) & (v_{i2}-\mu_2)^2 & (v_{i2}-\mu_2)(v_{i3}-\mu_3) \\ (v_{i1}-\mu_1)(v_{i3}-\mu_3) & (v_{i2}-\mu_2)(v_{i3}-\mu_3) & (v_{i3}-\mu_3)^2 \end{bmatrix}$$

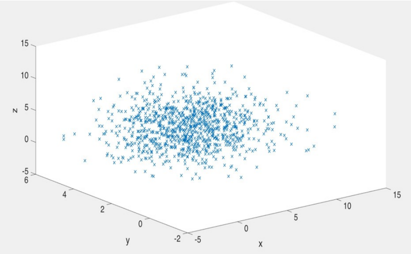
A Covariance matrix is always:

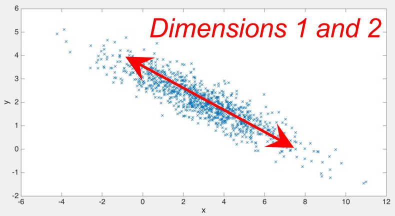
- square
- symmetric
- variances on the diagonal
- covariance between each pair of dimensions in non-diagonal elements

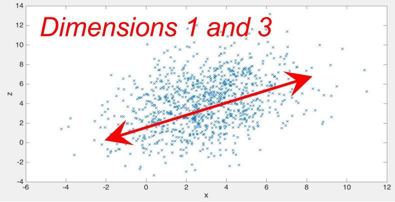
Covariance Matrix example

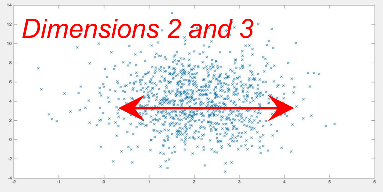
For the covariance matrix,

$$\mathbf{c} = \begin{bmatrix} 5 & -2 & 2 \\ -2 & 1 & 0 \\ 2 & 0 & 7 \end{bmatrix}$$



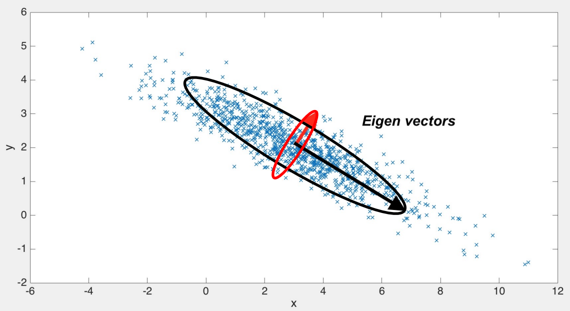






Covariance Matrix: Eigen analysis

- Eigenvectors and eigenvalues define the principal axes and spread of points along directions
- **Major axis** - eigenvector corresponding to larger eigenvalue (i.e. larger variance)
- **Minor axis** - eigenvector corresponding to smaller eigenvalue (i.e. smaller variance)
- These can be represented using major and minor axes of ellipses



Covariance Matrix: Eigen analysis

Definition

For a square matrix $\mathbf{C}$,
if there exists a non-zero column vector $\mathbf{v}$ where

$$\mathbf{C}v = \lambda v$$

then,

$v \rightarrow$ eigenvector of matrix C
$\lambda \rightarrow$ eigenvalue of matrix C

e.g.

$$\mathbf{C} = \begin{bmatrix} 0 & -1 \\ 2 & 3 \end{bmatrix}, v_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}, \lambda_1 = 1$$

Covariance Matrix: Eigen analysis

- To calculate eigenvectors of a square matrix, e.g. a covariance matrix, then solve

$$|\mathbf{C} - \lambda \boldsymbol{I}| = 0$$

where

- $\boldsymbol{I}$ is the identity matrix
- $|\mathbf{C}|$ is the determinant of the matrix

For 2×2 matrices, there are two eigenvalues λ_1, λ_2

$$\mathbf{C} - \lambda \boldsymbol{I} = \begin{bmatrix} 0 & -1 \\ 2 & 3 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} = \begin{bmatrix} -\lambda & -1 \\ 2 & 3 - \lambda \end{bmatrix}$$

$$|\mathbf{C} - \lambda \boldsymbol{I}| = \lambda^2 - 3\lambda + 2 = (\lambda - 1)(\lambda - 2)$$

$$\lambda_1 = 1 \quad and \quad \lambda_2 = 2$$

Covariance Matrix: Eigen analysis

- After the eigenvalues are found, the eigenvectors can be calculated

For $\lambda_1 = 1$

$$\begin{bmatrix} 0 & -1 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} = \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} \tag{2}$$

- This simplifies to:

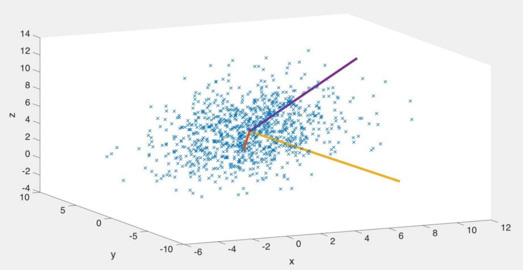
$$\begin{bmatrix} -v_{12} \\ 2v_{11} + 3v_{12} \end{bmatrix} = \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} \tag{3}$$

- If we set $v_{12} = 1$, then we get the eigenvector:

$$\begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \tag{4}$$

- Verify that this is indeed a valid eigenvector by calculating $\mathbf{C}v = \lambda v$

Covariance Matrix: another example



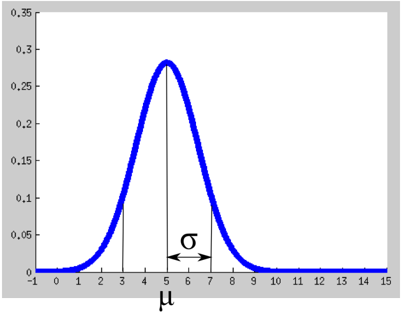
- Eigenvalues → $\lambda_1 = 0.08$ $\lambda_2 = 4.52$ $\lambda_3 = 8.40$
- Eigenvectors → $v_1 = \begin{bmatrix} -0.42 \\ -0.90 \\ 0.12 \end{bmatrix}$ $v_2 = \begin{bmatrix} 0.71 \\ -0.40 \\ -0.57 \end{bmatrix}$ $v_3 = \begin{bmatrix} 0.57 \\ -0.15 \\ 0.81 \end{bmatrix}$
- Principal/Major axis is v_3 (corresponding to the largest eigenvalue)

Normal or Gaussian Distribution (Reminder)

For a normal distribution $N(\mu, \sigma^2)$ in one dimension, the probability density function (pdf) can be calculated as:

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

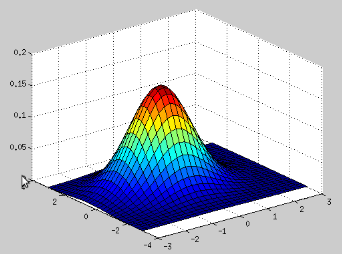
68% of data within 1σ of μ
92% within 2σ of μ
99% within 3σ of μ

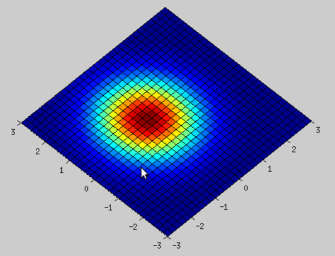


Normal Distribution - Multi-dimensional (reminder)

For multi-dimensional normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, the probability density function (pdf) can be calculated as

$$p(\mathbf{x}) = \frac{1}{2\pi \|\boldsymbol{\Sigma}\|^{1/2}} \exp\left(-\tfrac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \ \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

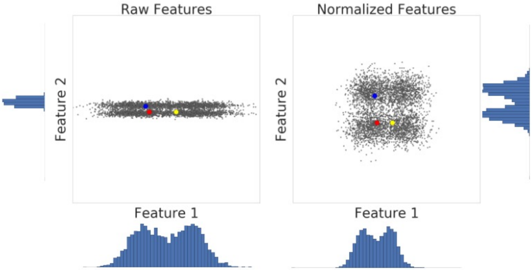




WARNING: Σ **is the capital letter of** σ**, not the summation sign!**

So here Σ **is the covariance matrix.**

Next



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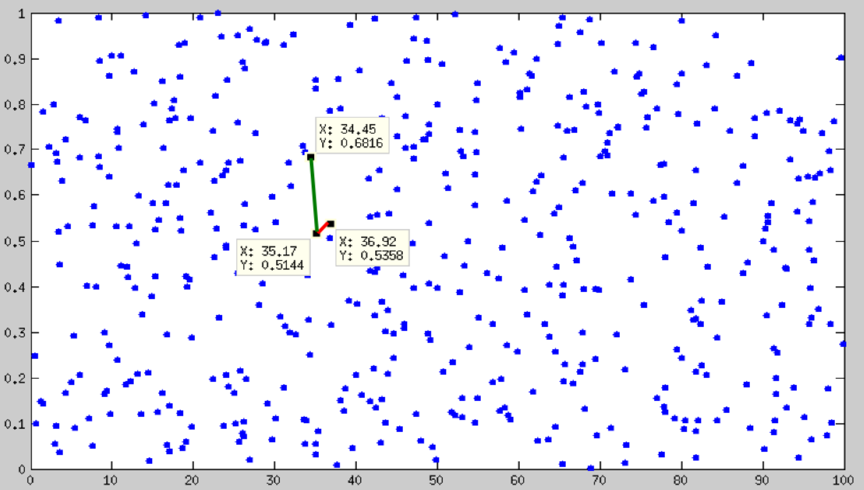
- ➢ Data characteristics: distance measures
- ➢ Data characteristics: summary statistics [*reminder*]
- ➢ **Data normalisation and outliers**

Data Characteristic - Data Normalisation

- Note the difference in magnitude between the two dimensions below!
- Data may need to be normalised before distance is calculated



Data Characteristic - Data Normalisation

- Methods for normalisation:

1. Rescaling

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

rescales the range of features to [0, 1]

2. Standardisation (also known as *z*-score)

$$x' = \frac{x - \mu}{\sigma}$$

makes the values of each feature in the data have zero-mean and unit-variance

3. Scaling to unit length

$$x' = \frac{x}{||\mathbf{x}||}$$

scales components of feature vector so that the complete vector has length one

Brief return to Distance Measures

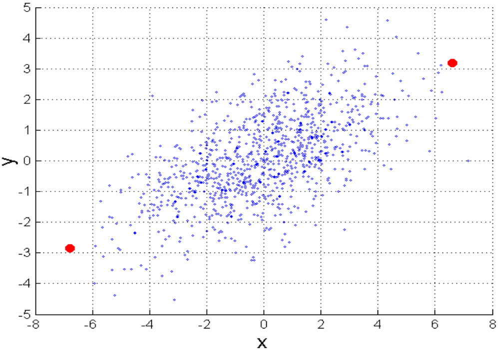
Mahalanobis Distance is a measure of distance between a data vector and a set of data, or a variation that measures the distance between two vectors from the same dataset:

$$mahalanobis(a,b) = (a-b)^T \Sigma^{-1} (a - b)$$

$$\text{where } \operatorname{cov}(X,Y) = \Sigma = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})(y_i - \bar{y})$$

Warning: Σ is the covariance matrix of the input data D

For red points, the Euclidean distance is 14.7, and the Mahalanobis distance is 6.



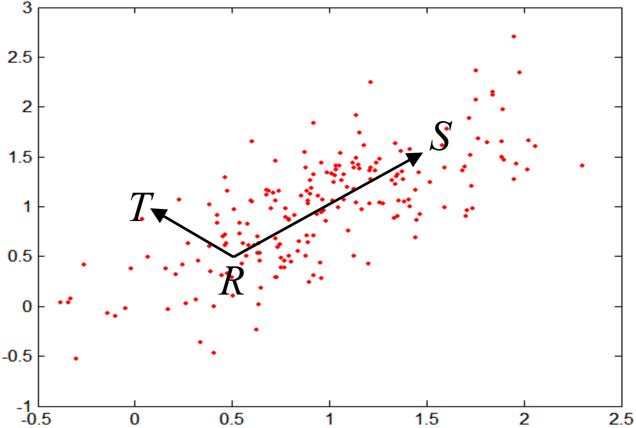
Brief return to Distance Measures

Mahalanobis Distance example:

Given $R = (0.5,0.5)$, $S = (1.5,1.5)$, $T = (0.0,1.0)$, find the mahalanobis distance RT and RS.

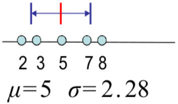
$$\sum = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

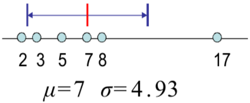
$RS = 4$
$RT = 5$

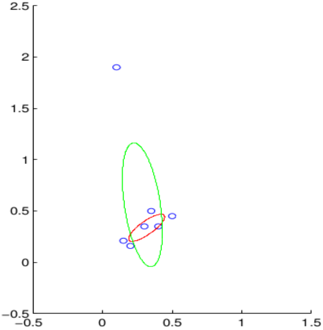


Data Characteristic - Outliers

- Mean, variance and covariance can provide concise description of ‘average’ and ‘spread’, but not when outliers are present in the data
- **outliers**: An *outlier* is an observation that lies an abnormal distance from other values in a random sample from a population.
- usually due to fault in measurement and not always easy to remove







Next in COMS20011

- Least Squares and Regression
- Clustering data
- Classification of data
- The Fourier transform
- Principal Components Analysis
- Convolutions