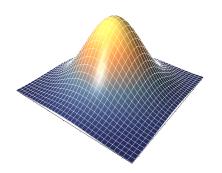
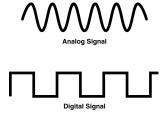
COMS20011 – Data-Driven Computer Science



February 2021
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This lecture



- Data acquisition
- Data characteristics: distance measures
- Data characteristics: summary statistics [reminder]

Data normalisation and outliers

Mean and Variance

For one-dimensional data $\mathbf{v} = \{v_1, ..., v_n\},$

Mean: [average]

$$\mu = \frac{1}{N} \sum_{i} v_i$$

Variance: [spread]

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

Standard Deviation:

$$\sigma = \sqrt{\frac{1}{N-1} \sum_{i} (v_i - \mu)^2}$$

Mean and Covariance

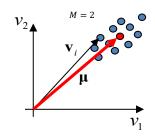
For multi-dimensional data:

e.g. M dimensions with $\{v_1, ..., v_N\}$, i.e there are N vectors/datapoints where each vector has M elements.



Computed independently for each dimension

$$\mu = \frac{1}{N} \sum_{i} \mathbf{v}_{i}$$



Covariance:

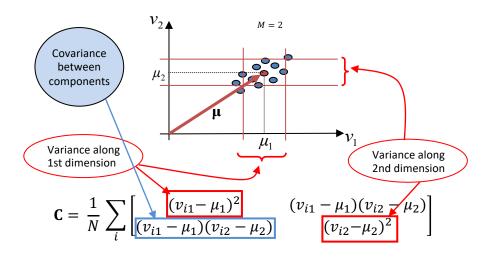
Gives both spread and correlation

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

$$\mathbf{C} = \frac{1}{N-1} \sum_{i} (\mathbf{v}_{i} - \boldsymbol{\mu})^{\mathrm{T}} (\mathbf{v}_{i} - \boldsymbol{\mu})$$

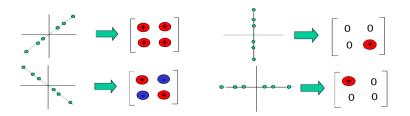
$$\mathbf{C} = \frac{1}{N} \sum_{i} \begin{bmatrix} (v_{i1} - \mu_1)^2 & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ (v_{i1} - \mu_1)(v_{i2} - \mu_2) & (v_{i2} - \mu_2)^2 \end{bmatrix}$$

Mean and Covariance



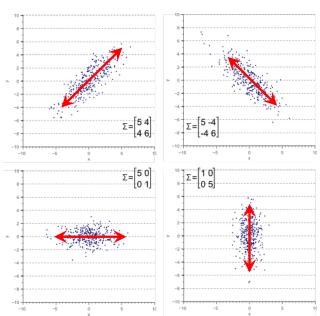
Covariance Matrix

$$\mathbf{C} = \frac{1}{N} \sum_{i} \begin{bmatrix} (v_{i1} - \mu_1)^2 & (v_{i1} - \mu_1)(v_{i2} - \mu_2) \\ (v_{i1} - \mu_1)(v_{i2} - \mu_2) & (v_{i2} - \mu_2)^2 \end{bmatrix} \quad \longrightarrow \quad \begin{bmatrix} \bullet & 0 \\ 0 & \bullet \end{bmatrix}$$



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,

$$\mathbf{C} = \frac{1}{N} \sum_{i} \begin{bmatrix} (v_{i1} - \mu_{1})^{2} & (v_{i1} - \mu_{1})(v_{i2} - \mu_{2}) & (v_{i1} - \mu_{1})(v_{i3} - \mu_{3}) \\ (v_{i1} - \mu_{1})(v_{i2} - \mu_{2}) & (v_{i2} - \mu_{2})^{2} & (v_{i2} - \mu_{2})(v_{i3} - \mu_{3}) \\ (v_{i1} - \mu_{1})(v_{i3} - \mu_{3}) & (v_{i2} - \mu_{1})(v_{i3} - \mu_{3}) & (v_{i3} - \mu_{3})^{2} \end{bmatrix}$$

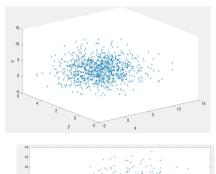
A Covariance matrix is always:

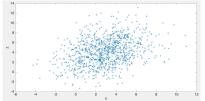
- square and symmetric
- variances on the diagonal
- covariance between each pair of dimensions is included in non-diagonal elements

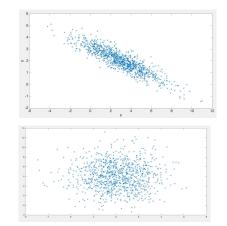
Covariance Matrix example

For the covariance matrix,

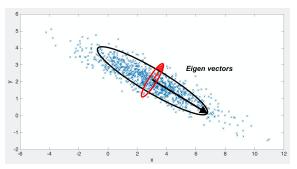
$$\mathbf{c} = \begin{bmatrix} 5 & -2 & 2 \\ -2 & 1 & 0 \\ 2 & 0 & 7 \end{bmatrix}$$







- Eigenvectors and eigenvalues define 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



Definition

For a square matrix C, if there exists a non-zero column vector v where

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

then,

 $v \rightarrow {
m eigenvector\ of\ matrix\ } {\it C}$ $\lambda \rightarrow {
m eigenvalue\ of\ matrix\ } {\it C}$

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

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

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

where

- ► *I* is the identity matrix
- ▶ |C| is the determinant of the matrix

For 2 \times 2 matrices, there are two eigenvalues λ_1 , λ_2

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

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

$$\lambda_1 = 1, \lambda_2 = 2$$

After the eigenvalues are found, the eigenvectors can be calculated

For $\lambda_1 = 1$

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

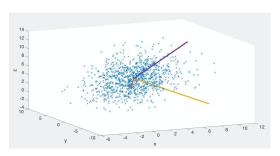
This simplifies to:

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

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

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

Covariance Matrix: another example



$$\triangleright$$
 Eigenvalues \rightarrow $\lambda_1 = 0.08$ $\lambda_2 = 4.52$ $\lambda_3 = 8.40$

$$\lambda_1 = 0.08$$

$$\lambda_2 = 4.52$$

$$\lambda_3 = 8.40$$

$$v_1 = \begin{bmatrix} -0.42 \\ -0.90 \\ 0.12 \end{bmatrix}$$

➤ Eigenvectors →
$$v_1 = \begin{bmatrix} -0.42 \\ -0.90 \\ 0.12 \end{bmatrix}$$
 $v_1 = \begin{bmatrix} 0.71 \\ -0.40 \\ -0.57 \end{bmatrix}$ $v_3 = \begin{bmatrix} 0.57 \\ -0.15 \\ 0.81 \end{bmatrix}$

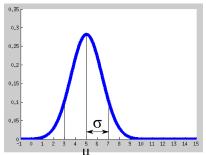
$$v_3 = \begin{bmatrix} 0.57 \\ -0.15 \\ 0.81 \end{bmatrix}$$

 \triangleright 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:

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

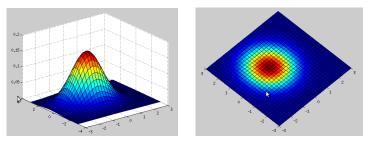


68% of data within 1σ of μ 92% within 2σ of μ 99% within 3σ of μ

Normal Distribution - Multi-dimensional (reminder)

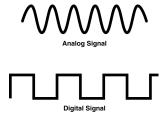
For multi-dimensional normal distribution $N(\mu, \Sigma)$, the probability density function (pdf) can be calculated as

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



WARNING: Σ is the capital letter of σ , not the summation sign! So here Σ is the covariance matrix.

This lecture

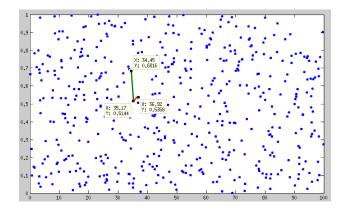


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- Data characteristics: summary statistics [reminder]

Data normalisation and outliers

Data Characteristic - Data Normalisation

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



Data Characteristic - Data Normalisation

Methods for normalisation:

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

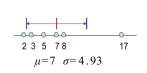
2. Standardisation (also known as z-score)
$$x' = \frac{x - \mu}{\sigma}$$

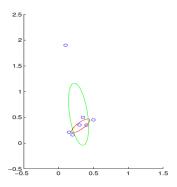
3. Scaling to unit length
$$x' = \frac{x}{\|x\|}$$

Data Characteristic - Outliers

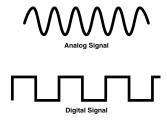
- Mean, variance and covariance can provide concise description of 'average' and 'spread', but not when outliers are present in the data
- outliers: small number of points with values significantly different from that of the other points
- usually due to fault in measurement and not always easy to remove







Concluding initial part of COMS20011



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Data normalisation and outliers