Multivariate Statistics and Machine Learning

Lecture Notes
MATH38161

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Preface

About these notes

This is the course text for MATH38161, an introductory course in **Multivariate Statistics and Machine Learning** for third year mathematics students.

These notes will be updated from time to time. To view the current version in your browser visit the online MATH38161 lecture notes. You may also downlad the MATH38161 lecture notes as PDF.

About the author

My name is Korbinian Strimmer and I am a Professor in Statistics in the Statistics group of the Department of Mathematics at the University of Manchester. You can find more information about me on my home page.

I have first taught this module in the Winter term 2018 at the University of Manchester.

I hope you enjoy the course. If you have any questions, comments, or corrections then please email me at korbinian.strimmer@manchester.ac.uk

About the module

Topics covered

The MATH38161 module is designed to run over the course of 11 weeks. It has six parts, each covering a particular aspect of multivariate statistics and machine learning:

1. Multivariate random variables and estimation in large and small sample settings (W1 and W2)
2. Transformations and dimension reduction (W3 and W4)
3. Unsupervised learning/clustering (W5 and W6)
4. Supervised learning/classification (W7 and W8)
5. Measuring and modelling multivariate dependencies (W9)
6. Nonlinear and nonparametric models (W10, W11)

This module focuses on:

- *Concepts and methods* (not on theory)
- *Implementation and application in R*
- *Practical data analysis and interpretation* (incl. report writing)
- *Modern tools in data science and statistics* (R markdown, R studio)

Additional support material

Accompanying these notes are

- a weekly learning plan for an 11 week study period,
- corresponding worksheets with examples (theory and application in R) and solutions in R Markdown,
- lecture videos (visualiser style).

Organisatorical information is available from the course home page and on Blackboard.

If you are a University of Manchester student and enrolled for this module you can find the exam questions of previous years (without solution) as well as the coursework instructions on Blackboard.

Furthermore, there is also an MATH38161 online reading list hosted by the University of Manchester library.

Acknowledgements

Many thanks to Beatriz Costa Gomes for her help to compile the first draft of these course notes in the winter term 2018 while she was a graduate teaching assistant for this course. I also thank the many students who suggested corrections.

Chapter 1

Multivariate random variables

1.1 Why multivariate statistics?

Science uses experiments to verify hypotheses about the world. Statistics provides tools to quantify this procedure and offers methods to link data (experiments) with probabilistic models (hyptheses). Since the world is complex we need complex models and complex data, hence the need for multivariate statistics and machine learning.

Specifically, multivariate statistics (as opposed to univariate statistics) is concerned with methods and models for **random vectors** and **random matrices**, rather than just random univariate (scalar) variables. Therefore, in multivariate statistics we will frequently make use of matrix notation.

Closely related to multivariate statistics (traditionally a subfield of statistics) is machine learning (ML) which is traditionally a subfield of computer science. ML used to focus more on on algorithms rather on probabilistic modeling but nowadays most machine learning methods are fully based on statistical multivariate approaches, so the two fields are converging.

Learning multivariate models allows us to learn dependencies and interactions among the components of the random variables which in turns allows to draw conclusion about the world.

Two main tasks:

- unsupervised learning (finding structure, clustering)
- supervised learning (training from labeled data, followed by prediction)

Challenges:

- complexity of model needs to be appropriate for problem and available data,
- high dimensions make estimation and inference difficult
- computational issues.

1.2 Essentials in multivariate statistics

1.2.1 Univariate vs. multivariate random variables

Univariate random variable (dimension $d = 1$):

$$x \sim F$$

where x is a **scalar** and F is the distribution. $\mathrm{E}(x) = \mu$ denotes the mean and $\mathrm{Var}(x) = \sigma^2$ the variance of x.

Multivariate random **vector** of dimension d:

$$\boldsymbol{x} = (x_1, x_2, ..., x_d)^T \sim F$$

$\boldsymbol{x}$ is **vector** valued random variable.

The vector $\boldsymbol{x}$ is column vector (=matrix of size $d \times 1$). Its components $x_1, x_2, ..., x_d$ are univariate random variables. The dimension d is also often denoted by p or q.

1.2.2 Mean of a random vector

The mean / expectation of a random vector with dimensions d is also a vector with dimensions d:

$$\mathrm{E}(\boldsymbol{x}) = \boldsymbol{\mu} = \begin{pmatrix} \mathrm{E}(x_1) \\ \mathrm{E}(x_2) \\ \vdots \\ \mathrm{E}(x_d) \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_d \end{pmatrix}$$

1.2.3 Variance of a random vector

Recall the definition of mean and variance for a univariate random variable:

$$\mathrm{E}(x) = \mu$$

$$\mathrm{Var}(x) = \sigma^2 = \mathrm{E}((x-\mu)^2) = \mathrm{E}((x-\mu)(x-\mu)) = \mathrm{E}(x^2) - \mu^2$$

Definition of **variance of a random vector:**

$$\mathrm{Var}(\boldsymbol{x}) = \underbrace{\boldsymbol{\Sigma}}_{d \times d} = \mathrm{E}\left(\underbrace{(\boldsymbol{x} - \boldsymbol{\mu})}_{d \times 1} \underbrace{(\boldsymbol{x} - \boldsymbol{\mu})^T}_{1 \times d} \right) = \mathrm{E}(\boldsymbol{x}\boldsymbol{x}^T) - \boldsymbol{\mu}\boldsymbol{\mu}^T$$

The variance of a random vector is, therefore, **not** a vector but a **matrix**!

$$\boldsymbol{\Sigma} = (\sigma_{ij}) = \begin{pmatrix} \sigma_{11} & \dots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \dots & \sigma_{dd} \end{pmatrix}$$

This matrix is called the **Covariance Matrix**, with off-diagonal elements $\sigma_{ij} = \mathrm{Cov}(x_i, x_j)$ and the diagonal $\sigma_{ii} = \mathrm{Var}(X_i) = \sigma_i^2$.

1.2.4 Properties of the covariance matrix

1. $\mathbf{\Sigma}$ is real valued: $\sigma_{ij} \in \mathbb{R}$
2. $\mathbf{\Sigma}$ is symmetric: $\sigma_{ij} = \sigma_{ji}$
3. The diagonal of $\mathbf{\Sigma}$ contains $\sigma_{ii} = \mathrm{Var}(x_i) = \sigma_i^2$, i.e. the variances of the components of $\boldsymbol{x}$.
4. Off-diagonal elements $\sigma_{ij} = \mathrm{Cov}(x_i, x_j)$ represent linear dependencies among the x_i. $\Longrightarrow$ linear regression, correlation

How many separate entries does $\mathbf{\Sigma}$ have?

$$\mathbf{\Sigma} = (\sigma_{ij}) = \underbrace{\begin{pmatrix} \sigma_{11} & \dots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \dots & \sigma_{dd} \end{pmatrix}}_{d \times d}$$

with $\sigma_{ij} = \sigma_{ji}$.

Number of separate entries: $\frac{d(d+1)}{2}$.

This numbers grows with the square of the dimension d, i.e. is of order $\mathrm{O}(d^2)$:

d	# entries
1	1
10	55
100	5050
1000	500500
10000	50005000

For large dimension d the covariance matrix has many components!

–> computationally expensive (both for storage and in handling) –> very challenging to estimate in high dimensions d.

Note: matrix inversion requires $\mathrm{O}(d^3)$ operations! So, computing $\mathbf{\Sigma}^{-1}$ is difficult for large d!

1.2.5 Eigenvalue decomposition of $\mathbf{\Sigma}$

Recall the orthogonal eigendecomposition from matrix analysis and linear algebra: A symmetric matrix with real entries has real eigenvalues and a complete set of orthogonal eigenvectors.

Applying eigenvalue decomposition to the covariance matrix yields

$$\mathbf{\Sigma} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$

where $\boldsymbol{U}$ is an orthogonal matrix containing the eigenvectors and

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_d \end{pmatrix}$$

contains the eigenvalues λ_i.

Importantly, the eigenvalues of the covariance matrix are not only real valued but they are further constrained to be non-negative. This can be seen by computing the quadratic form $z^T \boldsymbol{\Sigma} z$ for a non-zero non-random vector z which yields

$$\begin{aligned} z^T \boldsymbol{\Sigma} z &= z^T \mathrm{E}\left((\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T \right) z \\ &= \mathrm{E}\left(z^T (\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T z \right) \\ &= \mathrm{E}\left(\left(z^T (\boldsymbol{x} - \boldsymbol{\mu}) \right)^2 \right) \geq 0 \,. \end{aligned}$$

Hence the covariance matrix **$\boldsymbol{\Sigma}$ is always positive semi-definite**.

In fact, **unless there is collinearity** (i.e. a variable is a linear function the other variables) all eigenvalues will be positive and **$\boldsymbol{\Sigma}$ is positive definite**.

1.2.6 Quantities related to the covariance matrix

1.2.6.1 Correlation matrix $\boldsymbol{P}$

The correlation matrix $\boldsymbol{P}$ (= upper case greek "rho") is the standardised covariance matrix

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}} = \mathrm{Cor}(x_i, x_j)$$

$$\rho_{ii} = 1 = \mathrm{Cor}(x_i, x_i)$$

$$\boldsymbol{P} = (\rho_{ij}) = \begin{pmatrix} 1 & \dots & \rho_{1d} \\ \vdots & \ddots & \vdots \\ \rho_{d1} & \dots & 1 \end{pmatrix}$$

where $\boldsymbol{P}$ ("capital rho") is a symmetric matrix ($\rho_{ij} = \rho_{ji}$).

Note the **variance-correlation decomposition**

$$\boldsymbol{\Sigma} = \boldsymbol{V}^{\frac{1}{2}} \boldsymbol{P} \boldsymbol{V}^{\frac{1}{2}}$$

where $\boldsymbol{V}$ is a diagonal matrix containing the variances:

$$\boldsymbol{V} = \begin{pmatrix} \sigma_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{dd} \end{pmatrix}$$

$$\boldsymbol{P} = \boldsymbol{V}^{-\frac{1}{2}} \boldsymbol{\Sigma} \boldsymbol{V}^{-\frac{1}{2}}$$

This is the definition of correlation written in matrix notation.

1.2.6.2 Precision matrix or concentration matrix

$$\boldsymbol{\Omega} = (\omega_{ij}) = \boldsymbol{\Sigma}^{-1}$$

$\boldsymbol{\Omega}$ ("Omega") is the inverse of the covariance matrix.

The inverse of the covariance matrix can be obtained via the spectral decomposition, followed by inverting the eigenvalues λ_i:

$$\boldsymbol{\Sigma}^{-1} = \boldsymbol{U} \boldsymbol{\Lambda}^{-1} \boldsymbol{U}^T = \boldsymbol{U} \begin{pmatrix} \lambda_1^{-1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_d^{-1} \end{pmatrix} \boldsymbol{U}^T$$

Note that **all eigenvalues λ_i need to be positive so that $\boldsymbol{\Sigma}$ can be inverted.** (i.e., $\boldsymbol{\Sigma}$ needs to be positive definite).
If any $\lambda_i = 0$ then $\boldsymbol{\Sigma}$ is singular and not invertible.

Importance of $\boldsymbol{\Sigma}^{-1}$: - Natural parameter in exponential family. - Many expressions in multivariate statistics contain $\boldsymbol{\Sigma}^{-1}$ and not $\boldsymbol{\Sigma}$ - $\boldsymbol{\Sigma}^{-1}$ has close connection with graphical models (e.g. conditional independence graph, partial correlations, see later chapter)

1.2.6.3 Partial correlation matrix

This is a standardised version of the precision matrix, see later chapter on graphical models.

1.2.6.4 Total variation and generalised variance

To summarise the covariance matrix $\boldsymbol{\Sigma}$ in a single scalar value there are two commonly used measures:

- **total variation**: $\mathrm{Tr}(\boldsymbol{\Sigma}) = \sum_{i=1}^{d} \lambda_i$
- **generalised variance**: $\det(\boldsymbol{\Sigma}) = \prod_{i=1}^{d} \lambda_i$

If all eigenvalues are positive then $\log\det(\boldsymbol{\Sigma}) = \sum_{i=1}^{d} \log \lambda_i = \mathrm{Tr}(\log \boldsymbol{\Sigma})$.

$\log \boldsymbol{\Sigma}$ is the matrix logarithm of $\boldsymbol{\Sigma}$ and is given by $\log \boldsymbol{\Sigma} = \boldsymbol{U} \begin{pmatrix} \log \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \log \lambda_d \end{pmatrix} \boldsymbol{U}^T$

1.3 Multivariate normal distribution

The multivariate normal model is a generalisation of the univariate normal distribution from dimension 1 to dimension d.

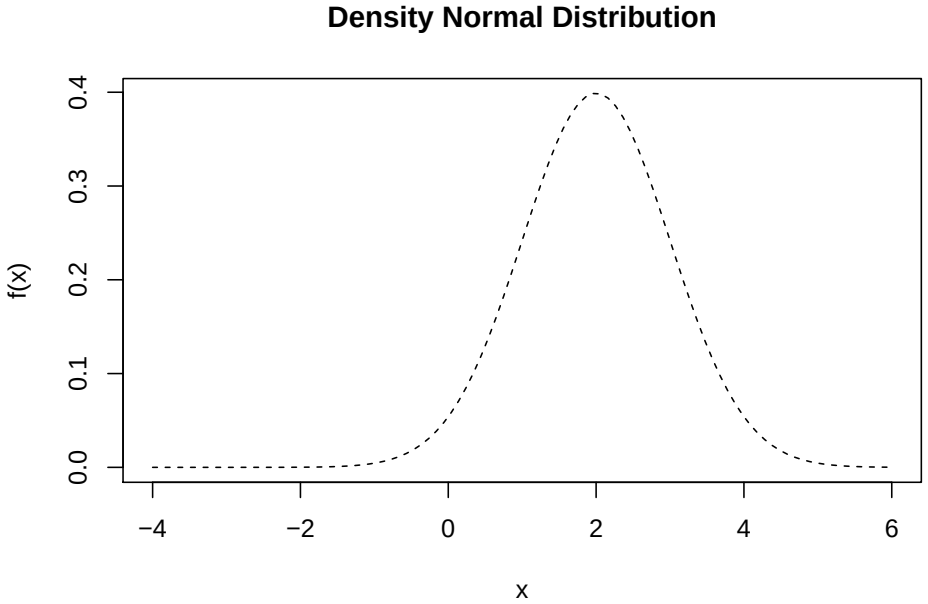
1.3.1 Univariate normal distribution:

$$\text{Dimension } d = 1$$
$$x \sim N(\mu, \sigma^2)$$
$$\mathrm{E}(x) = \mu, \mathrm{Var}(x) = \sigma^2$$

Density:

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

Plot of univariate normal density :
- Unimodal with peak at μ, the width is determined by σ (in this plot: $\mu = 2, \sigma = 1$)



Special case: **standard normal** with $\mu = 0$ and $\sigma^2 = 1$:

$$f(x|\mu = 0, \sigma^2 = 1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

Maximum entropy characterisation: the normal distribution is the unique distribution that has the highest (differential) entropy over all continuous distributions with support from minus infinity to plus infinity with a given mean and variance.

This is in fact one of the reasons why the normal distribution is so important (und useful) – if we only know that a random variable has a mean and variance, and not much else, then using the normal distribution will be a reasonable and well justified working assumption!

1.3.2 Multivariate normal model

$$\text{Dimension } d$$
$$\boldsymbol{x} \sim N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
$$\boldsymbol{x} \sim \text{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
$$\text{E}(\boldsymbol{x}) = \boldsymbol{\mu}, \text{Var}(\boldsymbol{x}) = \boldsymbol{\Sigma}$$

Density:

$$f(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{d}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(\underbrace{-\frac{1}{2} \underbrace{(\boldsymbol{x}-\boldsymbol{\mu})^T}_{1\times d} \underbrace{\boldsymbol{\Sigma}^{-1}}_{d\times d} \underbrace{(\boldsymbol{x}-\boldsymbol{\mu})}_{d\times 1}}_{1\times 1=\text{scalar!}} \right)$$

- note that density contains precision matrix $\boldsymbol{\Sigma}^{-1}$
- inverting $\boldsymbol{\Sigma}$ implies inverting the eigenvalues λ_i of $\boldsymbol{\Sigma}$ (thus we need $\lambda_i > 0$)
- density also contains $\det(\boldsymbol{\Sigma}) = \prod_{i=1}^{d} \lambda_i \equiv$ product of eigenvalues of $\boldsymbol{\Sigma}$

Special case: **standard multivariate normal** with

$$\boldsymbol{\mu} = \boldsymbol{0}, \boldsymbol{\Sigma} = \boldsymbol{I} = \begin{pmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{pmatrix}$$

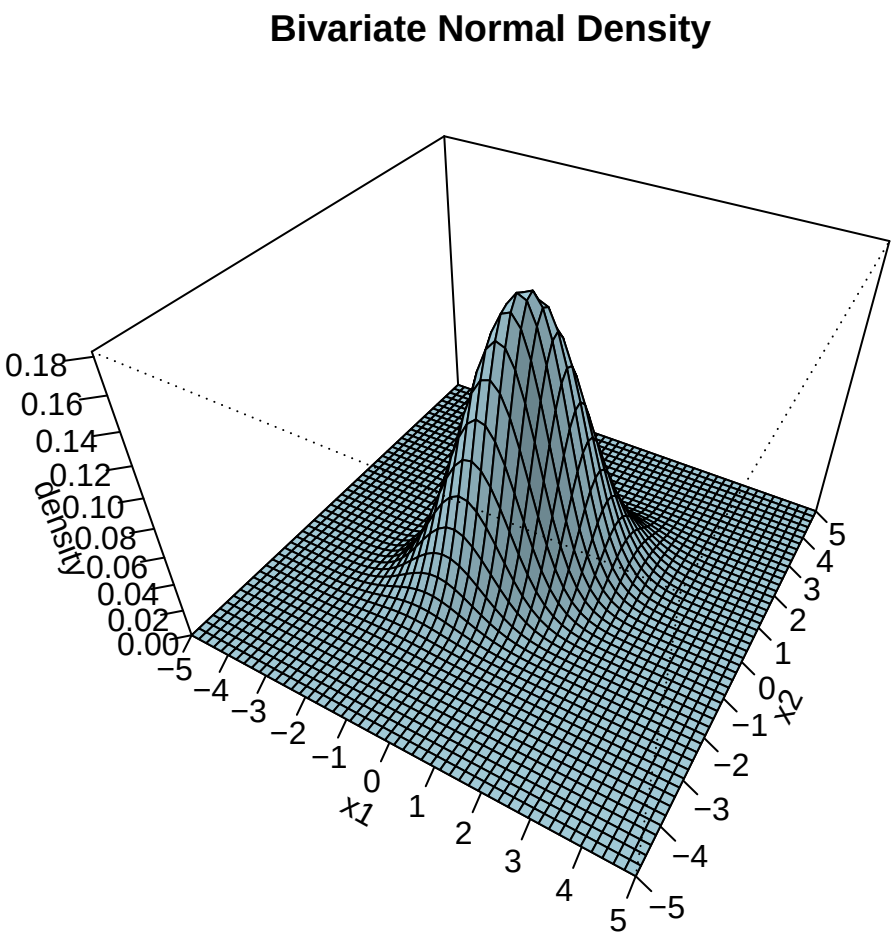
$$f(\boldsymbol{x}|\boldsymbol{\mu} = \boldsymbol{0}, \boldsymbol{\Sigma} = \boldsymbol{I}) = (2\pi)^{-d/2} \exp\left(-\frac{1}{2}\boldsymbol{x}^T\boldsymbol{x}\right) = \prod_{i=1}^{d} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x_i^2}{2}\right)$$

which is equivalent to the product of d univariate standard normals!

Misc:

- for $d = 1$, multivariate normal reduces to normal.
- for $\boldsymbol{\Sigma}$ diagonal (i.e. $\boldsymbol{P} = \boldsymbol{I}$, no correlation), MVN is the product of univariate normals (see Worksheet 2).

Plot of MVN density:



- Location: $\boldsymbol{\mu}$
- Shape: $\boldsymbol{\Sigma}$
- Unimodal: **one** peak
- Support from $-\infty$ to $+\infty$ in each dimension

You can find an interactive R Shiny web app of the bivariate normal density online at https://minerva.it.manchester.ac.uk/shiny/strimmer/bvn/ .

1.3.3 Shape of the contour lines of the multivariate normal density

Now show that the contour lines of the multivariate normal density always take on the form of an ellipse, and that the radii of the ellipse is determined by the eigenvalues of $\boldsymbol{\Sigma}$.

We start by observing that a circle with radius r around the origin can be

described as the set of points (x_1, x_2) satisfying $x_1^2 + x_2^2 = r^2$, or equivalently, $\frac{x_1^2}{r^2} + \frac{x_2^2}{r^2} = 1$. This is generalised to the shape of an ellipse by allowing (in two dimensions) for two radii r_1 and r_2 with $\frac{x_1^2}{r_1^2} + \frac{x_2^2}{r_2^2} = 1$, or in vector notation $\boldsymbol{x}^T \text{Diag}(r_1^2, r_2^2)^{-1} \boldsymbol{x} = 1$. In d dimensions and allowing for rotation of the axes and a shift of the origin from 0 to $\boldsymbol{\mu}$ the condition for an ellipse is

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{Q} \, \text{Diag}(r_1^2, \ldots, r_d^2)^{-1} \boldsymbol{Q}^T (\boldsymbol{x} - \boldsymbol{\mu}) = 1$$

where $\boldsymbol{Q}$ is an orthogonal rotation matrix.

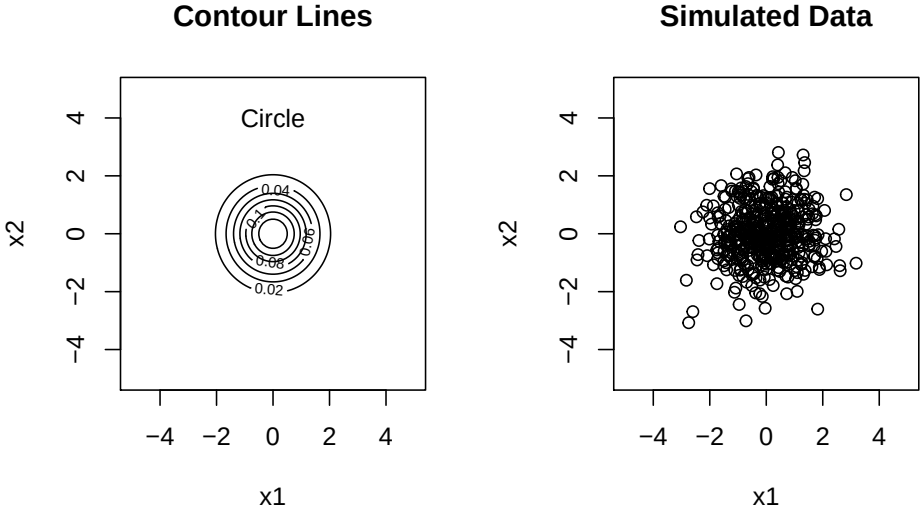
A contour line of a probability density function is a set of connected points where the density assumes the same constant value. In the case of the multivariate normal distribution keeping the density at some fixed value implies that $(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) = c$ where c is a constant. Using the eigenvalue decomposition of $\boldsymbol{\Sigma} = \boldsymbol{U} \boldsymbol{\Lambda} \boldsymbol{U}^T$ we can rewrite this condition as

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{U} \boldsymbol{\Lambda}^{-1} \boldsymbol{U}^T (\boldsymbol{x} - \boldsymbol{\mu}) = c \, .$$

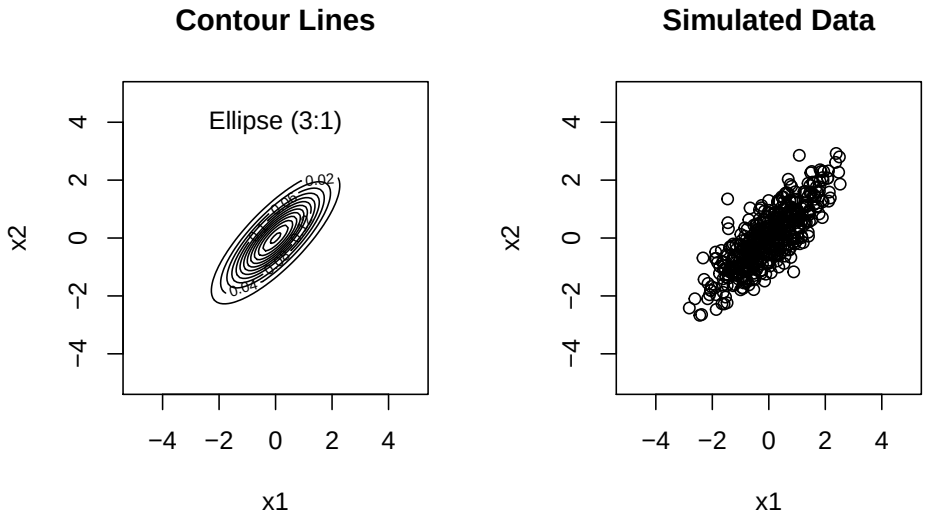
This implies that contour lines of the multivariate normal density are indeed ellipses and that the squared radii are proportional to the eigenvalues of $\boldsymbol{\Sigma}$. Equivalently, the positive square roots of the eigenvalues are proportional to the radii of the ellipse. Hence, for singular covariance matrix with one or more $\lambda_i = 0$ the corresponding radii are zero.

Two examples:

Case 1: No Correlation / Diagonal / Isotropic / Spherical Covariance $\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ with $\sqrt{\lambda_1 / \lambda_2} = 1$:



Case 2: with correlation $\Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$ with $\sqrt{\lambda_1/\lambda_2} = 3$:



Small λ_i indicates collinearity!

1.4 Estimation in large sample and small sample settings

In practical application of multivariate normal model we need to learn its parameters from data. We first consider the case when there are many measurements available, and then second the case when the number of data points is small compared to the number of parameters.

In a previous course in year 2 ("Statistical Methods" MATH20802) the method of maximum likelihood
as well as essential of Bayesian statistics were introduced. Here we apply these approaches in the setting of the multivariate normal distribution.

1.4.1 Multivariate data

Vector notation:

Samples from a multivariate normal distribution are *vectors* (not scalars as for univariate normal):

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n \overset{\text{iid}}{\sim} N_d\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$$

Matrix and component notation:

All the data points are commonly collected into a matrix $\boldsymbol{X}$.

In statistics the convention is to store each data vector in the rows of $\boldsymbol{X}$:

$$\boldsymbol{X} = (\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n)^T = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & & & \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{pmatrix}$$

Therefore,

$$\boldsymbol{x}_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1d} \end{pmatrix}, \boldsymbol{x}_2 = \begin{pmatrix} x_{21} \\ \vdots \\ x_{2d} \end{pmatrix}, \dots, \boldsymbol{x}_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{nd} \end{pmatrix}$$

Thus, in statistics the first index runs over $(1, ..., n)$ and denotes the samples while the second index runs over $(1, ..., d)$ and refers to the variables.

The statistics convention on data matrices is *not* universal! In fact, in most of the machine learning literature in engineering and computer science the data samples are stored in the columns so that the variables appear in the rows (thus in the engineering convention the data matrix is transposed compared to the statistics convention).

In order to avoid confusion it is recommended to use vector notation for data instead of matrix notation because this is not ambiguous.

1.4.2 Strategies for large sample estimation

1.4.2.1 Empirical estimators (outline)

For large n we have thanks to the law of large numbers:

$$\underbrace{F}_{\text{true}} \approx \underbrace{\widehat{F}}_{\text{empirical}}$$

We now would like to estimate A which is a functional of F, i.e. $A = m(F)$. For example the mean, the median or some other quantity.

The *empirical estimate* is obtained by replacing the unknown true distribution F with the observed empirical distribution: $\hat{A} = m(\widehat{F})$.

For example, the expectation of a random variable is approximated/estimated as the average over the observation:

$$\mathrm{E}_F(\boldsymbol{x}) \approx \mathrm{E}_{\widehat{F}}(\boldsymbol{x}) = \frac{1}{n} \sum_{k=1}^{n} \boldsymbol{x}_k$$

$$\mathrm{E}_F(g(\boldsymbol{x})) \approx \mathrm{E}_{\widehat{F}}(g(\boldsymbol{x})) = \frac{1}{n} \sum_{k=1}^{n} g(\boldsymbol{x}_k)$$

Simple recipe to obtain an empirical estimator: simply replace the expectation operator by the sample average in the quantity of interest.

What does this work: the empirical distribution $\widehat{F}$ is actually the nonparametric maximum likelihood estimate of F (see below for likelihood estimation).

Note: the approximation of F by $\widehat{F}$ also the basis other approaches such as Efron's bootstrap method.

1.4.2.2 Maximum likelihood estimation (outline)

R.A. Fisher (1922): model-based estimators using the density or probability mass function

log-likelihood function:

$$\log L(\boldsymbol{\theta}) = \sum_{k=1}^{n} \underbrace{\log f}_{\text{log-density}} \; (\underbrace{x_i}_{\text{data}} \mid \underbrace{\boldsymbol{\theta}}_{\text{parameters}})$$

likelihood = probability to observe data given the model parameters

Maximum likelihood estimate:

$$\hat{\boldsymbol{\theta}}^{\text{ML}} = \arg\max_{\boldsymbol{\theta}} \log L(\boldsymbol{\theta})$$

Maximum likelihood (ML) finds the parameters that make the observed data most likely (it does *not* find the most probable model!)

Recall from MATH20802 that maximum likelihood is closely linked to minimising the relative entropy (KL divergence) $I^{KL}(F, F_{\boldsymbol{\theta}})$ between the unknown true model F to the specified model $F_{\boldsymbol{\theta}}$. Specifically, for large sample size n the model $F_{\hat{\boldsymbol{\theta}}}$ fit by maximum likelihood is indeed the model that is closest to F.

Correspondingly, the great appeal of **maximum likelihood estimates** (MLEs) is that they **are optimal for large n**, i.e. so that **for large sample size no estimator can be constructed that outperforms the MLE** (note the emphasis on "for large n"!). A further advantage of the method of maximum likelihood is that it does not only provide a point estimate but also the asymptotic error (via the Fisher information which is related to the curvature of the log-likelihood function).

1.4.3 Large sample estimates of mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$

1.4.3.1 Empirical estimates:

Recall the definitions:

$$\boldsymbol{\mu} = \mathrm{E}(\boldsymbol{x})$$

and

$$\boldsymbol{\Sigma} = \mathrm{E}\left((\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T \right)$$

For the empirical estimate we replace the expectations by the corresponding sample averages.

These resulting estimators can be written in three different ways:

Vector notation:

$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{k=1}^{n} \boldsymbol{x}_k$$

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{k=1}^{n}(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})^T = \frac{1}{n}\sum_{k=1}^{n}\boldsymbol{x}_k\boldsymbol{x}_k^T - \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}^T$$

Data matrix notation:

The empirical mean and covariance can also be written in terms of the data matrix $\boldsymbol{X}$ (using statistics convention):

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\boldsymbol{X}^T\mathbf{1}_n$$

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} - \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}^T$$

See Worksheet 2 for details.

Component notation:

The corresponding component notation with $\boldsymbol{X} = (x_{ki})$ is:

$$\hat{\mu}_i = \frac{1}{n}\sum_{k=1}^{n}x_{ki}$$

$$\hat{\sigma}_{ij} = \frac{1}{n}\sum_{k=1}^{n}(x_{ki} - \hat{\mu}_i)(x_{kj} - \hat{\mu}_j)$$

$$\hat{\boldsymbol{\mu}} = \begin{pmatrix}\hat{\mu}_1\\ \vdots \\ \hat{\mu}_d\end{pmatrix}, \widehat{\boldsymbol{\Sigma}} = (\hat{\sigma}_{ij})$$

Variance estimate:

$$\hat{\sigma}_{ii} = \frac{1}{n}\sum_{k=1}^{n}(x_{ki} - \hat{\mu}_i)^2$$

Note the factor $\frac{1}{n}$ (not $\frac{1}{n-1}$)

Engineering and machine learning convention:

Using the engineering and machine learning convention for the data matrix $\boldsymbol{X}$ the estimators are written as

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\boldsymbol{X}\mathbf{1}_n$$

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n}\boldsymbol{X}\boldsymbol{X}^T - \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}^T$$

In the corresponding component notation the two indices for the columns and rowns are interchanged.

To avoid confusion when using matrix or component notation you need to always state which convention is used! In these notes we strictly follow the statistics convention.

1.4.3.2 Maximum likelihood estimates

We now derive the MLE of the parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ of the multivariate normal distribution. The corresponding log-likelihood function is

$$\begin{aligned}\log L(\boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \sum_{k=1}^{n} \log f(\boldsymbol{x}_k|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\ &= -\frac{nd}{2}\log(2\pi) - \frac{n}{2}\log\det(\boldsymbol{\Sigma}) - \frac{1}{2}\sum_{k=1}^{n}(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}_k - \boldsymbol{\mu})\,.\end{aligned}$$

Written in terms of the precision matrix $\boldsymbol{\Omega} = \boldsymbol{\Sigma}^{-1}$ this becomes

$$\log L(\boldsymbol{\mu}, \boldsymbol{\Omega}) = -\frac{nd}{2}\log(2\pi) + \frac{n}{2}\log\det(\boldsymbol{\Omega}) - \frac{1}{2}\sum_{k=1}^{n}(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Omega}(\boldsymbol{x}_k - \boldsymbol{\mu})\,.$$

Exploiting identities for the trace and log det (see Appendix) we can rewrite $(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Omega}(\boldsymbol{x}_k - \boldsymbol{\mu}) = \mathrm{Tr}((\boldsymbol{x}_k - \boldsymbol{\mu})(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Omega})$ and $\log\det(\boldsymbol{\Omega}) = \mathrm{Tr}(\log\boldsymbol{\Omega})$ we rewrite the log-likelihood as

$$\log L(\boldsymbol{\mu}, \boldsymbol{\Omega}) = -\frac{nd}{2}\log(2\pi) + \frac{n}{2}\mathrm{Tr}(\log\boldsymbol{\Omega}) - \frac{1}{2}\sum_{k=1}^{n}\mathrm{Tr}((\boldsymbol{x}_k - \boldsymbol{\mu})(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Omega})\,.$$

First, to find the MLE for $\boldsymbol{\mu}$ we compute (see Appendix for some rules in vector and matrix calculus)

$$\frac{\partial \log L(\boldsymbol{\mu}, \boldsymbol{\Omega})}{\partial \boldsymbol{\mu}} = \sum_{k=1}^{n}(\boldsymbol{x}_k - \boldsymbol{\mu})^T\boldsymbol{\Omega}\,.$$

Setting this equal to zero we get $\sum_{k=1}^{n}\boldsymbol{x}_k = n\hat{\boldsymbol{\mu}}_{ML}$ and thus

$$\hat{\boldsymbol{\mu}}_{ML} = \frac{1}{n}\sum_{k=1}^{n}\boldsymbol{x}_k\,.$$

Next, to obtain the MLE for $\boldsymbol{\Omega}$ we compute

$$\frac{\partial \log L(\boldsymbol{\mu}, \boldsymbol{\Omega})}{\partial \boldsymbol{\Omega}} = \frac{n}{2}\boldsymbol{\Omega}^{-1} - \frac{1}{2}\sum_{k=1}^{n}(\boldsymbol{x}_k - \boldsymbol{\mu})(\boldsymbol{x}_k - \boldsymbol{\mu})^T\,.$$

Setting this equal to zero and substituting the MLE for $\boldsymbol{\mu}$ we get

$$\widehat{\boldsymbol{\Omega}}_{ML}^{-1} = \frac{1}{n}\sum_{k=1}^{n}(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})^T = \widehat{\boldsymbol{\Sigma}}_{ML}\,.$$

Therefore, the MLEs are identical to the empirical estimates.

Note the factor $\frac{1}{n}$ in the MLE of the covariance matrix.

1.4.3.3 Distribution of the empirical / maximum likelihood estimates

With $\boldsymbol{x}_1, ..., \boldsymbol{x}_n \sim N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ one can find the exact distributions of the estimators.

1. Distribution of the estimate of the mean:

$$\hat{\boldsymbol{\mu}}_{ML} \sim N_d\left(\boldsymbol{\mu}, \frac{\boldsymbol{\Sigma}}{n}\right)$$

Since $\mathrm{E}(\hat{\boldsymbol{\mu}}_{ML}) = \boldsymbol{\mu} \Longrightarrow \hat{\boldsymbol{\mu}}_{ML}$ is unbiased.

2. Distribution of the covariance estimate:

$$\widehat{\boldsymbol{\Sigma}}_{ML} \sim \text{Wishart}(\frac{\boldsymbol{\Sigma}}{n}, n-1)$$

Since $\mathrm{E}(\widehat{\boldsymbol{\Sigma}}_{ML}) = \frac{n-1}{n}\boldsymbol{\Sigma} \Longrightarrow \widehat{\boldsymbol{\Sigma}}_{ML}$ is biased, with $\text{Bias}(\widehat{\boldsymbol{\Sigma}}_{ML}) = \boldsymbol{\Sigma} - \mathrm{E}(\widehat{\boldsymbol{\Sigma}}_{ML}) = -\frac{\boldsymbol{\Sigma}}{n}$.

Easy to make unbiased: $\widehat{\boldsymbol{\Sigma}}_{UB} = \frac{n}{n-1}\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-1}\sum_{k=1}^{n}(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_k - \hat{\boldsymbol{\mu}})^T$ is unbiased.

But unbiasedness of an estimator is **not** a very relevant criterion in multivariate statistics as we will see in the next section.

1.4.4 Problems with maximum likelihood in small sample settings and high dimensions

Modern data is high dimensional!

Data sets with $n < d$, i.e. high dimension d and small sample size n are now common in many fields, e.g., medicine, biology but also finance and business analytics.

$$n = 100 \,(\text{e.g, patients/samples})$$
$$d = 20000 \,(\text{e.g., genes/SNPs/proteins/variables})$$

Reasons:

- the number of measured variables is increasing quickly with technological advances (e.g. genomics)
- but the number of samples cannot be similary increased (for cost and ethical reasons)

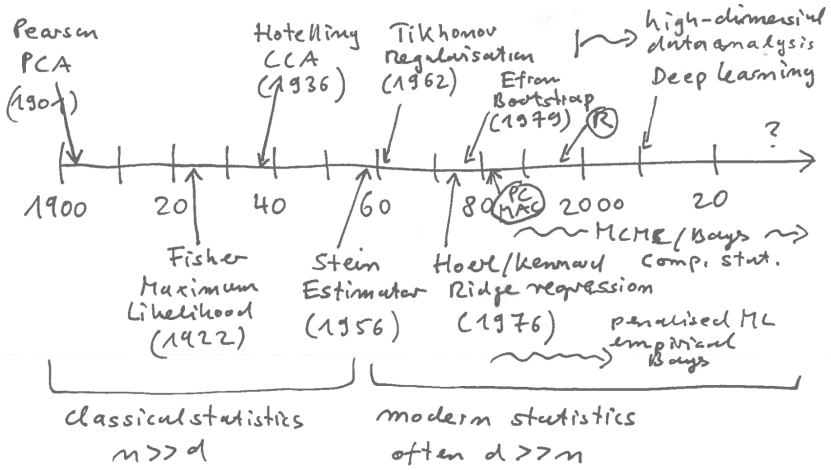
General problems of MLEs:

1. ML estimators are optimal only if **sample size is large** compared to the number of parameters. However, this optimality is not any more valid if sample size is moderate or smaller than the number of parameters.
2. If there is not enough data the **ML estimate overfits**. This means ML fits the current data perfectly but the resulting model does not generalise well (i.e. model will perform poorly in prediction)
3. If there is a choice between different models with different complexity **ML will always select the model with the largest number of parameters**.

-> for high-dimensional data with small sample size maximum likelihood estimation does not work!!!

History of Statistics:

Much of modern statistics (from 1960 onwards) is devoted to the development of inference and estimation techniques that work with complex, high-dimensional data.



- Maximum likelihood is a method from classical statistics (time up to about 1960).
- From 1960 modern (computational) statistics emerges, starting with **"Stein Paradox" (1956):** Charles Stein showed that in a **multivariate setting** ML estimators are **dominated by** (= are always worse than) shrinkage estimators!
- For example, there is a shrinkage estimator for the mean that is better (in terms of MSE) than the average (which is the MLE)!

Modern statistics has developed many different (but related) methods for use in high-dimensional, small sample settings:

- regularised estimators
- shrinkage estimators
- penalised maximum likelihood estimators
- Bayesian estimators
- Empirical Bayes estimators
- KL / entropy-based estimators

Most of this is out of scope for our class, but will be covered in advanced statistical courses.

Next, we describe a **simple regularised estimator for the estimation of the covariance** that we will use later (i.e. in classification).

1.4.5 Estimation of covariance matrix in small sample settings

Problems with ML estimate of Σ

1. Σ has $O(d^2)$ number of parameters! $\implies \hat{\boldsymbol{\Sigma}}^{\text{MLE}}$ requires *a lot* of data! $n \gg d$ or d^2
2. if $n < d$ then $\hat{\boldsymbol{\Sigma}}$ is positive **semi**-definite (even if Σ is p.d.f.!)
   $\implies \hat{\boldsymbol{\Sigma}}$ will have **vanishing eigenvalues** (some $\lambda_i = 0$) and thus **cannot be inverted** and is singular!

Simple regularised estimate of Σ

Regularised estimator $\boldsymbol{S}^*$ = convex combination of $\boldsymbol{S} = \hat{\boldsymbol{\Sigma}}^{\text{MLE}}$ and $\boldsymbol{I}_d$ (identity matrix) to get

Regularisation:

$$\underbrace{\boldsymbol{S}^*}_{\text{regularised estimate}} = \underbrace{\lambda}_{\text{shrinkage intensity}} \underbrace{\boldsymbol{I}_d}_{\text{target}} + (1-\lambda) \underbrace{\boldsymbol{S}}_{\text{ML estimate}}$$

Next, choose $\lambda \in [0,1]$ such that $\boldsymbol{S}^*$ is better (in terms of MSE) than both $\boldsymbol{S}$ and $\boldsymbol{I}_d$.

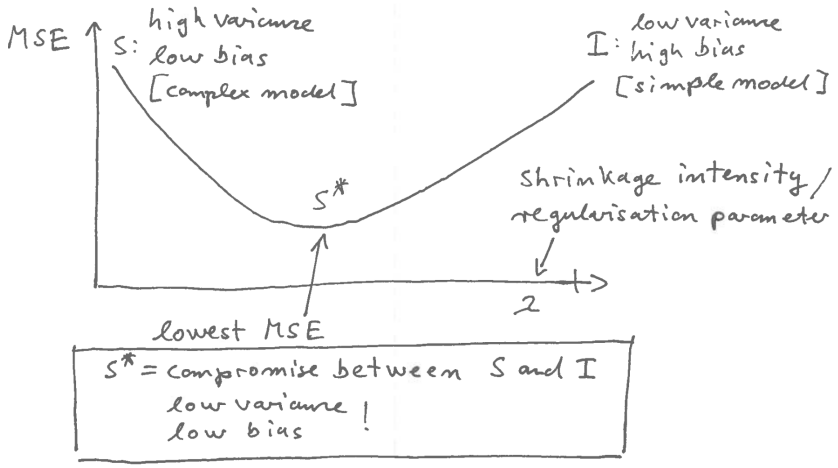
Bias-variance trade-off

MSE is the Mean Squared Error, composed of squared bias and variance.

$$\text{MSE}(\theta) = \text{E}((\hat{\theta} - \theta)^2) = \text{Bias}(\hat{\theta})^2 + \text{Var}(\hat{\theta})$$

with $\text{Bias}(\hat{\theta}) = \text{E}(\hat{\theta}) - \theta$

$\boldsymbol{S}$: ML estimate, many parameters, low bias, high variance
$\boldsymbol{I}_d$: "target", no parameters, high bias, low variance
$\implies$ **reduce high variance of $\boldsymbol{S}$ by *introducing* a bit of bias through $\boldsymbol{I}_d$!**
$\implies$ overall, MSE is decreased



How to find optimal shrinkage / regularisation parameter λ? Minimise MSE!

Challenge: since we don't know the true $\boldsymbol{\Sigma}$ we cannot actually compute the MSE directly but have to estimate it! How is this done in practise?

- by cross-validation (=resampling procedure)
- by using some analytic approximation (e.g. Stein's formula)

Why does regularisation of $\hat{\boldsymbol{\Sigma}}$ work?

1. $\boldsymbol{S}^*$ is **positive definite**:
   Matrix Theory:

$$\underbrace{\boldsymbol{M}_1}_{\text{symmetric positive definite, } \lambda \boldsymbol{I}} + \underbrace{\boldsymbol{M}_2}_{\text{symmetric positive semi-definite, } (1-\lambda)\boldsymbol{S}} = \underbrace{\boldsymbol{M}_3}_{\text{symmetric positive definite, } \boldsymbol{S}^*}$$

   $\Longrightarrow \boldsymbol{S}^*$ can be inverted even if $n < d$

(see Appendix A for details).

2. It's **Bayesian** in disguise!

$$\underbrace{\boldsymbol{S}^*}_{\text{posterior mean}} = \underbrace{\lambda \boldsymbol{I}_d}_{\text{prior information}} + (1-\lambda) \underbrace{\boldsymbol{S}}_{\text{data summarised by maximum likelihood}}$$

   - Prior information helps to infer $\boldsymbol{\Sigma}$ even in small samples
   - Since λ is chosen from data, it is actually an empirical Bayes.
   - also called shrinkage estimator since the off-diagonal entries are shrunk towards zero
   - this type of linear shrinkage/regularisation is natural for models in the exponential family (Diaconis and Ylvisaker, 1979)

In Worksheet 2 the empirical estimator of covariance is compared with the covariance estimator implemented in the R package "corpcor". This uses a regularisation similar as above (but for the correlation rather than covariance matrix) and it employs an analytic data-adaptive estimate of the shrinkage intensity λ. This estimator is a variant of an empirical Bayes / James-Stein estimator (see the year 2 Statistical Methods 20802 module).

Summary

- In multivariate statistics, it is useful (and often necessary) to utilise prior information!
- Regularisation introduces bias and reduces variance, minimising overall MSE
- Unbiased estimation (a highly valued property in classical statistics!) is not a good idea in multivariate settings and often leads to poor estimators.

1.5 Discrete multivariate distributions

Most univariate distributions have multivariate counterparts. Here are some of the most important ones. First we discuss discrete distributions, then later continuous distributions.

1.5.1 Categorical distribution

1.5.1.1 Univariate case

Bernoulli distribution (=coin tossing model)

$$x \sim \text{Ber}(\pi)$$

$$x \in \{0, 1\}$$

$$\pi \in [0, 1]$$

$$\text{Pr}(x = 1) = \pi$$

$$\text{Pr}(x = 0) = 1 - \pi$$

$$\text{E}(x) = \pi$$

$$\text{Var}(x) = \pi(1 - \pi)$$

1.5.1.2 Multivariate case

$$\boldsymbol{x} \sim \text{Categ}(\boldsymbol{\pi})$$

$$\boldsymbol{x} = (x_1, ..., x_d)^T;\ x_i \in \{0, 1\};\ \sum_{i=1}^{d} x_i = 1$$

$$\boldsymbol{\pi} = (\pi_1, ..., \pi_d)^T;\ \sum_{i=1}^{d} \pi_i = 1$$

$$\text{Pr}(x_i = 1) = \pi_i$$

$$\text{Pr}(x_i = 0) = 1 - \pi_i$$

$$\text{E}(\boldsymbol{x}) = \boldsymbol{\pi}$$

$$\text{Var}(x_i) = \pi_i(1 - \pi_i)$$

$$\text{Cov}(x_i, x_j) = -\pi_i \pi_j$$

1.5.2 Multinomial distribution

1.5.2.1 Univariate case

Binomial Distribution

Repeat Bernoulli experiment r times

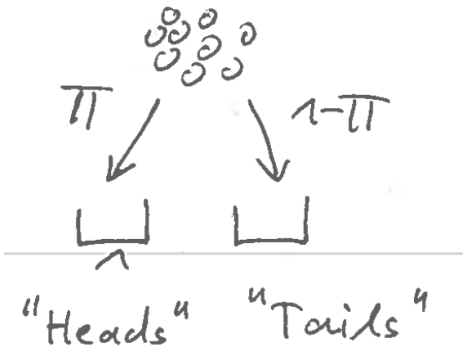
$$x \sim \text{Binom}(\pi, r)$$
$$x \in \{0, ..., r\}$$
$$\text{E}(x) = r\,\pi$$
$$\text{Var}(x) = r\,\pi(1-\pi)$$

Standardised to unit interval:

$$\frac{x}{r} \in \left\{0, \frac{1}{r}, ..., 1\right\}$$
$$\text{E}\left(\frac{x}{r}\right) = \pi$$
$$\text{Var}\left(\frac{x}{r}\right) = \frac{\pi(1-\pi)}{r}$$

Urn model:

distribute r balls into two bins



1.5.2.2 Multivariate case

Multinomial distribution

Draw r times from categorical distribution

$$\boldsymbol{x} \sim Multinom(\boldsymbol{\pi}, r)$$
$$x_i \in \{0, 1, ..., r\};\ \sum_{i=1}^{d} x_i = r$$

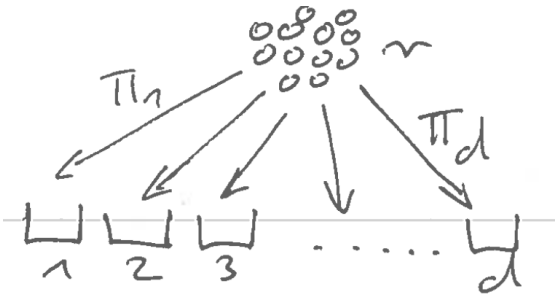
$$\mathrm{E}(\boldsymbol{x}) = r\,\boldsymbol{\pi}$$
$$\mathrm{Var}(x_i) = r\,\pi_i(1-\pi_i)$$
$$\mathrm{Cov}(x_i, x_j) = -r\,\pi_i\pi_j$$

Standardised to unit interval:

$$\frac{x_i}{r} \in \left\{0, \frac{1}{r}, \frac{2}{r}, ..., 1\right\}$$
$$\mathrm{E}\left(\frac{\boldsymbol{x}}{r}\right) = \boldsymbol{\pi}$$
$$\mathrm{Var}\left(\frac{x_i}{r}\right) = \frac{\pi_i(1-\pi_i)}{r}$$
$$\mathrm{Cov}\left(\frac{x_i}{r}, \frac{x_j}{r}\right) = -\frac{\pi_i\pi_j}{r}$$

Urn model:

distribute r balls into d bins



1.6 Continuous multivariate distributions

1.6.1 Dirichlet distribution

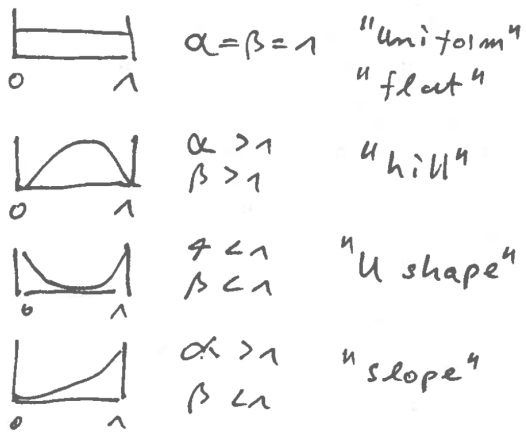
1.6.1.1 Univariate case

Beta distribution

$$x \sim \mathrm{Beta}(\alpha, \beta)$$
$$x \in [0, 1]$$
$$\alpha > 0; \beta > 0$$
$$m = \alpha + \beta$$
$$\mu = \frac{\alpha}{m} \in [0, 1]$$
$$\mathrm{E}(x) = \mu$$
$$\mathrm{Var}(x) = \frac{\mu(1-\mu)}{m+1}$$

compare with unit standardised binomial!

Different shapes



Useful as distribution for a proportion π

Bayesian Model:

Beta prior: $\pi \sim Beta(\alpha, \beta)$

Binomial likelihood: $x|\pi \sim Binom$

1.6.1.2 Multivariate case

Dirichlet distribution

$$\boldsymbol{x} \sim \text{Dirichlet}(\boldsymbol{\alpha})$$

$$x_i \in [0,1]; \sum_{i=1}^{d} x_i = 1$$

$$\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_d)^T > 0$$

$$m = \sum_{i=1}^{d} \alpha_i$$

$$\mu_i = \frac{\alpha_i}{m} \in [0,1]$$

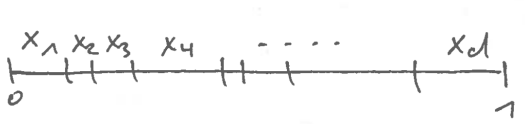
$$\text{E}(x_i) = \mu_i$$

$$\text{Var}(x_i) = \frac{\mu_i(1-\mu_i)}{m+1}$$

$$\text{Cov}(x_i, x_j) = -\frac{\mu_i \mu_j}{m+1}$$

compare with unit standardised multinomial!

Stick breaking" model



Useful as distribution for a proportion $\boldsymbol{\pi}$

Bayesian Model:

Dirichlet prior: $\boldsymbol{\pi} \sim Dirichlet(\boldsymbol{\alpha})$

Multinomial likelihood: $\boldsymbol{x}|\boldsymbol{\pi} \sim Multinom$

1.6.2 Wishart distribution

This multivariate distribution generalises the univariate scaled χ^2 distribution (also known as Gamma distribution).

1.6.2.1 Univariate case

Scaled χ^2 distribution (=Gamma distribution, see below)

$$z_1, z_2, \ldots, z_m \overset{\text{iid}}{\sim} N(0, \sigma^2)$$

$$x = \sum_{i=1}^{m} z_i^2$$

$$x \sim \sigma^2 \chi^2_m = \mathrm{W}_1(\sigma^2, m)$$

$$\mathrm{E}(x) = m\,\sigma^2$$

$$\mathrm{Var}(x) = m\,2\sigma^4$$

Useful as the distribution of sample variance:

$$y_1, \ldots, y_n \sim N(\mu, \sigma^2)$$

Known mean μ:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \mu)^2 \sim \mathrm{W}_1\left(\frac{\sigma^2}{n}, n\right)$$

Unknown mean μ (estimated by $\bar{y}$):

$$\widehat{\sigma^2}_{ML} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2 \sim \mathrm{W}_1\left(\frac{\sigma^2}{n}, n-1\right)$$

$$\widehat{\sigma^2}_{UB} = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2 \sim \mathrm{W}_1\left(\frac{\sigma^2}{n-1}, n-1\right)$$

1.6.2.2 Multivariate case

Wishart distribution

$$z_1, z_2, \ldots, z_m \overset{\text{iid}}{\sim} N_d(0, \boldsymbol{\Sigma})$$
$$\underbrace{\boldsymbol{X}}_{d\times d} = \sum_{i=1}^{m} \underbrace{z_i z_i^T}_{d\times d}$$

Note that $\boldsymbol{X}$ is a *matrix*!

$$\boldsymbol{X} \sim \mathrm{W}_d(\boldsymbol{\Sigma}, m)$$
$$\mathrm{E}(\boldsymbol{X}) = m\boldsymbol{\Sigma}$$
$$\mathrm{Var}(x_{ij}) = m\left(\sigma_{ij}^2 + \sigma_{ii}\sigma_{jj}\right)$$

Useful as distribution of sample covariance:

$$\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n \sim N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
$$\frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{y}_i - \boldsymbol{\mu})(\boldsymbol{y}_i - \boldsymbol{\mu})^T \sim \mathrm{W}_d(\boldsymbol{\Sigma}/n, n)$$
$$\widehat{\boldsymbol{\Sigma}}_{ML} = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{y}_i - \bar{\boldsymbol{y}})(\boldsymbol{y}_i - \bar{\boldsymbol{y}})^T \sim \mathrm{W}_d(\boldsymbol{\Sigma}/n, n-1)$$
$$\widehat{\boldsymbol{\Sigma}}_{UB} = \frac{1}{n-1}\sum_{i=1}^{n}(\boldsymbol{y}_i - \bar{\boldsymbol{y}})(\boldsymbol{y}_i - \bar{\boldsymbol{y}})^T \sim \mathrm{W}_d(\boldsymbol{\Sigma}/(n-1), n-1)$$

1.6.2.3 Relationship to Gamma distribution

The scaled χ^2 distribution (=one-dimensional Wishart distribution) with parameters σ^2 and m is in fact a reparameterised **Gamma distribution** with shape parameter α and scale parameter β:

$$\mathrm{Gamma}\left(\underbrace{\frac{m}{2}}_{\text{shape}}, \underbrace{2\sigma^2}_{\text{scale}}\right) = \sigma^2\chi_m^2 = \mathrm{W}_1(\sigma^2, m)$$

or, equivalently ($m = 2\alpha$, $\sigma^2 = \beta/2$)

$$\mathrm{Gamma}\left(\underbrace{\alpha}_{\text{shape}}, \underbrace{\beta}_{\text{scale}}\right) = \frac{\beta}{2}\chi_{2\alpha}^2 = \mathrm{W}_1(\frac{\beta}{2}, 2\alpha)$$

The mean of the Gamma distribution is $\mathrm{E}(x) = \alpha\beta = \mu$ and the variance is $\mathrm{Var}(x) = \alpha\beta^2 = \mu^2/\alpha$.

The **exponential distribution** with rate parameter λ is a special case of the Gamma distribution with $\alpha = 1$:

$$\text{Exp}(\lambda) = \text{Gamma}(1, \frac{1}{\lambda}) = \frac{1}{2\lambda}\chi^2_2 = \text{W}_1(\frac{1}{2\lambda}, 2)$$

The corresponding mean is $1/\lambda = \mu$ and variance $1/\lambda^2 = \mu^2$.

1.6.3 Inverse Wishart distribution

1.6.3.1 Univariate case

Inverse χ^2 Distribution

$$x \sim \text{W}_1^{-1}(\psi, k+2) = \psi \ \text{Inv-}\chi^2_{k+2}$$

$$\text{E}(x) = \frac{\psi}{k}$$

$$\text{Var}(x) = \frac{2\psi^2}{k^2(k-2)}$$

Relationship to scaled χ^2 :

$$\frac{1}{x} \sim W_1(\psi^{-1}, k+2) = \psi^{-1}\chi^2_{k+2}$$

1.6.3.2 Multivariate case

Inverse Wishart distribution

$$\underbrace{\boldsymbol{X}}_{d\times d} \sim \text{W}_d^{-1}\left(\underbrace{\boldsymbol{\Psi}}_{d\times d}, k+d+1\right)$$

$$\text{E}(\boldsymbol{X}) = \boldsymbol{\Psi}/k$$

$$\text{Var}(x_{ij}) = \frac{2}{k^2(k-2)}\frac{(k+2)\psi_{ij} + k\,\psi_{ii}\psi_{jj}}{2k+2}$$

Relationship to Wishart:

$$\boldsymbol{X}^{-1} \sim \text{W}_d\left(\boldsymbol{\Psi}^{-1}, k+d+1\right)$$

1.6.3.3 Relationship to inverse Gamma distribution

Another way to express the univariate inverse Wishart distribution is via the **inverse Gamma distribution**:

$$IG(\underbrace{1+\frac{k}{2}}_{\text{shape }\alpha}, \underbrace{\frac{\psi}{2}}_{\text{scale }\beta}) = \psi \ \text{Inv-}\chi^2_{k+2} = \text{W}_1^{-1}(\psi, k+2)$$

or equivalently ($k = 2(\alpha - 1)$ and $\psi = 2\beta$)

$$IG(\alpha, \beta) = 2\beta \text{ Inv-}\chi^2_{2\alpha} = \text{W}_1^{-1}(2\beta, 2\alpha)$$

The mean of the inverse Gamma distribution is $\text{E}(x) = \frac{\beta}{\alpha - 1} = \mu$ the variance $\text{Var}(x) = \frac{\beta^2}{(\alpha-1)^2(\alpha-2)} = \frac{2\mu^2}{k-2}$.

The inverse of x is Gamma distributed:

$$\frac{1}{x} \sim \text{Gamma}(1 + \frac{k}{2}, 2\psi^{-1}) = \text{Gamma}(\alpha, \beta^{-1})$$

The inverse Wishart distribution is useful as conjugate distribution for Bayesian modelling of the variance, with k the sample size parameter and $\Psi = k\Sigma$ (or $\psi = k\sigma^2$).

1.6.4 Further distributions

https://en.wikipedia.org/wiki/List_of_probability_distributions

Wikipedia is a quite good source for information on distributions!

Chapter 2

Transformations and dimension reduction

Motivation: In the following we study transformations of random vectors and their distributions. These transformation are very important since they either transform simple distributions into more complex distributions or allow to simplify complex models. In machine learning invertible mappings of transformations for probability distributions are known as "normalising flows" (these play a key role e.g. in neural networks).

2.1 Linear Transformations

2.1.1 Location-scale transformation

Also known as affine transformation.

$$\boldsymbol{y} = \underbrace{\boldsymbol{a}}_{\text{location parameter}} + \underbrace{\boldsymbol{B}}_{\text{scale parameter}} \boldsymbol{x}$$

$\boldsymbol{y}$: $m \times 1$ random vector

$\boldsymbol{a}$: $m \times 1$ vector, location parameter

$\boldsymbol{B}$: $m \times d$ matrix, scale parameter , $m \geq 1$

$\boldsymbol{x}$: $d \times 1$ random vector

$$\begin{array}{l} \mathrm{E}(\boldsymbol{x}) = \boldsymbol{\mu} \\ \mathrm{Var}(\boldsymbol{x}) = \boldsymbol{\Sigma} \end{array} \implies \begin{array}{l} \mathrm{E}(\boldsymbol{y}) = \boldsymbol{a} + \boldsymbol{B}\boldsymbol{\mu} \\ \mathrm{Var}(\boldsymbol{y}) = \boldsymbol{B}\boldsymbol{\Sigma}\boldsymbol{B}^T \end{array}$$

Special cases/examples:

1. Univariate case ($d = 1, m = 1$)

- $\mathrm{E}(y) = a + b\mu$
- $\mathrm{Var}(y) = b^2\sigma^2$

2. Sum of two random univariate variables
   $y = x_1 + x_2$, i.e. $a = 0$ and $\boldsymbol{B} = (1, 1)$
   - $\mathrm{E}(x_1 + x_2) = \mu_1 + \mu_2$
   - $\mathrm{Var}(x_1 + x_2) = (1,1)\begin{pmatrix}\sigma_1^2 & \sigma_{12}\\ \sigma_{21} & \sigma_2^2\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \sigma_1^2 + \sigma_2^2 + 2\sigma_{12} = \mathrm{Var}(x_1) + \mathrm{Var}(x_2) + 2\mathrm{Cov}(x_1, x_2)$
3. $y_1 = a_1 + b_1 x_1$ and $y_2 = a_2 + b_2 x_2$, i.e. $\boldsymbol{a} = \begin{pmatrix}a_1\\a_2\end{pmatrix}$ and $\boldsymbol{B} = \begin{pmatrix}b_1 & 0\\0 & b_2\end{pmatrix}$
   - $\mathrm{E}(\boldsymbol{y}) = \begin{pmatrix}a_1 + b_1\mu_1\\a_2 + b_2\mu_2\end{pmatrix}$
   - $\mathrm{Var}(\boldsymbol{y}) = \begin{pmatrix}b_1 & 0\\0 & b_2\end{pmatrix}\begin{pmatrix}\sigma_1^2 & \sigma_{12}\\ \sigma_{21} & \sigma_2^2\end{pmatrix}\begin{pmatrix}b_1 & 0\\0 & b_2\end{pmatrix} = \begin{pmatrix}b_1^2\sigma_1^2 & b_1 b_2 \sigma_{12}\\ b_1 b_2 \sigma_{21} & b_2^2\sigma_2^2\end{pmatrix}$
     i.e. $\mathrm{Cov}(a_1 + b_1 x_1, a_2 + b_2 x_2) = b_1 b_2 \mathrm{Cov}(x_1, x_2)$

2.1.2 Invertible location-scale transformation

If $m = d$ and $\det(\boldsymbol{B}) \neq 0$ then we get an **invertible** transformation:

$$\boldsymbol{y} = \boldsymbol{a} + \boldsymbol{B}\boldsymbol{x}$$

$$\boldsymbol{x} = \boldsymbol{B}^{-1}(\boldsymbol{y} - \boldsymbol{a})$$

Transformation of density: $\boldsymbol{x} \sim F_{\boldsymbol{x}}$ with density $f_{\boldsymbol{x}}(\boldsymbol{x})$

$\implies \boldsymbol{y} \sim F_{\boldsymbol{y}}$ with density

$$f_{\boldsymbol{y}}(\boldsymbol{y}) = |\det(\boldsymbol{B})|^{-1} f_{\boldsymbol{x}}\left(\boldsymbol{B}^{-1}(\boldsymbol{y} - \boldsymbol{a})\right)$$

Example 2.1. Mahalanobis transform $\boldsymbol{y} = \boldsymbol{\Sigma}^{-1/2}(\boldsymbol{x} - \boldsymbol{\mu})$

We assume a positive definite and thus invertible $\boldsymbol{\Sigma}$, so that the inverse principal matrix square root $\boldsymbol{\Sigma}^{-1/2}$ can be computed, and the transformation itself is invertible.

$$\boldsymbol{a} = -\boldsymbol{\Sigma}^{-1/2}\boldsymbol{\mu}$$

$$\boldsymbol{B} = \boldsymbol{\Sigma}^{-1/2}$$

$$\mathrm{E}(\boldsymbol{x}) = \boldsymbol{\mu} \text{ and } \mathrm{Var}(\boldsymbol{x}) = \boldsymbol{\Sigma}$$

$$\implies \mathrm{E}(\boldsymbol{y}) = \boldsymbol{0} \text{ and } \mathrm{Var}(\boldsymbol{y}) = \boldsymbol{I}_d$$

Mahalanobis transformation performs three functions:

1. Centering ($-\boldsymbol{\mu}$)
2. Standardisation $\mathrm{Var}(y_i) = 1$
3. Decorrelation $\mathrm{Cor}(y_i, y_j) = 0$ for $i \neq j$

Univariate case ($d = 1$)

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

= centering + standardisation

The **Mahalanobis transformation** appears implicitly in many places in multivariate statistics, e.g. in the multivariate normal density.

It is a particular example of a whitening transformation (of which there are infinitely many, see later chapters).

Example 2.2. Inverse Mahalanobis transformation $\boldsymbol{y} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{x}$

This transformation is the **inverse** of the Mahalanobis transformation. As the Mahalanobis transform is a particular whitening transform the inverse transform is sometimes called the Mahalanobis colouring transformation.

$$\boldsymbol{a} = \boldsymbol{\mu}$$
$$\boldsymbol{B} = \boldsymbol{\Sigma}^{1/2}$$

$$\mathrm{E}(\boldsymbol{x}) = \boldsymbol{0} \text{ and } \mathrm{Var}(\boldsymbol{x}) = \boldsymbol{I}_d$$
$$\implies \mathrm{E}(\boldsymbol{y}) = \boldsymbol{\mu} \text{ and } \mathrm{Var}(\boldsymbol{y}) = \boldsymbol{\Sigma}$$

Assume $\boldsymbol{x}$ is multivariate standard normal $\boldsymbol{x} \sim N_d(\boldsymbol{0}, \boldsymbol{I}_d)$ with density

$$f_{\boldsymbol{x}}(\boldsymbol{x}) = (2\pi)^{-d/2} \exp\left(-\frac{1}{2}\boldsymbol{x}^T\boldsymbol{x}\right)$$

Then the density after applying this inverse Mahalanobis transform is

$$f_{\boldsymbol{y}}(\boldsymbol{y}) = |\det(\boldsymbol{\Sigma}^{1/2})|^{-1}(2\pi)^{-d/2} \exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1/2}\,\boldsymbol{\Sigma}^{-1/2}(\boldsymbol{y} - \boldsymbol{\mu})\right)$$

$$= (2\pi)^{-d/2} \det(\boldsymbol{\Sigma})^{-1/2} \exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{y} - \boldsymbol{\mu})\right)$$

$\implies \boldsymbol{y}$ has multivariate normal density!!

Application: e.g. random number generation: draw from $N_d(\boldsymbol{0}, \boldsymbol{I}_d)$ (easy!) then convert to multivariate normal by tranformation.

2.2 Nonlinear transformations

2.2.1 General transformation

$$\boldsymbol{y} = \boldsymbol{h}(\boldsymbol{x})$$

with $\boldsymbol{h}$ an arbitrary vector-valued function

- linear case: $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{a} + \boldsymbol{B}\boldsymbol{x}$

2.2.2 Delta method

Assume that we know the mean $\mathrm{E}(\boldsymbol{x}) = \boldsymbol{\mu}$ and variance $\mathrm{Var}(\boldsymbol{x}) = \boldsymbol{\Sigma}$ of $\boldsymbol{x}$. Is it possible to say something about the mean and variance of the transformed random variable $\boldsymbol{y}$?

$$\mathrm{E}(\boldsymbol{y}) = \mathrm{E}(\boldsymbol{h}(\boldsymbol{x})) = ?$$
$$\mathrm{Var}(\boldsymbol{y}) = \mathrm{Var}(\boldsymbol{h}(\boldsymbol{x})) = ?$$

In general, for a transformation $\boldsymbol{h}(\boldsymbol{x})$ the exact mean and variance of the transformed variable cannot be obtained analytically.

However, we can find a **linear approximation** and then compute its mean and variance. This approximation is called the "Delta Method", or the "law of propagation of errors", and is credited to Gauss.[1]

Linearisation of $\boldsymbol{h}(\boldsymbol{x})$ is achieved by a Taylor series approximation of first order of $\boldsymbol{h}(\boldsymbol{x})$ around $\boldsymbol{x}_0$:

$$\boldsymbol{h}(\boldsymbol{x}) \approx \boldsymbol{h}(\boldsymbol{x}_0) + \underbrace{\boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{x}_0)}_{\text{Jacobi matrix}} (\boldsymbol{x} - \boldsymbol{x}_0) = \underbrace{\boldsymbol{h}(\boldsymbol{x}_0) - \boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{x}_0)\, \boldsymbol{x}_0}_{\boldsymbol{a}} + \underbrace{\boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{x}_0)}_{\boldsymbol{B}} \boldsymbol{x}$$

∇, the nabla operator, is the row vector $(\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_d})$, which when applied to univariate h gives the gradient:

$$\nabla h(\boldsymbol{x}) = \left(\frac{\partial h}{\partial x_1}, ..., \frac{\partial h}{\partial x_d} \right)$$

The **Jacobi matrix** is the **generalisation of the gradient** if $\boldsymbol{h}$ is vector-valued:

$$\boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{x}) = \begin{pmatrix} \nabla h_1(\boldsymbol{x}) \\ \nabla h_2(\boldsymbol{x}) \\ \vdots \\ \nabla h_m(\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} \frac{\partial h_1}{\partial x_1} & \cdots & \frac{\partial h_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_m}{\partial x_1} & \cdots & \frac{\partial h_m}{\partial x_d} \end{pmatrix}$$

First order approximation of $\boldsymbol{h}(\boldsymbol{x})$ around $\boldsymbol{x}_0 = \boldsymbol{\mu}$ yields $\boldsymbol{a} = \boldsymbol{h}(\boldsymbol{\mu}) - \boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{\mu})\, \boldsymbol{\mu}$ $\boldsymbol{B} = \boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{\mu})$ and leads directly to the **multivariate Delta method**:

$$\mathrm{E}(\boldsymbol{y}) \approx \boldsymbol{h}(\boldsymbol{\mu})$$
$$\mathrm{Var}(\boldsymbol{y}) \approx \boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{\mu})\, \boldsymbol{\Sigma}\, \boldsymbol{J}_{\boldsymbol{h}}(\boldsymbol{\mu})^T$$

The **univariate Delta method** is a special case:

$$\mathrm{E}(y) \approx h(\mu)$$
$$\mathrm{Var}(y) \approx \sigma^2 h'(\mu)^2$$

Note that the Delta approximation breaks down if $\mathrm{Var}(\boldsymbol{y})$ is singular, for example if the first derivative (or gradient or Jacobi matrix) at $\boldsymbol{\mu}$ is zero.

[1] Gorroochurn, P. 2020. Who Invented the Delta Method, Really? The Mathematical Intelligencer **42**:46–49. https://doi.org/10.1007/s00283-020-09982-0

Example 2.3. Variance of the odds ratio

The proportion $\hat{p} = \frac{n_1}{n}$ resulting from n repeats of a Bernoulli experiment has expectation $\mathrm{E}(\hat{p}) = p$ and variance $\mathrm{Var}(\hat{p}) = \frac{p(1-p)}{n}$. What are the (approximate) mean and the variance of the corresponding odds ratio $\widehat{OR} = \frac{\hat{p}}{1-\hat{p}}$?

With $h(x) = \frac{x}{1-x}$, $\widehat{OR} = h(\hat{p})$ and $h'(x) = \frac{1}{(1-x)^2}$ we get using the Delta method $\mathrm{E}(\widehat{OR}) \approx h(p) = \frac{p}{1-p}$ and $\mathrm{Var}(\widehat{OR}) \approx h'(p)^2 \mathrm{Var}(\hat{p}) = \frac{p}{n(1-p)^3}$.

Example 2.4. Log-transform as variance stabilisation

Assume x has some mean $\mathrm{E}(x) = \mu$ and variance $\mathrm{Var}(x) = \sigma^2\mu^2$, i.e. the standard deviation $\mathrm{SD}(x)$ is proportional to the mean μ. What are the (approximate) mean and the variance of the log-transformed variable $\log(x)$?

With $h(x) = \log(x)$ and $h'(x) = \frac{1}{x}$ we get using the Delta method $\mathrm{E}(\log(x)) \approx h(\mu) = \log(\mu)$ and $\mathrm{Var}(\log(x)) \approx h'(\mu)^2 \mathrm{Var}(x) = \left(\frac{1}{\mu}\right)^2 \sigma^2\mu^2 = \sigma^2$. Thus, after applying the log-transform the variance does not depend any more on the mean!

2.2.3 Transformation of densities under general invertible transformation

Assume $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{y}(\boldsymbol{x})$ is invertible: $\boldsymbol{h}^{-1}(\boldsymbol{y}) = \boldsymbol{x}(\boldsymbol{y})$

$\boldsymbol{x} \sim F_{\boldsymbol{x}}$ with probability density function $f_{\boldsymbol{x}}(\boldsymbol{x})$

The density $f_{\boldsymbol{y}}(\boldsymbol{y})$ of the transformed random vector $\boldsymbol{y}$ is then given by

$$f_{\boldsymbol{y}}(\boldsymbol{y}) = |\det\left(\boldsymbol{J}_{\boldsymbol{x}}(\boldsymbol{y})\right)| \; f_{\boldsymbol{x}}\left(\boldsymbol{x}(\boldsymbol{y})\right)$$

where $\boldsymbol{J}_{\boldsymbol{x}}(\boldsymbol{y})$ is the Jacobi matrix of the inverse transformation

Special cases:

- Univariate version: $f_y(y) = |\frac{dx}{dy}| f_x\left(x(y)\right)$
- Linear transformation $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{a} + \boldsymbol{B}\boldsymbol{x}$, with $\boldsymbol{x}(\boldsymbol{y}) = \boldsymbol{B}^{-1}(\boldsymbol{y} - \boldsymbol{a})$ and $\boldsymbol{J}_{\boldsymbol{x}}(\boldsymbol{y}) = \boldsymbol{B}^{-1}$:
  $f_{\boldsymbol{y}}(\boldsymbol{y}) = |\det(\boldsymbol{B})|^{-1} f_{\boldsymbol{x}}\left(\boldsymbol{B}^{-1}(\boldsymbol{y} - \boldsymbol{a})\right)$

2.2.4 Normalising flows

In machine learning (sequences of) invertible nonlinear transformations are known as "normalising flows". They are used both in a generative way (building complex models from simple models) and also in a simplification and dimension reduction context.

In this module we will focus mostly on linear transformations as these underpin much of classical multivariate statistics, but it is important to keep in mind for later study the importance of nonlinear transformations —see, e.g, the review paper by Kobyzev et al. "Normalizing Flows: Introduction and Ideas", available from https://arxiv.org/abs/1908.09257 .

2.3 Whitening transformations

2.3.1 Overview

The *Mahalanobis* transform (also know as "zero-phase component analysis" or short ZCA transform in machine learning) is a specific example of a **whitening transformation**. These constitute an important and widely used class of invertible location-scale transformations.

Terminology: whitening refers to the fact that after the transformation the covariance matrix is spherical, isotrop, white ($\boldsymbol{I}_d$)

Whitening is **useful in preprocessing**, to **turn multivariate problems into simple univariate models** and some **reduce the dimension in an optimal way**.

In so-called latent variable models whitening procedures link observed and latent variables (which usually are uncorrelated and standardised random variables):

$$\begin{array}{cc} \text{Whitening} & \boldsymbol{x} \quad \text{Observed variable (can be measured), external, typically correlated} \\ \downarrow & \uparrow \\ & \boldsymbol{z} \quad \text{Unobserved "latent" variable, internal, typically not correlated} \end{array}$$

2.3.2 General whitening transformation

Starting point:

Random vector $\boldsymbol{x} \sim F_{\boldsymbol{x}}$ (not necessarily from multivariate normal).

The random variance $\boldsymbol{x}$ has some mean $\mathrm{E}(\boldsymbol{z}) = \boldsymbol{\mu}$ and a positive definite (invertible) covariance matrix $\mathrm{Var}(\boldsymbol{x}) = \boldsymbol{\Sigma}$. The covariance can be split into positive variances $\boldsymbol{V}$ and a positive definite invertible correlation matrix $\boldsymbol{P}$ so that $\boldsymbol{\Sigma} = \boldsymbol{V}^{1/2}\boldsymbol{P}\boldsymbol{V}^{1/2}$.

Whitening transformation:

$$\underbrace{\boldsymbol{z}}_{d\times 1 \text{ vector}} = \underbrace{\boldsymbol{W}}_{d\times d \text{ whitening matrix}} \underbrace{\boldsymbol{x}}_{d\times 1 \text{ vector}}$$

Objective: choose $\boldsymbol{W}$ so that $\mathrm{Var}(\boldsymbol{z}) = \boldsymbol{I}_d$

For Mahalanobis/ZCA whitening we already know that $\boldsymbol{W}^{\mathrm{ZCA}} = \boldsymbol{\Sigma}^{-1/2}$.

In general, the whitening matrix $\boldsymbol{W}$ needs to satisfy a constraint:

$$\begin{array}{lll} & \mathrm{Var}(\boldsymbol{z}) & = \boldsymbol{I}_d \\ \Longrightarrow & \mathrm{Var}(\boldsymbol{W}\boldsymbol{x}) & = \boldsymbol{W}\boldsymbol{\Sigma}\boldsymbol{W}^T = \boldsymbol{I}_d \\ \Longrightarrow & \boldsymbol{W}\,\boldsymbol{\Sigma}\,\boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{W} & \end{array}$$

$$\Longrightarrow \text{constraint on whitening matrix: } \boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{\Sigma}^{-1}$$

Clearly, the ZCA whitening matrix satisfies this constraint: $(\boldsymbol{W}^{ZCA})^T\boldsymbol{W}^{ZCA} = \boldsymbol{\Sigma}^{-1/2}\boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Sigma}^{-1}$

2.3.3 Solution of whitening constraint (covariance-based)

A general way to specify a valid whitening matrix is

$$\boldsymbol{W} = \boldsymbol{Q}_1 \boldsymbol{\Sigma}^{-1/2}$$

where $\boldsymbol{Q}_1$ is an orthogonal matrix

Recall that an orthogonal matrix $\boldsymbol{Q}$ has the property that $\boldsymbol{Q}^{-1} = \boldsymbol{Q}^T$ and and as a consequence $\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$.

As a result, the above $\boldsymbol{W}$ satisfies the whitening constraint:

$$\boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{\Sigma}^{-1/2} \underbrace{\boldsymbol{Q}_1^T\boldsymbol{Q}_1}_{\boldsymbol{I}} \boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Sigma}^{-1}$$

Note the converse is also true: any whitening whitening matrix, i.e. any $\boldsymbol{W}$ satisfying the whitening constraint, can be written in the above form as $\boldsymbol{Q}_1 = \boldsymbol{W}\boldsymbol{\Sigma}^{1/2}$ is orthogonal by construction.

$\Longrightarrow$ instead of choosing $\boldsymbol{W}$, **we choose the orthogonal matrix $\boldsymbol{Q}_1$!**

- recall that orthogonal matrices geometrically represent rotations (plus reflections).
- it is now clear that there are infinitely many whitening procedures, because there are infinitely many rotations! This also means we need to find ways to choose/select among whitening procedures.
- for the Mahalanobis/ZCA transformation $\boldsymbol{Q}_1^{\text{ZCA}} = \boldsymbol{I}$
- **whitening** can be interpreted as **Mahalanobis transform** followed by **rotation**

2.3.4 Another solution (correlation-based)

Instead of working with the covariance matrix $\boldsymbol{\Sigma}$, we can express $\boldsymbol{W}$ also in terms of the corresponding correlation matrix $\boldsymbol{P} = (\rho_{ij}) = \boldsymbol{V}^{-1/2}\boldsymbol{\Sigma}\boldsymbol{V}^{-1/2}$ where $\boldsymbol{V}^{1/2}$ is the diagonal matrix containing the variances.

Specifically we can specify the whitening matrix as

$$\boldsymbol{W} = \boldsymbol{Q}_2\boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}$$

It is easy to verify that this $\boldsymbol{W}$ also satisfies the whitening constraint:

$$\begin{aligned}\boldsymbol{W}^T\boldsymbol{W} &= \boldsymbol{V}^{-1/2}\boldsymbol{P}^{-1/2} \underbrace{\boldsymbol{Q}_2^T\boldsymbol{Q}_2}_{\boldsymbol{I}} \boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2} \\ &= \boldsymbol{V}^{-1/2}\boldsymbol{P}^{-1}\boldsymbol{V}^{-1/2} = \boldsymbol{\Sigma}^{-1}\end{aligned}$$

Conversely, any whitening matrix $\boldsymbol{W}$ can also be written in this form as $\boldsymbol{Q}_2 = \boldsymbol{W}\boldsymbol{V}^{1/2}\boldsymbol{P}^{1/2}$ is orthogonal by construction.

- **Another interpretation of whitening**: first **standardising** ($\boldsymbol{V}^{-1/2}$), then **decorrelation** ($\boldsymbol{P}^{-1/2}$), followed by **rotation** ($\boldsymbol{Q}_2$)

- for Mahalanobis/ZCA transformation $Q_2^{\text{ZCA}} = \boldsymbol{\Sigma}^{-1/2}\boldsymbol{V}^{1/2}\boldsymbol{P}^{1/2}$

Both forms to write W using Q_1 and Q_2 are equally valid (and interchangeable).

Note that for the same $\boldsymbol{W}$

$$Q_1 \neq Q_2 \text{ Two different orthogonal matrices!}$$

and also

$$\underbrace{\boldsymbol{\Sigma}^{-1/2}}_{\text{Symmetric}} \neq \underbrace{\boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}}_{\text{Not Symmetric}}$$

even though

$$\boldsymbol{\Sigma}^{-1/2}\boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Sigma}^{-1} = \boldsymbol{V}^{-1/2}\boldsymbol{P}^{-1/2}\boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}$$

2.3.5 Cross-covariance and cross-correlation

A useful criterion to distinguish whitening transformation is to consider the cross-covariance and cross-correlation:

a) **Cross-covariance $\boldsymbol{\Phi} = \Sigma_{zx}$** between $\boldsymbol{z}$ and $\boldsymbol{x}$:

$$\begin{aligned}\boldsymbol{\Phi} = \text{Cov}(\boldsymbol{z}, \boldsymbol{x}) &= \text{Cov}(\boldsymbol{W}\boldsymbol{x}, \boldsymbol{x}) \\ &= \boldsymbol{W}\boldsymbol{\Sigma} \\ &= \boldsymbol{Q}_1\boldsymbol{\Sigma}^{-1/2}\boldsymbol{\Sigma} \\ &= \boldsymbol{Q}_1\boldsymbol{\Sigma}^{1/2}\end{aligned}$$

Cross-covariance is linked with Q_1! Thus, choosing cross-covariance determines Q_1 (and vice versa). The whitening matrix expressed in terms of cross-covariance is $\boldsymbol{W} = \boldsymbol{\Phi}\boldsymbol{\Sigma}^{-1}$.

b) **Cross-correlation $\boldsymbol{\Psi} = \boldsymbol{P}_{zx}$** between $\boldsymbol{z}$ and $\boldsymbol{x}$:

$$\begin{aligned}\boldsymbol{\Psi} = \text{Cor}(\boldsymbol{z}, \boldsymbol{x}) &= \boldsymbol{\Phi}\boldsymbol{V}^{-1/2} \\ &= \boldsymbol{W}\boldsymbol{\Sigma}\boldsymbol{V}^{-1/2} \\ &= \boldsymbol{Q}_2\boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}\boldsymbol{\Sigma}\boldsymbol{V}^{-1/2} \\ &= \boldsymbol{Q}_2\boldsymbol{P}^{1/2}\end{aligned}$$

Cross-correlation is linked with Q_2! Hence, choosing cross-correlation determines Q_2 (and vice versa). The whitening matrix expressed in terms of cross-correlation is $\boldsymbol{W} = \boldsymbol{\Psi}\boldsymbol{P}^{-1}\boldsymbol{V}^{-1/2}$.

Note that the factorisation of the cross-covariance $\boldsymbol{\Phi} = \boldsymbol{Q}_1\boldsymbol{\Sigma}^{1/2}$ and the cross-correlation $\boldsymbol{\Psi} = \boldsymbol{Q}_2\boldsymbol{P}^{1/2}$ into the product of an orthogonal matrix and a positive semi-definite symmetric matrix is the called *polar decomposition*.

2.3.6 Inverse whitening transformation, loadings, and multiple correlation

Reverse transformation:

Recall that $\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x}$. Therefore, the reverse transformation going from the whitened to the original variable is $\boldsymbol{x} = \boldsymbol{W}^{-1}\boldsymbol{z}$. This can be expressed also in terms of cross-covariance and cross-correlation. With $\boldsymbol{W} = \boldsymbol{Q}_1\boldsymbol{\Sigma}^{-1/2}$ we get for the inverse $\boldsymbol{W}^{-1} = \boldsymbol{\Sigma}^{1/2}\boldsymbol{Q}_1^{-1} = \boldsymbol{\Sigma}^{1/2}\boldsymbol{Q}_1^{-T} = \boldsymbol{\Phi}^T$ so that

$$\boldsymbol{x} = \boldsymbol{\Phi}^T\boldsymbol{z}\,.$$

Furthermore, since $\boldsymbol{\Psi} = \boldsymbol{\Phi}\boldsymbol{V}^{-1/2}$ we have $\boldsymbol{W}^{-1} = \boldsymbol{V}^{1/2}\boldsymbol{\Psi}^T$ and

$$\boldsymbol{V}^{-1/2}\boldsymbol{x} = \boldsymbol{\Psi}^T\boldsymbol{z}\,.$$

Definition of loadings:

Loadings are the coefficients of the linear transformation from the latent variable back to the observed variable. If the variables are standardised to unit variance then the loadings are also called *correlation loadings*.

Hence, the cross-covariance matrix plays the role of *loadings* linking the latent variable $\boldsymbol{z}$ with the original $\boldsymbol{x}$. Similarly, the cross-correlation matrix are the *correlation loadings* linking the (already standardised) latent variable $\boldsymbol{z}$ with the standardised $\boldsymbol{x}$.

Multiple correlation coefficients from z to x:

Consider the backtransformation from $\boldsymbol{z}$ to $\boldsymbol{x}$. The components of $\boldsymbol{z}$ are all uncorrelated. Therefore, we can compute the squared multiple correlation coefficient between each x_j and $\boldsymbol{z}$ as the sum of the squared correlations $\mathrm{Cor}(z_i, x_j)^2$:

$$\mathrm{Cor}(\boldsymbol{z}, x_j)^2 = \sum_{i=1}^{d} \mathrm{Cor}(z_i, x_j)^2 = \sum_{i=1}^{d} \psi_{ij}^2$$

In vector notation with $\boldsymbol{\Psi} = (\psi_{ij})$ we get

$$\begin{aligned}(\mathrm{Cor}(\boldsymbol{z}, x_j)^2)^T &= \mathrm{Diag}(\boldsymbol{\Psi}^T\boldsymbol{\Psi}) \\ &= \mathrm{Diag}(\boldsymbol{P}^{1/2}\boldsymbol{Q}_2^T\boldsymbol{Q}_2\boldsymbol{P}^{1/2}) \\ &= \mathrm{Diag}(\boldsymbol{P}) \\ &= (1, \ldots, 1)^T\end{aligned}$$

Therefore the column sums of the matrix (ψ_{ij}^2) are all 1 regardless of the choice of $\boldsymbol{Q}_2$:

$$\sum_{i=1}^{d} \psi_{ij}^2 = 1 \text{ for all } j$$

It is easy to understand why we get multiple squared correlations of value 1 — because x_j is a linear function of the $z_1, \ldots, z_d$ with no noise term, which means x_j can be predicted perfectly from $\boldsymbol{z}$ with no error.

Multiple correlation coefficients from x to z:

For the original direction going from $x_1, \ldots, x_d$ to the z_i the corresponding squared multiple correlations $\text{Cor}(z_i, \boldsymbol{x})^2$ are also 1, but because the x_j are correlated we cannot simply sum the squared correlations to get $\text{Cor}(z_i, \boldsymbol{x})^2$ but we also need take account of the correlations among the $\boldsymbol{x}_j$ (i.e. $\boldsymbol{P}$). In vector notation:

$$\begin{aligned}(\text{Cor}(z_i, \boldsymbol{x})^2)^T &= \text{Diag}(\boldsymbol{\Psi}\boldsymbol{P}^{-1}\boldsymbol{\Psi}^T) \\ &= \text{Diag}(\boldsymbol{Q}_2\boldsymbol{P}^{1/2}\boldsymbol{P}^{-1}\boldsymbol{P}^{1/2}\boldsymbol{Q}_2^T) \\ &= \text{Diag}(\boldsymbol{I}) \\ &= (1, \ldots, 1)^T\end{aligned}$$

2.4 Natural whitening procedures

Now we discuss several strategies (maximise correlation between individual components, maximise compression, etc.) to arrive at optimal whitening transformation.

This leads to the following "natural" whitening transformations:

- **Mahalanobis** whitening, also known as **ZCA** (zero-phase component analysis) whitening in machine learning
- **ZCA-cor** whitening
- **PCA** whitening
- **PCA-cor** whitening
- **Cholesky** whitening

In the following $\boldsymbol{x}_c = \boldsymbol{x} - \boldsymbol{\mu}_{\boldsymbol{x}}$ and $\boldsymbol{z}_c = \boldsymbol{z} - \boldsymbol{\mu}_{\boldsymbol{z}}$ denote the mean-centered variables.

2.4.1 ZCA whitening

Aim: remove correlations but otherwise make sure that after whitening $\boldsymbol{z}$ does not differ too much from $\boldsymbol{x}$. Specifically, each element z_i should be as close as as possible to the corresponding element x_i:

$$\begin{aligned} z_1 &\leftrightarrow x_1 \\ z_2 &\leftrightarrow x_2 \\ z_3 &\leftrightarrow x_3 \\ &\vdots \end{aligned}$$

One possible way to implement this is to compute the expected squared difference between the two centered random vectors $\boldsymbol{z}_c$ and $\boldsymbol{x}_c$.

ZCA objective function: minimise $\text{E}\left((\boldsymbol{z}_c - \boldsymbol{x}_c)^T(\boldsymbol{z}_c - \boldsymbol{x}_c)\right)$ to find an optimal whitening procedure.

The ZCA objective function can be simplified as follows:

$$\begin{aligned}
&= \mathrm{E}(\boldsymbol{z}_c^T \boldsymbol{z}_c) - 2\mathrm{E}(\boldsymbol{x}_c^T \boldsymbol{z}_c) + \mathrm{E}(\boldsymbol{x}_c^T \boldsymbol{x}_c) \\
&= \mathrm{E}(\mathrm{Tr}(\boldsymbol{z}_c \boldsymbol{z}_c^T)) - 2\mathrm{E}(\mathrm{Tr}(\boldsymbol{z}_c \boldsymbol{x}_c^T)) + \mathrm{E}(\mathrm{Tr}(\boldsymbol{x}_c \boldsymbol{x}_c^T)) \\
&= \mathrm{Tr}(\mathrm{E}(\boldsymbol{z}_c \boldsymbol{z}_c^T)) - 2\mathrm{Tr}(\mathrm{E}(\boldsymbol{z}_c \boldsymbol{x}_c^T)) + \mathrm{Tr}(\mathrm{E}(\boldsymbol{x}_c \boldsymbol{x}_c^T)) \\
&= \mathrm{Tr}(\mathrm{Var}(\boldsymbol{z})) - 2\mathrm{Tr}(\mathrm{Cov}(\boldsymbol{z}, \boldsymbol{x})) + \mathrm{Tr}(\mathrm{Var}(\boldsymbol{x})) \\
&= d - 2\mathrm{Tr}(\boldsymbol{\Phi}) + \mathrm{Tr}(\boldsymbol{V})
\end{aligned}$$

The only term that depends on the whitening transformation is $-2\mathrm{Tr}(\boldsymbol{\Phi})$ as it is a function of $\boldsymbol{Q}_1$. Therefore we can use the following alternative objective:

ZCA equivalent objective: maximise $\mathrm{Tr}(\boldsymbol{\Phi}) = \mathrm{Tr}(\boldsymbol{Q}_1 \boldsymbol{\Sigma}^{1/2})$ to find optimal $\boldsymbol{Q}_1$

This is the sum $\sum_{i=1}^{d} \mathrm{Cov}(z_i, x_i)$ of all covariances between corresponding elements in $\boldsymbol{z}$ and $\boldsymbol{x}$.

Solution:

i) Apply eigendecomposition to $\boldsymbol{\Sigma} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$. Note that $\boldsymbol{\Lambda}$ is diagonal with positive entries $\lambda_i > 0$ as $\boldsymbol{\Sigma}$ is positive definite.
ii) The objective function becomes

$$\begin{aligned}
\mathrm{Tr}(\boldsymbol{Q}_1 \boldsymbol{\Sigma}^{1/2}) &= \mathrm{Tr}(\boldsymbol{Q}_1 \boldsymbol{U} \boldsymbol{\Lambda}^{1/2} \boldsymbol{U}^T) \\
&= \mathrm{Tr}(\boldsymbol{\Lambda}^{1/2} \boldsymbol{U}^T \boldsymbol{Q}_1 \boldsymbol{U}) \\
&= \mathrm{Tr}(\boldsymbol{\Lambda}^{1/2} \boldsymbol{B}) \\
&= \sum_{i=1}^{d} \lambda_i b_{ii}.
\end{aligned}$$

Note that the product of the orthogonal matrices $\boldsymbol{B} = \boldsymbol{U}^T \boldsymbol{Q}_1 \boldsymbol{U}$ is itself an orthogonal matrix, and $\boldsymbol{Q}_1 = \boldsymbol{U}\boldsymbol{B}\boldsymbol{U}^T$.
iii) As $\lambda_i > 0$ the objective function is maximised for the orthogonal matrix $\boldsymbol{B} = \boldsymbol{I}$.
iv) Thus, the optimal $\boldsymbol{Q}_1$ matrix is

$$\boldsymbol{Q}_1^{\mathrm{ZCA}} = \boldsymbol{I}$$

The corresponding whitening matrix for ZCA is

$$\boldsymbol{W}^{\mathrm{ZCA}} = \boldsymbol{\Sigma}^{-1/2}$$

and the cross-covariance matrix is

$$\boldsymbol{\Phi}^{\mathrm{ZCA}} = \boldsymbol{\Sigma}^{1/2}$$

and the cross-correlation matrix

$$\boldsymbol{\Psi}^{\mathrm{ZCA}} = \boldsymbol{\Sigma}^{1/2} \boldsymbol{V}^{-1/2}$$

Note that for ZCA $\mathrm{Cov}(z_i, x_i) > 0$ and $\mathrm{Cor}(z_i, x_i) > 0$ so two corresponding components z_i and x_i are always positively correlated!

Summary:

- ZCA/Mahalanobis transform is the unique transformation that minimises the expected total squared component-wise difference between $\boldsymbol{x}_c$ and $\boldsymbol{z}_c$.
- As corresponding components in the whitened and original variables are always positively correlated this facilitates interpretation of the whitening variables.
- Use ZCA aka Mahalanobis whitening if you want to "just" remove correlations.

2.4.2 ZCA-Cor whitening

Aim: same as above but remove scale in $\boldsymbol{x}$ first before comparing to $\boldsymbol{z}$

ZCA-cor objective function: minimise $\mathrm{E}\left((\boldsymbol{z}_c - \boldsymbol{V}^{-1/2}\boldsymbol{x}_c)^T(\boldsymbol{z}_c - \boldsymbol{V}^{-1/2}\boldsymbol{x}_c)\right)$ to find an optimal whitening procedure.

This can be simplified as follows:

$$\begin{aligned}
&= \mathrm{E}(\boldsymbol{z}_c^T\boldsymbol{z}_c) - 2\mathrm{E}(\boldsymbol{x}_c^T\boldsymbol{V}^{-1/2}\boldsymbol{z}_c) + \mathrm{E}(\boldsymbol{x}_c^T\boldsymbol{V}^{-1}\boldsymbol{x}_c)\\
&= \mathrm{Tr}(\mathrm{Var}(\boldsymbol{z})) - 2\mathrm{Tr}(\mathrm{Cor}(\boldsymbol{z},\boldsymbol{x})) + \mathrm{Tr}(\mathrm{Cor}(\boldsymbol{x},\boldsymbol{x}))\\
&= d - 2\mathrm{Tr}(\boldsymbol{\Psi}) + d\\
&= 2d - 2\mathrm{Tr}(\boldsymbol{\Psi})
\end{aligned}$$

The only term that depends on the whitening transformation via $\boldsymbol{Q}_2$ is $-2\mathrm{Tr}(\boldsymbol{\Psi})$ so we can use the following alternative objective instead:

ZCA-cor equivalent objective: maximise $\mathrm{Tr}(\boldsymbol{\Psi}) = \mathrm{Tr}(\boldsymbol{Q}_2\boldsymbol{P}^{1/2})$ to find optimal $\boldsymbol{Q}_2$

This is the sum $\sum_{i=1}^{d}\mathrm{Cor}(z_i, x_i)$ of all correlations between corresponding elements in $\boldsymbol{z}$ and $\boldsymbol{x}$.

Solution: same as above for ZCA but using correlation instead of covariance:

i) Apply eigendecomposition to $\boldsymbol{P} = \boldsymbol{G}\boldsymbol{\Theta}\boldsymbol{G}^T$ with positive diagonal $\boldsymbol{\Theta}$.
ii) The objective function becomes $\mathrm{Tr}(\boldsymbol{Q}_2\boldsymbol{P}^{1/2})) = \mathrm{Tr}(\boldsymbol{\Theta}^{1/2}\boldsymbol{G}^T\boldsymbol{Q}_2\boldsymbol{G})$
iii) This is maximised for
$$\boldsymbol{Q}_2^{\text{ZCA-Cor}} = \boldsymbol{I}$$

The corresponding whitening matrix for ZCA-cor is

$$\boldsymbol{W}^{\text{ZCA-Cor}} = \boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}$$

and the cross-covariance matrix is

$$\boldsymbol{\Phi}^{\text{ZCA-Cor}} = \boldsymbol{P}^{1/2}\boldsymbol{V}^{1/2}$$

and the cross-correlation matrix is

$$\boldsymbol{\Psi}^{\text{ZCA-Cor}} = \boldsymbol{P}^{1/2}$$

As a result for ZCA-cor $\mathrm{Cov}(z_i, x_i) > 0$ and $\mathrm{Cor}(z_i, x_i) > 0$ so two corresponding components z_i and x_i are always positively correlated!

Summary:

- ZCA-cor whitening is the unique whitening transformation maximising the total correlation between corresponding elements in $\boldsymbol{x}$ and $\boldsymbol{z}$.
- ZCA-cor leads to interpretable $\boldsymbol{z}$ because each individual element in $\boldsymbol{z}$ is (typically strongly) positively correlated with the corresponding element in the original $\boldsymbol{x}$.
- As ZCA-cor is explicitly constructed to maximise the total pairwise correlations it achieves the higher correlation than ZCA.
- If $\boldsymbol{x}$ is standardised to $\text{Var}(x_i) = 1$ then ZCA and ZCA-cor are identical but otherwise they are different whitening transformations.

2.4.3 PCA whitening

Aim: remove correlations and at the same compress information into a few latent variables. Specfically, we would like that the first latent component z_1 is maximally linked with all variables in $\boldsymbol{x}$, followed by the second component z_2 and so on:

$$\begin{array}{llll} z_1 & \leftarrow x_1 & z_2 & \leftarrow x_1 \quad \dots \\ z_1 & \leftarrow x_2 & z_2 & \leftarrow x_2 \\ \vdots & & & \\ z_1 & \leftarrow x_d & z_2 & \leftarrow x_d \end{array}$$

One way to measure the total link of each z_i with all x_j is the sum of the corresponding squared covariances

$$p_i = \sum_{j=1}^{d} \text{Cov}(z_i, x_j)^2 = \sum_{j=1}^{d} \phi_{ij}^2$$

In vector notation we write

$$\boldsymbol{p} = (p_1, ..., p_d)^T = \text{Diag}(\boldsymbol{\Phi}\boldsymbol{\Phi}^T)$$

With $\boldsymbol{\Phi} = \boldsymbol{Q}_1\boldsymbol{\Sigma}^{1/2}$ this can be written $\boldsymbol{p} = \text{Diag}(\boldsymbol{Q}_1\boldsymbol{\Sigma}\boldsymbol{Q}_1^T)$ as a function of $\boldsymbol{Q}_1$.

PCA objective functions: maximise $p_1, \dots, p_{d-1}$ in $\boldsymbol{p} = \text{Diag}(\boldsymbol{Q}_1\boldsymbol{\Sigma}\boldsymbol{Q}_1^T)$ such that $p_1 \geq p_2 \geq \cdots \geq p_d$ to find an optimal optimal $\boldsymbol{Q}_1$ and the corresponding whitening transformation.

Note that $\sum_{i=1}^{d} p_i = \text{Tr}(\boldsymbol{Q}_1\boldsymbol{\Sigma}\boldsymbol{Q}_1) = \text{Tr}(\boldsymbol{\Sigma})$ is constant regardless of the choice $\boldsymbol{Q}_1$ so there are only $d-1$ independent p_i.

Solution:

i) Apply eigendecomposition to $\boldsymbol{\Sigma} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$. Note that $\boldsymbol{\Lambda}$ is diagonal with positive entries $\lambda_1 \geq \lambda_2 \dots \geq \lambda_d > 0$ as $\boldsymbol{\Sigma}$ is positive definite and that the eigenvalues are already arranged non-increasing order. Also recall that $\boldsymbol{U}$ is not uniquely defined — you are free to change the columns signs.

ii) The objective functions become $\boldsymbol{p} = \text{Diag}((\boldsymbol{Q}_1\boldsymbol{U})\boldsymbol{\Lambda}(\boldsymbol{Q}_1\boldsymbol{U})^T) = \text{Diag}(\boldsymbol{B}\boldsymbol{\Lambda}\boldsymbol{B}^T)$ where $\boldsymbol{B}$ is an orthogonal matrix, and $\boldsymbol{Q}_1 = \boldsymbol{B}\boldsymbol{U}^T$.

iii) The optimal (maximum) values are achieved for $\boldsymbol{B} = \boldsymbol{I}$, with $p_i^{\text{PCA}} = \lambda_i$. However, this is not the only solution — you can arbitrarily change the column signs of the matrix $\boldsymbol{B}$ to arrive at the same maximum!

iv) The corresponding optimal value for the $\boldsymbol{Q}_1$ matrix is

$$\boldsymbol{Q}_1^{\text{PCA}} = \boldsymbol{U}^T$$

The corresponding whitening matrix is

$$\boldsymbol{W}^{\text{PCA}} = \boldsymbol{U}^T\boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Lambda}^{-1/2}\boldsymbol{U}^T$$

and the cross-covariance matrix is

$$\boldsymbol{\Phi}^{\text{PCA}} = \boldsymbol{\Lambda}^{1/2}\boldsymbol{U}^T$$

and the cross-correlation matrix is

$$\boldsymbol{\Psi}^{\text{PCA}} = \boldsymbol{\Lambda}^{1/2}\boldsymbol{U}^T\boldsymbol{V}^{-1/2}$$

Note that all of the above (i.e. $\boldsymbol{Q}_1^{\text{PCA}}, \boldsymbol{W}^{\text{PCA}}, \boldsymbol{\Phi}^{\text{PCA}}, \boldsymbol{\Psi}^{\text{PCA}}$) is not unique as we still have the sign ambiguity in the columns of $\boldsymbol{U}$ (which also has absorbed the sign ambiguity of $\boldsymbol{B}$)!

Identifiability:

Therefore, for identifiability reasons we need to impose a further constraint on $\boldsymbol{Q}_1^{\text{PCA}}$. A useful condition is to require a positive diagonal, i.e. $\text{Diag}(\boldsymbol{Q}_1^{\text{PCA}}) > 0$ and also $\text{Diag}(\boldsymbol{U}) > 0$. As a result, $\text{Diag}(\boldsymbol{\Phi}^{\text{PCA}}) > 0$ and $\text{Diag}(\boldsymbol{\Psi}^{\text{PCA}}) > 0$. With this constraint in place all pairs of x_i and z_i are positively correlated.

It is particularly important to pay attention to the sign ambiguity if different computer implementations of PCA whitening (and the related PCA approach) are used.

Proportion of total variation:

The sum of the maximised squared covariances for each latent component z_i is $\sum_{i=1}^{d} p_i^{\text{PCA}} = \sum_{i=1}^{d} \lambda_i$ and equals the total variation $\text{Tr}(\boldsymbol{\Sigma})$.

The fraction $\frac{\lambda_i}{\sum_{j=1}^{d} \lambda_j}$ is the proportional contribution of each element in $\boldsymbol{z}$ to explain the total variation. Thus, low ranking components z_i with small $p_i^{\text{PCA}} = \lambda_i$ may be discarded. In fact, the aim of PCA whitening is to achieve this kind of compression and the resuling reduction in dimension in the latent space.

Summary:

- PCA whitening is a whitening transformation that maximises compression with the sum of squared cross-covariances as underlying optimality criterion.
- There are sign ambiguities in the PCA whitened variables which are inherited from the sign ambiguities in eigenvectors.
- If a positive-diagonal condition on the orthogonal matrices is imposed then these sign ambiguities are fully resolved and corresponding components z_i and x_i are always positively correlated.

2.4.4 PCA-cor whitening

Aim: same as for PCA whitening but remove scale in $\boldsymbol{x}$ first. This means we use squared correlations rather than squared covariances to measure compression, i.e.

$$p_i = \sum_{j=1}^{d} \mathrm{Cor}(z_i, x_j)^2 = \sum_{j=1}^{d} \psi_{ij}^2$$

In vector notation this becomes

$$\boldsymbol{p} = \mathrm{Diag}(\boldsymbol{\Psi}\boldsymbol{\Psi}^T) = \mathrm{Diag}(\boldsymbol{Q}_2\boldsymbol{P}\boldsymbol{Q}_2^T)$$

PCA-cor objective functions: maximise $p_1, \ldots, p_{d-1}$ in $\boldsymbol{p} = \mathrm{Diag}(\boldsymbol{Q}_2\boldsymbol{P}\boldsymbol{Q}_2^T)$ such that $p_1 \geq p_2 \geq \cdots \geq p_d$ to find an optimal optimal $\boldsymbol{Q}_2$ and the corresponding whitening transformation.

Note that $\sum_{i=1}^{d} p_i = \mathrm{Tr}(\boldsymbol{Q}_2\boldsymbol{P}\boldsymbol{Q}_2) = \mathrm{Tr}(\boldsymbol{P}) = d$ is constant regardless of the choice $\boldsymbol{Q}_2$ so there are only $d-1$ independent p_i.

Solution:

i) Apply eigendecomposition to $\boldsymbol{P} = \boldsymbol{G}\boldsymbol{\Theta}\boldsymbol{G}^T$. Note that $\boldsymbol{\Theta}$ is diagonal with positive entries $\theta_1 \geq \theta_2 \ldots \geq \theta_d > 0$ as $\boldsymbol{P}$ is positive definite and that the eigenvalues are already arranged non-increasing order. Also recall that $\boldsymbol{G}$ is not uniquely defined — you are free to change the columns signs.

ii) The objective functions become $\boldsymbol{p} = \mathrm{Diag}((\boldsymbol{Q}_2\boldsymbol{G})\boldsymbol{\Theta}(\boldsymbol{Q}_2\boldsymbol{G})^T) = \mathrm{Diag}(\boldsymbol{B}\boldsymbol{\Theta}\boldsymbol{B}^T)$ where $\boldsymbol{B}$ is an orthogonal matrix, and $\boldsymbol{Q}_2 = \boldsymbol{B}\boldsymbol{G}^T$.

iii) The optimal (maximum) values are achieved for $\boldsymbol{B} = \boldsymbol{I}$, with $p_i^{\text{PCA-Cor}} = \theta_i$. However, this is not the only solution — you can arbitrarily change the column signs of the matrix $\boldsymbol{B}$ to arrive at the same maximum!

iv) The corresponding optimal value for the $\boldsymbol{Q}_2$ matrix is

$$\boldsymbol{Q}_2^{\text{PCA-Cor}} = \boldsymbol{G}^T$$

The corresponding whitening matrix is

$$\boldsymbol{W}^{\text{PCA-Cor}} = \boldsymbol{\Theta}^{-1/2}\boldsymbol{G}^T\boldsymbol{V}^{-1/2}$$

and the cross-covariance matrix is

$$\boldsymbol{\Phi}^{\text{PCA-Cor}} = \boldsymbol{\Theta}^{1/2}\boldsymbol{G}^T\boldsymbol{V}^{1/2}$$

and the cross-correlation matrix is

$$\boldsymbol{\Psi}^{\text{PCA-Cor}} = \boldsymbol{\Theta}^{1/2}\boldsymbol{G}^T$$

As with PCA whitening, there are sign ambiguities in the above because the column signs of $\boldsymbol{G}$ can be freely chosen.

Identifiability:

For identifiability we choose to set $\text{Diag}(\boldsymbol{Q}_2^{\text{PCA-Cor}}) > 0$ and also $\text{Diag}(\boldsymbol{G}) > 0$ so that $\text{Diag}(\boldsymbol{\Phi}^{\text{PCA-Cor}}) > 0$ and $\text{Diag}(\boldsymbol{\Psi}^{\text{PCA-Cor}}) > 0$.

Proportion of total variation:

The sum of the maximised squared correlations for each latent component z_i is $\sum_{i=1}^{d} p_i^{\text{PCA-Cor}} = \sum_{i=1}^{d} \theta_i = d$ and equals the total variation $\text{Tr}(\boldsymbol{P})$. Therefore the fraction $\frac{\theta_i}{\sum_{j=1}^{d} \theta_j} = \frac{\theta_j}{d}$ is the proportional contribution of each element in $\boldsymbol{z}$ to explain the total variation.

Summary:

- PCA-cor whitening is a whitening transformation that maximises compression with the sum of squared cross-correlations as underlying optimality criterion.
- There are sign ambiguities in the PCA-cor whitened variables which are inherited from the sign ambiguities in eigenvectors.
- If a positive-diagonal condition on the orthogonal matrices is imposed then these sign ambiguities are fully resolved and corresponding components z_i and x_i are always positively correlated.
- If $\boldsymbol{x}$ is standardised to $\text{Var}(x_i) = 1$, then PCA and PCA-cor whitening are identical.

2.4.5 Cholesky whitening

Aim: find a whitening transformation such that the cross-covariance $\boldsymbol{\Phi}$ and cross-correlation $\boldsymbol{\Psi}$ have triangular structure. This is useful in some models such as time course data, e.g. to ensure that the future cannot influence the past.

Solution: Apply a Cholesky decomposition to $\boldsymbol{\Sigma}^{-1} = \boldsymbol{L}\boldsymbol{L}^T$

The Cholesky descomposition requires positive definite $\boldsymbol{\Sigma}$ and is unique. $\boldsymbol{L}$ is a lower triangular matrix with positive diagonal elements. Its inverse $\boldsymbol{L}^{-1}$ is also lower triangular with positive diagonal elements.

The resulting whitening matrix is

$$\boldsymbol{W}^{\text{Chol}} = \boldsymbol{L}^T$$

By construction, $\boldsymbol{W}^{\text{Chol}}$ satisfies the whitening constraint since $(\boldsymbol{W}^{\text{Chol}})^T\boldsymbol{W}^{\text{Chol}} = \boldsymbol{\Sigma}^{-1}$.

The cross-covariance matrix is (with $\boldsymbol{\Sigma} = (\boldsymbol{L}^{-1})^T\boldsymbol{L}^{-1}$)

$$\boldsymbol{\Phi}^{\text{Chol}} = \boldsymbol{L}^T\boldsymbol{\Sigma} = \boldsymbol{L}^{-1}$$

and the cross-correlation matrix is

$$\boldsymbol{\Psi}^{\text{Chol}} = \boldsymbol{L}^T\boldsymbol{\Sigma}\boldsymbol{V}^{-1/2} = \boldsymbol{L}^{-1}\boldsymbol{V}^{-1/2}$$

Note that the both $\boldsymbol{\Phi}^{\text{Chol}}$ and $\boldsymbol{\Psi}^{\text{Chol}}$ are also lower triangular matrices with positive diagonal elements!

Finally, the corresponding orthogonal matrices are

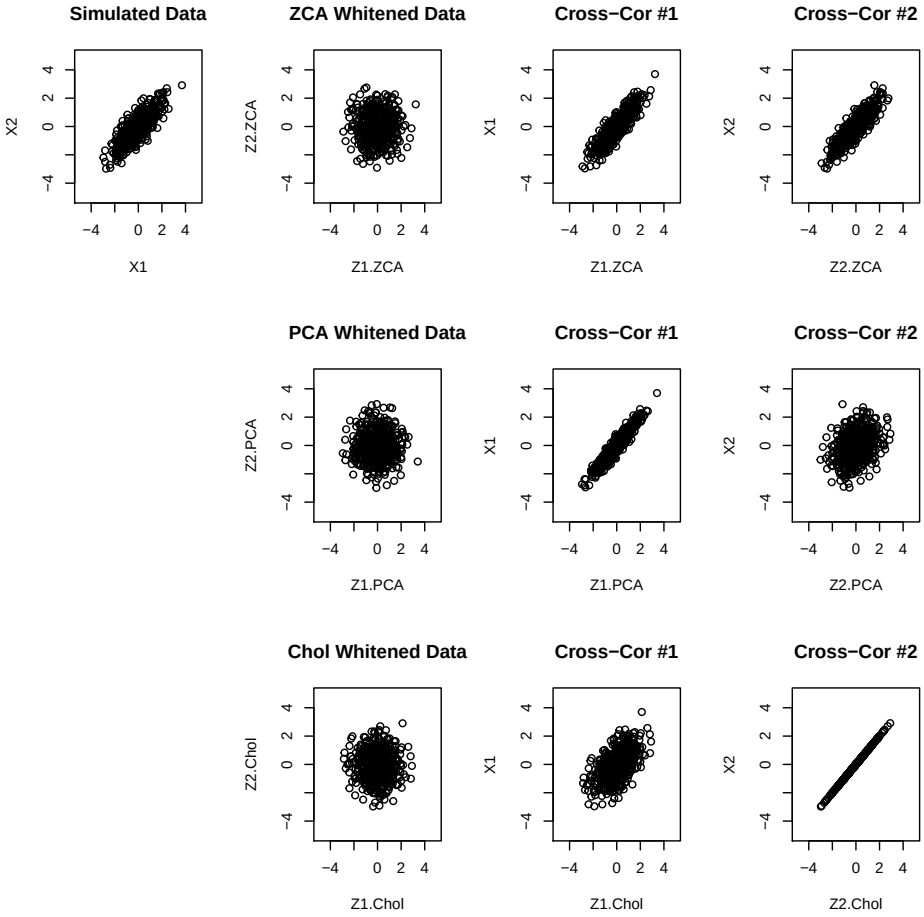
$$Q_1^{\text{Chol}} = \boldsymbol{L}^T \boldsymbol{\Sigma}^{1/2}$$

and

$$Q_2^{\text{Chol}} = \boldsymbol{L}^T \boldsymbol{V}^{1/2} \boldsymbol{P}^{1/2}$$

2.4.6 Comparison of ZCA, PCA and Cholesky whitening

For comparison, here are the results of ZCA, PCA and Cholesky whitening applied to a simulated bivariate normal data set with correlation $\rho = 0.8$.



In column 1 you can see the simulated data as scatter plot.

Column 2 shows the scatter plots of the whitened data — as expect all three methods removed correlation produce isotropic covariance.

The three approached differ differ in the cross-correlations. Columns 3 and 4 show the cross-correlations between the first two corresponding components (x_1 and z_1, and x_2 and z_2) for ZCA, PCA and Cholesky whitening. As expected, in ZCA both pairs show strong correlation, but this is not the case for PCA and Cholesky whitening.

2.4.7 Recap

Method	Type of usage
ZCA, ZCA-cor:	pure decorrelate, maintain similarity to original data set, interpretability
PCA, PCA-cor:	compression, find effective dimension, reduce dimensionality, feature identification
Cholesk y	time course data, triangular W, $\mathbf{\Phi}$ and $\boldsymbol{P}$

Related models not discussed in this course:

- Factor models: essentially whitening plus an additional error term, factors have rotational freedom just like in whitening
- PLS: similar to PCA but in regression setting (with the choice of latent variables depending on the response)

2.5 Principal Component Analysis (PCA)

2.5.1 PCA transformation

Traditional PCA was invented 1901 by Karl Pearson[2] and is very closely related to **PCA whitening**.

Assume random vector $\boldsymbol{x}$ with $\text{Var}(\boldsymbol{x}) = \mathbf{\Sigma} = \boldsymbol{U}\mathbf{\Lambda}\boldsymbol{U}^T$. PCA is a particular orthogonal transformation of the original $\boldsymbol{x}$ such that the resulting components are orthogonal:

$$\underbrace{\boldsymbol{t}^{\text{PCA}}}_{\text{Principal components}} = \underbrace{\boldsymbol{U}^T}_{\text{Orthogonal matrix}} \boldsymbol{x}$$

$$\text{Var}(\boldsymbol{t}^{\text{PCA}}) = \mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_d \end{pmatrix}$$

Note that while principal components are *orthogonal* they do *not* have unit variance but the variance of principal components t_i equals the eigenvalues λ_i.

Thus PCA itself is *not* a whitening procedure. However, you arrive at PCA whitening by simply by standardising the PCA components: $\boldsymbol{z}^{\text{PCA}} = \mathbf{\Lambda}^{-1/2}\boldsymbol{t}^{\text{PCA}}$

Compression properties:

The total variation is $\text{Tr}(\text{Var}(\boldsymbol{t}^{\text{PCA}})) = \text{Tr}(\mathbf{\Lambda}) = \sum_{j=1}^{d} \lambda_j$. With principle components the fraction $\frac{\lambda_i}{\sum_{j=1}^{d} \lambda_j}$ can be interpreted as the proportion of variation contributed by each component in $\boldsymbol{t}^{\text{PCA}}$ to the total variation. Thus, low ranking components in $\boldsymbol{t}^{\text{PCA}}$ with low variation may be discarded, thus leading to a reduction in dimension.

[2] Pearson, K. 1901. On lines and planes of closest fit to systems of points in space. Philosophical Magazine **2**:559–572.

2.5.2 Application to data

Written in terms of a data matrix $\boldsymbol{X}$ instead of a random vector $\boldsymbol{x}$ PCA becomes:

$$\underbrace{\boldsymbol{T}}_{\text{Sample version of principal components}} = \underbrace{\boldsymbol{X}}_{\text{Data matrix}} \boldsymbol{U}$$

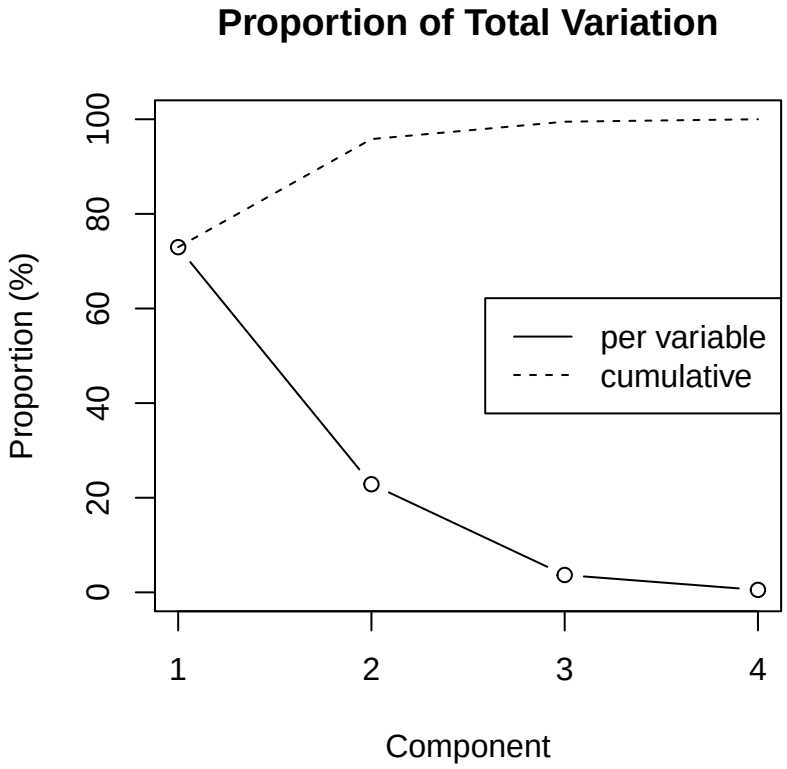
There are now two ways to obtain $\boldsymbol{U}$:

1. Estimate the covariance matrix, e.g. by $\hat{\boldsymbol{\Sigma}} = \frac{1}{n}\boldsymbol{X}_c^T\boldsymbol{X}_c$ where $\boldsymbol{X}_c$ is the column-centred data matrix; then apply the eigenvalue decomposition on $\hat{\boldsymbol{\Sigma}}$ to get $\boldsymbol{U}$.
2. Compute the singular value decomposition of $\boldsymbol{X}_c = \boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T$. As $\hat{\boldsymbol{\Sigma}} = \frac{1}{n}\boldsymbol{X}_c^T\boldsymbol{X}_c = \boldsymbol{U}(\frac{1}{n}\boldsymbol{D}^2)\boldsymbol{U}^T$ you can just use $\boldsymbol{U}$ from the SVD of $\boldsymbol{X}_c$ and there is no need to compute the covariance.

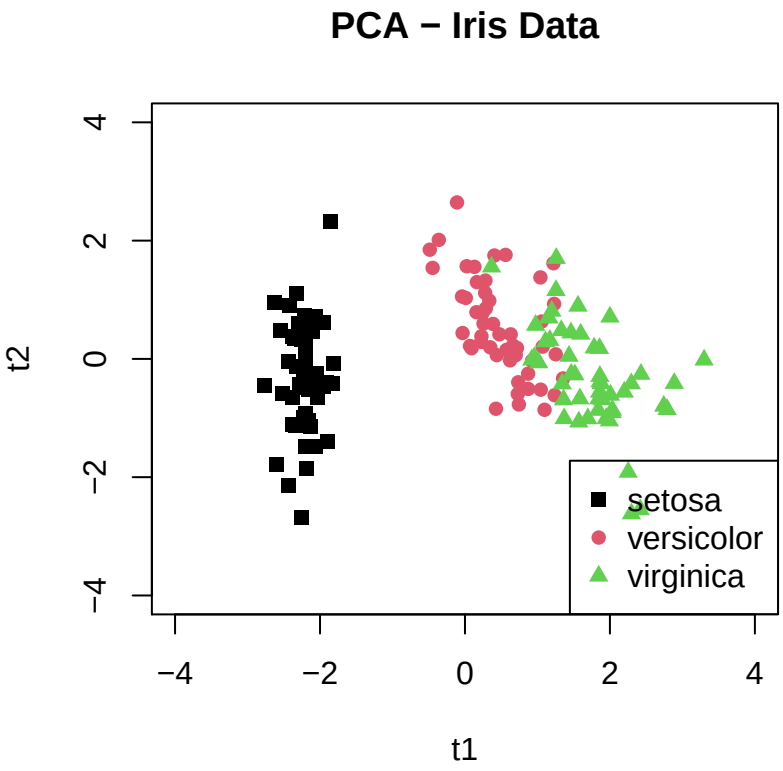
2.5.3 Iris data example

As an example we consider the famous iris flower data set. It consists of data for for botanical variables (sepal length, sepal width, petal length and petal width) measured on 150 flowers from three iris species (setosa, versicolr, virginica). Thus for this data set $d = 4$ and $n = 150$.

We first standardise the data, then compute PCA components and plot the proportion of total variance contributed by each component. This shows that only two PCA components are needed to achieve 95% of the total variation:



A scatter plot plot of the the first two principal components is also informative:



This shows that there groupings among the 150 flowers, corresponding to the species, and that these groups can be characterised by the the principal components.

2.6 Correlation loadings plot to interpret PCA components

2.6.1 PCA correlation loadings

In an earlier section we have learned that for a general whitening transformation the cross-correlations $\boldsymbol{\Psi} = \mathrm{Cor}(\boldsymbol{z}, \boldsymbol{x})$ play the role of correlation loadings in the inverse transformation:

$$\boldsymbol{V}^{-1/2}\boldsymbol{x} = \boldsymbol{\Psi}^T\boldsymbol{z}\,,$$

i.e. they are the coefficients linking the whitening variable $\boldsymbol{z}$ with the standardised $\boldsymbol{x}$. This relationship holds therefore also for PCA whitening with $\boldsymbol{z}^{\mathrm{PCA}} = \boldsymbol{\Lambda}^{-1/2}\boldsymbol{U}^T\boldsymbol{x}$ and $\boldsymbol{\Psi}^{\mathrm{PCA}} = \boldsymbol{\Lambda}^{1/2}\boldsymbol{U}^T\boldsymbol{V}^{-1/2}$.

The classical PCA is not a whitening approach because $\mathrm{Var}(\boldsymbol{t}^{\mathrm{PCA}}) \neq \boldsymbol{I}$. However, we can still compute cross-correlations between the principal components $\boldsymbol{t}^{\mathrm{PCA}}$ and $\boldsymbol{x}$, resulting in

$$\mathrm{Cor}(\boldsymbol{t}^{\mathrm{PCA}}, \boldsymbol{x}) = \boldsymbol{\Lambda}^{1/2}\boldsymbol{U}^T\boldsymbol{V}^{-1/2} = \boldsymbol{\Psi}^{\mathrm{PCA}}$$

Note these are the same as the cross-correlations for PCA-whitening since $\boldsymbol{t}^{\text{PCA}}$ and $\boldsymbol{z}^{\text{PCA}}$ only differ in scale.

The inverse PCA transformation is

$$\boldsymbol{x} = \boldsymbol{U}\boldsymbol{t}^{\text{PCA}}$$

In terms of standardised PCA components and standardised original components it becomes

$$\boldsymbol{V}^{-1/2}\boldsymbol{x} = \boldsymbol{\Psi}^T\boldsymbol{\Lambda}^{-1/2}\boldsymbol{t}^{\text{PCA}}$$

Thus the cross-correlation matrix $\boldsymbol{\Psi}$ plays the role of *correlation loadings* also in classical PCA, i.e. they are the coefficients linking the standardised PCA components with the standardised original components.

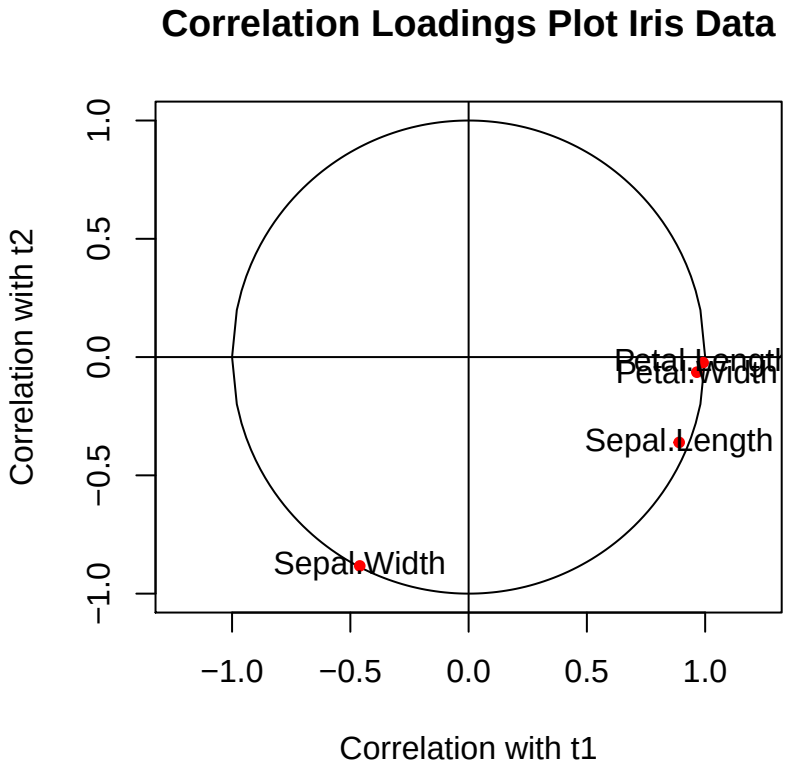
2.6.2 PCA correlation loadings plot

In PCA and PCA-cor whitening as well as in classical PCA the aim is compression, i.e. to find latent variables such that most of the total variation is contributed by a small number of components.

In order to be able to better interpret the top ranking PCA component we can use a visual device called *correlation loadings plot*. For this we compute the correlation between the PCA components 1 and 2 (t_1^{PCA} and t_2^{PCA}) with all original variables $x_1, \ldots, x_d$.

For each original variable x_j we therefore have two numbers betweem -1 and 1, the correlationa $\text{Cor}(t_1^{\text{PCA}}, x_j)$ and $cor(t_2^{\text{PCA}}, x_j)$ that we use as coordinates to draw a point in a plane. By construction, all points have to lie within a unit circle around the origin. As the sum of the squared correlation loadings from all latents component to one specific original variable sum up to one, the sum of the squared loadings from just the first two components is also at most 1. The orginal variables most strongly influenced by the two latent variables will have strong correlation and thus lie near the outer circle, whereas variables that are not influenced by the two latent variables will lie near the origin.

As an example, here is the correlation loadings plot showing the cross-correlation between the first two PCA components and all four variables of the iris flower data set discussed earlier.



The interpretation of this plot is discussed in Worksheet 4.

2.7 CCA whitening (Canonical Correlation Analysis)

Canonical correlation analysis was invented by Harald Hotelling in 1936.[3]

So far, we have looked only into whitening as a **single** vector $\boldsymbol{x}$. In CCA whitening we consider **two vectors** $\boldsymbol{x}$ and $\boldsymbol{y}$ simultaneously:

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix} \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_q \end{pmatrix} \qquad \begin{aligned} \mathrm{Var}(\boldsymbol{x}) &= \boldsymbol{\Sigma}_{\boldsymbol{x}} = \boldsymbol{V}_{\boldsymbol{x}}^{1/2} \boldsymbol{P}_{\boldsymbol{x}} \boldsymbol{V}_{\boldsymbol{x}}^{1/2} \\ \mathrm{Var}(\boldsymbol{y}) &= \boldsymbol{\Sigma}_{\boldsymbol{y}} = \boldsymbol{V}_{\boldsymbol{y}}^{1/2} \boldsymbol{P}_{\boldsymbol{y}} \boldsymbol{V}_{\boldsymbol{y}}^{1/2} \end{aligned}$$

Dimension p Dimension q

$$\begin{aligned} \text{Whitening of } \boldsymbol{x}\text{:} \quad & \boldsymbol{z}_{\boldsymbol{x}} = \boldsymbol{W}_{\boldsymbol{x}} \boldsymbol{x} = \boldsymbol{Q}_{\boldsymbol{x}} \boldsymbol{P}_{\boldsymbol{x}}^{-1/2} \boldsymbol{V}_{\boldsymbol{x}}^{-1/2} \boldsymbol{x} \\ \text{Whitening of } \boldsymbol{y}\text{:} \quad & \boldsymbol{z}_{\boldsymbol{y}} = \boldsymbol{W}_{\boldsymbol{y}} \boldsymbol{y} = \boldsymbol{Q}_{\boldsymbol{y}} \boldsymbol{P}_{\boldsymbol{y}}^{-1/2} \boldsymbol{V}_{\boldsymbol{y}}^{-1/2} \boldsymbol{y} \end{aligned}$$

(note we use the correlation-based form of $\boldsymbol{W}$)

Cross-correlation between $\boldsymbol{z}_{\boldsymbol{y}}$ and $\boldsymbol{z}_{\boldsymbol{y}}$:

[3] Hotelling, H. 1936. Relations between two sets of variates. Biometrika **28**:321–377.

$$\text{Cor}(\boldsymbol{z_x}, \boldsymbol{z_y}) = \boldsymbol{Q_x K Q_y^T}$$

with $\boldsymbol{K} = \boldsymbol{P_x^{-1/2} P_{xy} P_y^{-1/2}}$.

Idea: we can choose suitable orthogonal matrices $\boldsymbol{Q_x}$ and $\boldsymbol{Q_y}$ by putting constraints on the cross-correlation.

CCA: we aim for a *diagonal* $\text{Cor}(\boldsymbol{z_x}, \boldsymbol{z_y})$ so that each component in $\boldsymbol{z_x}$ only influences one (the corresponding) component in $\boldsymbol{z_y}$.

Motivation: pairs of "modules" represented by components of $\boldsymbol{z_x}$ and $\boldsymbol{z_y}$ influencing each other (and not anyone other module).

$$\boldsymbol{z_x} = \begin{pmatrix} z_1^x \\ z_2^x \\ \vdots \\ z_p^x \end{pmatrix} \quad \boldsymbol{z_y} = \begin{pmatrix} z_1^y \\ z_2^y \\ \vdots \\ z_q^y \end{pmatrix}$$

\end{align}

$$\text{Cor}(\boldsymbol{z_x}, \boldsymbol{z_y}) = \begin{pmatrix} d_1 & \dots & 0 \\ \vdots & \vdots & \\ 0 & \dots & d_m \end{pmatrix}$$

where d_i are the *canonical correlations* and $m = \min(p, q)$.

2.7.1 How to make cross-correlation matrix $\text{Cor}(\boldsymbol{z_x}, \boldsymbol{z_y})$ diagonal?

- Use Singular Value Decomposition (SVD) of matrix $\boldsymbol{K}$:

  $$\boldsymbol{K} = (\boldsymbol{Q_x^{\text{CCA}}})^T \boldsymbol{D} \boldsymbol{Q_y^{\text{CCA}}}$$

  where $\boldsymbol{D}$ is the diagonal matrix containing the singular values of $\boldsymbol{K}$
- This yields orthogonal matrices $\boldsymbol{Q_x^{\text{CCA}}}$ and $\boldsymbol{Q_y^{\text{CCA}}}$ and thus the desired whitened matrices $\boldsymbol{W_x^{\text{CCA}}}$ and $\boldsymbol{W_y^{\text{CCA}}}$
- As a result $\text{Cor}(\boldsymbol{z_x}, \boldsymbol{z_y}) = \boldsymbol{D}$ i.e. singular values of $\boldsymbol{K}$ are identical to canonical correlations d_i!

$\longrightarrow$ $\boldsymbol{Q_x^{\text{CCA}}}$ and $\boldsymbol{Q_y^{\text{CCA}}}$ are determined by the diagonality constraint (and are different to the other previously discussed whitening methods).

Note that the signs of corresponding in columns in $\boldsymbol{Q_x^{\text{CCA}}}$ and $\boldsymbol{Q_y^{\text{CCA}}}$ are not identified. Traditionally, in an SVD the signs are chosen such that the singular values are positive. However, if we impose positive-diagonality on $\boldsymbol{Q_x^{\text{CCA}}}$ and $\boldsymbol{Q_y^{\text{CCA}}}$, and thus positive-diagonality on the cross-correlations $\boldsymbol{\Psi_x}$ and $\boldsymbol{\Psi_y}$, then the canonical correlations may take on both positive and negative values.

2.7.2 Related methods

- O2PLS: similar to CCA but using orthogonal projections (thus in O2PLS the latent variables underlying $\boldsymbol{x}$ and $\boldsymbol{y}$ are not orthogonal)
- Vector correlation: aggregates the squared canonical correlations into a single overall measure of association between two random vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ (see Chapter 5 on multivariate dependencies).

Chapter 3

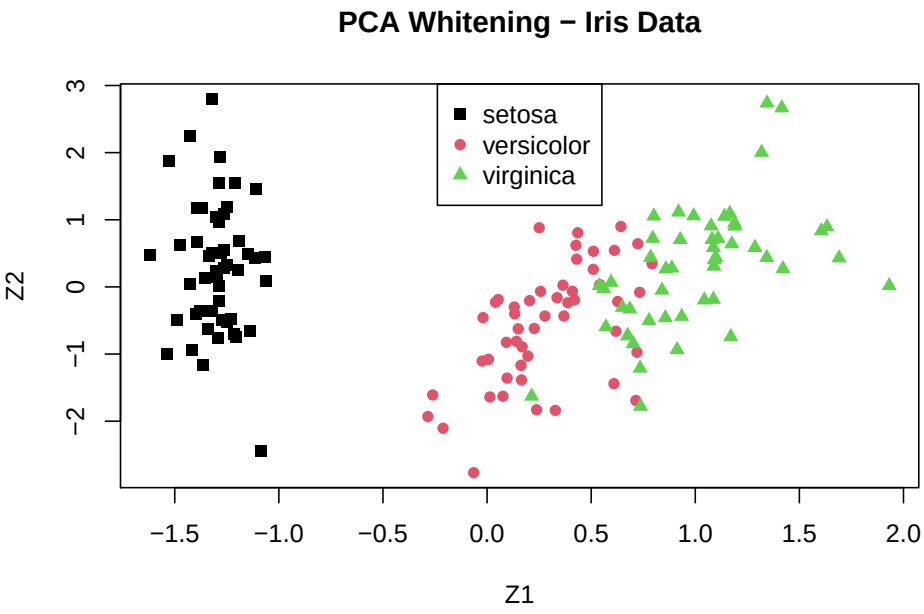
Unsupervised learning and clustering

3.1 Challenges in supervised learning

3.1.1 Objective

We observe data $x_1, \ldots, x_n$ for n objects (or subjects). Each sample x_i is a vector of dimension d. Thus, for each of the n objects / subjects we have measurements on d variables. The aim of unsupervised learning is to identify patters relating the objects/subjects based on the information available in x_i. Note that unsupervised learning *only* uses this information and nothing else.

For illustration consider the first two principal components of the Iris flower data (see e.g. Worksheet 4):



Clearly there is a group structure among the samples that is linked to particular patterns in the first two principal components.

Note that in this plot we have used additional information, the class labels (setosa, versicolor, virginica), to highlighting the true underlying structure (the three flower species).

In **unsupervised learning** the class labels are (assumed to be) unknown, and the aim is to infer the clustering and thus the classes labels.[1]

There are many methods for clustering and unsupervise learning, both purely algorithmic as well as probabilistic. In this chapter we will study a few of the most commonly used approaches.

3.1.2 Questions and problems

In order to implement unsupervised learning we need to address a number of questions:

- how do we define clusters?
- how do we learn / infer clusters?
- how many clusters are there? (this is surprisingly difficult!)
- how can we assess the uncertainty of clusters?

Once we know the clusters we are also interested in:

- which features define / separate each cluster?

(note this is a feature / variable selection problem, discussed in in supervised learning).

Many of these problems and questions are highly specific to the data at hand. Correspondingly, there are many different types of methods and models for clustering and unsupervised learning.

In terms of representing the data, unsupervised learning tries to balance between the following two extremes:

1) all objects are grouped into a single cluster (low complexity model)
2) all objects are put into their own cluster (high complexity model)

In practise, the aim is to find a compromise, i.e. a model that captures the structure in the data with appropriate complexity — not too low and not too complex.

3.1.3 Why is clustering difficult?

Partioning problem (combinatorics): How many partitions of n objects (say flowers) into K groups (say species) exists?

Answer:

[1] In contrast, in **supervised learning** (to be discussed in a subsequent chapter) the class labels are known for a subset of the data (the training data set) and are required to learn a prediction function.

$$S(n, K) = \left\{ \begin{array}{c} n \\ K \end{array} \right\}$$

this is the "Sterling number of the second type".

For large n:

$$S(n, K) \approx \frac{K^n}{K!}$$

Example:

n	K	Number of possible partitions
15	3	$\approx$ 2.4 million (10^6)
20	4	$\approx$ 2.4 billion (10^9)
$\vdots$		
100	5	$\approx 6.6 \times 10^{76}$

These are enormously big numbers even for relatively small problems!

$\Longrightarrow$ Clustering / partitioning / structure discovery is not easy!

$\Longrightarrow$ We cannot expect perfect answers or a single "true" clustering

In fact, as a model of the data many differnt clusterings may fit the data equally well.

$\Longrightarrow$ We need to assesse the uncertainty of the clustering

This can be done as part of probabilistic modelling or by resampling (e.g., bootstrap).

3.1.4 Common types of clustering methods

There are very many different clustering algorithms!

We consider the following two broad types of methods:

1) **Algorithmic clustering methods** (these are not explicitly based on a probabilistic model)

- K-means
- PAM
- hierarchical clustering (distance or similarity-based, divise and agglomerative)

  pros: fast, effective algorithms to find at least some grouping **cons:** no probabilistic interpretation, blackbox methods

2) **Model-based clustering** (based on a probabilistic model)

- mixture models (e.g. Gaussian mixture models, GMMs, non-hierarchical)
- graphical models (e.g. Bayesian networks, Gaussian graphical models GGM, trees and networks)

pros: full probabilistic model with all corresponding advantages
cons: computationally very expensive, sometimes impossible to compute exactly.

3.2 Hierarchical clustering

3.2.1 Tree-like structures

Often, categorisations of objects are nested, i.e. there sub-categories of categories etc. These can be naturally represented by **tree-like hierarchical structures**.

In many branches of science hierarchical clusterings are widely employed, for example in evolutionary biology: see e.g.

- Tree of Life explaining the biodiversity of life
- phylogenetic trees among species (e.g. vertebrata)
- population genetic trees to describe human evolution
- taxonomic trees for plant species
- etc.

Note that when visualising hierarchical structures typically the corresponding tree is depicted facing downwards, i.e. the root of the tree is shown on the top, and the tips/leaves of the tree are shown at the bottom!

In order to obtain such a hierarchical clustering from data two opposing strategies are commonly used:

1) **divisive or recursive partitioning algorithms**
   - grow the tree from the root downwards
   - first determine the main two clusters, then recursively refine the clusters further.
2) **agglomerative algorithms**
   - grow the tree from the leafs upwards
   - successively form partitions by first joining individual object together, then recursively join groups of items together, until all is merged.

In the following we discuss a number of popular hierarchical agglomerative clustering algorithms that are based on the pairwise distances / similarities (a $n \times n$ matrix) among all data points.

3.2.2 Agglomerative hierarchical clustering algorithms

A general algorithm for agglomerative construction of a hierarchical clustering works as follows:

Initialisation:

Compute a dissimilarity / distance matrix between all pairs of objects where "objects" are single data points at this stage but later are also be sets of data points.

Iterative procedure:

1) identify the pair of objects with the smallest distance. These two objects are then merged together into a common set. Create an internal node in the tree to describe this coalescent event.

2) update the distance matrix by computing the distances between the new set and all other objects. If the new set contains all data points the procedure terminates.

For actual implementation of this algorithm two key ingredients are needed:

1) a distance measure $d(\boldsymbol{a}, \boldsymbol{b})$ between two individual elementary data points $\boldsymbol{a}$ and $\boldsymbol{b}$.

   This is typically one of the following:

   - Euclidean distance $d(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{\sum_{i=1}^{d}(a_i - b_i)^2} = \sqrt{(\boldsymbol{a}-\boldsymbol{b})^T(\boldsymbol{a}-\boldsymbol{b})}$
   - Manhattan distance $d(\boldsymbol{a}, \boldsymbol{b}) = \sum_{i=1}^{d} |a_i - b_i|$
   - Maximum norm $d(\boldsymbol{a}, \boldsymbol{b}) = \max_{i \in \{1,\ldots,d\}} |a_i - b_i|$

   In the end, making the correct choice of distance will require subject knowledge about the data!

2) a distance measure $d(A, B)$ between two sets of objects $A = \{\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_{n_A}\}$ and $B = \{\boldsymbol{b}_1, \boldsymbol{b}_2, \ldots, \boldsymbol{b}_{n_B}\}$ of size n_A and n_B, respectively.

   To determine the distance $d(A, B)$ between these two sets the following measures are often employed:

   - **complete linkage** (max. distance): $d(A, B) = \max_{\boldsymbol{a}_i \in A, \boldsymbol{b}_i \in B} d(\boldsymbol{a}_i, \boldsymbol{b}_i)$
   - **single linkage** (min. distance): $d(A, B) = \min_{\boldsymbol{a}_i \in A, \boldsymbol{b}_i \in B} d(\boldsymbol{a}_i, \boldsymbol{b}_i)$
   - **average linkage** (avg. distance): $d(A, B) = \frac{1}{n_A n_B} \sum_{\boldsymbol{a}_i \in A} \sum_{\boldsymbol{b}_i \in B} d(\boldsymbol{a}_i, \boldsymbol{b}_i)$

3.2.3 Ward's clustering method

Another agglomerative hierarchical procedure is **Ward's minimum variance approach**. In this approach in each iteration the two sets A and B are merged that lead to the *smallest increase in within-group variation, or equivalenty, 5h3 total within-group sum of squares* (cf. K-means). The centroids of the two sets is given by $\boldsymbol{\mu}_A = \frac{1}{n_A} \sum_{\boldsymbol{a}_i \in A} \boldsymbol{a}_i$ and $\boldsymbol{\mu}_B = \frac{1}{n_B} \sum_{\boldsymbol{b}_i \in B} \boldsymbol{b}_i$.

The within-group sum of squares for group A is

$$w_A = \sum_{\boldsymbol{a}_i \in A} (\boldsymbol{a}_i - \boldsymbol{\mu}_A)^T (\boldsymbol{a}_i - \boldsymbol{\mu}_A)$$

and is computed here on the basis of the difference of the observations $\boldsymbol{a}_i$ relative to their mean $\boldsymbol{\mu}_A$. However, it is also possible to compute it from the pairwise differences between the observations using

$$w_A = \frac{1}{n_A} \sum_{\boldsymbol{a}_i, \boldsymbol{a}_j \in A, i<j} (\boldsymbol{a}_i - \boldsymbol{a}_j)^T (\boldsymbol{a}_i - \boldsymbol{a}_j)$$

This trick is used in Ward's clustering method by constructing a distance measure between to sets A and B as

$$d(A,B) = w_{A\cup B} - w_A - w_B\,.$$

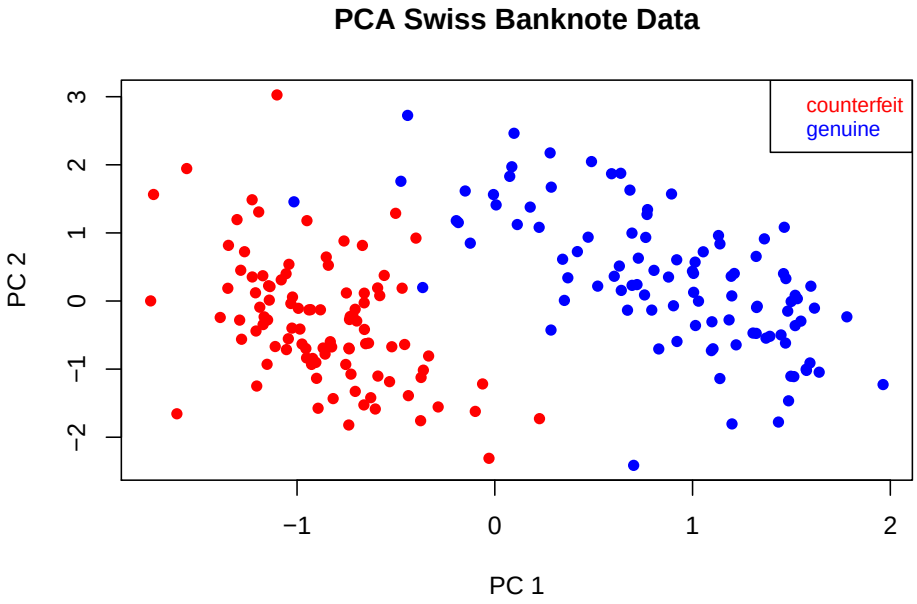
Correspondingly, the distance between two elementary data points $\boldsymbol{a}$ and $\boldsymbol{b}$ is the squared Euclidean distance

$$d(\boldsymbol{a},\boldsymbol{b}) = (\boldsymbol{a}-\boldsymbol{b})^T(\boldsymbol{a}-\boldsymbol{b})\,.$$

3.2.4 Application to Swiss banknote data set

This data set is reports 6 pysical measurements on 200 Swiss bank notes. Of the 200 notes 100 are genuine and 100 are counterfeit. The measurements are: length, left width, right width, bottom margin, top margin, diagonal length of the bank notes.

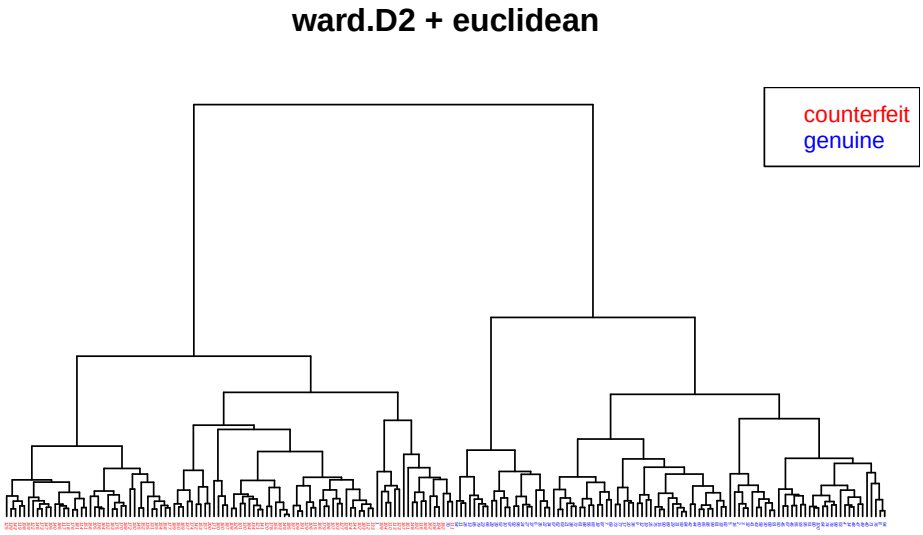
Plotting the first to PCAs of this data shows that there are indeed two well defined groups, and that these groups correspond precisely to the genuine and counterfeit banknotes:



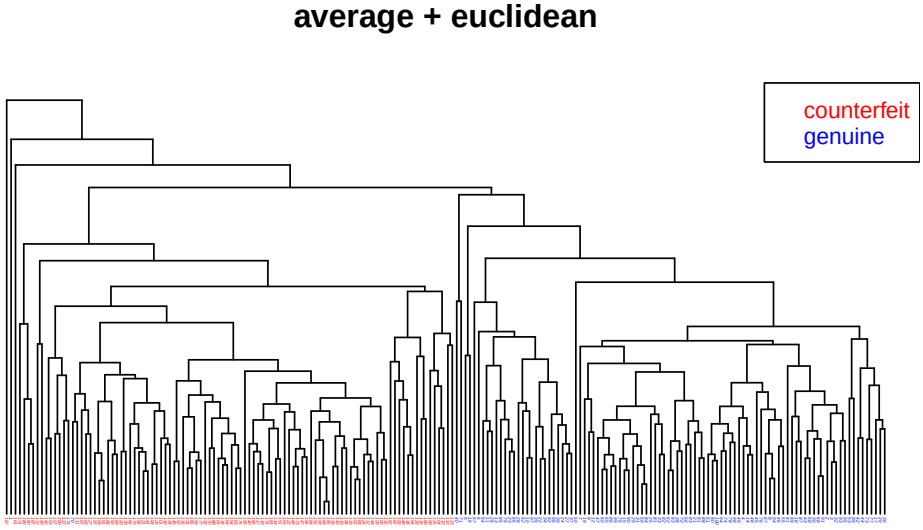
We now compare the hierarchical clusterings of the Swiss bank note data using four different methods using Euclidean distance.

An interactive R Shiny web app of this analysis (which also allows to explore further distance measures) is available online at https://minerva.it.manchester.ac.uk/shiny/strimmer/hclust/ .

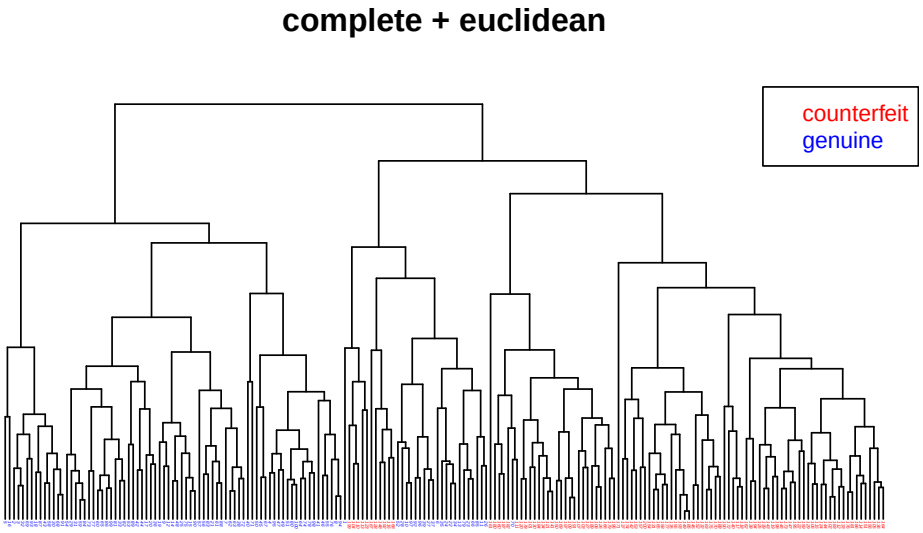
Ward.D2 (=Ward's method):



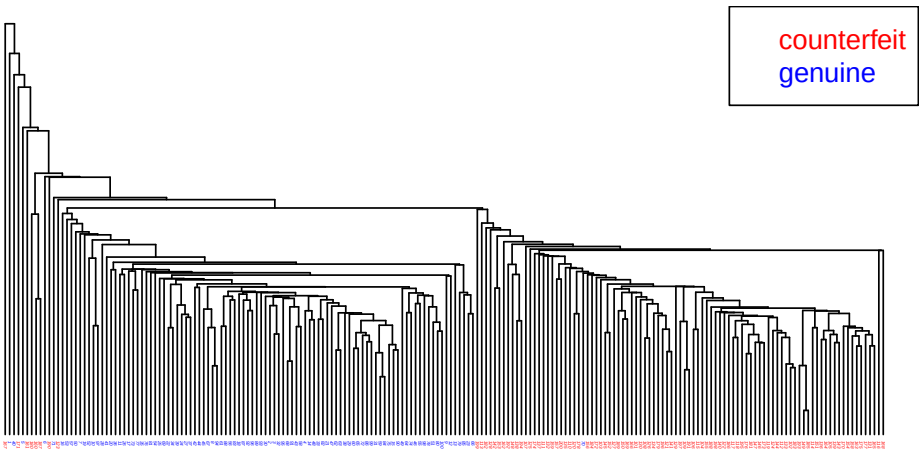
Average linkage:



Complete linkage:



Single linkage:



Result:

- All four trees / hierarchical clusterings are quite different!
- The Ward.D2 method is the only one that finds the correct grouping (except for a single error).

3.2.5 Assessment of the uncertainty of hierarchical clusterings

In practical application of hierarchical clustering methods is is essential to evaluate the stability and uncertainty of the obtained groupings. This is often done as follows using the "bootstrap":

- Sampling with replacement is used to generate a number of so-called bootstrap data sets (say $B = 200$) similar to the original one. Specifically, we create new data matrices by repeatedly randomly selecting columns (variables) from the original data matrix for inclusion in the bootstrap data matrix. Note that we sample columns as our aim is to cluster the samples.
- Subsequently, a hierarchical clustering is computed for each of the bootstrap data sets. As a result, we now have an "ensemble" of B bootstrap trees.
- Finally, analysis of the clusters (bipartions) shown in all the bootstrap trees allows to count the clusters that appear frequently, and also those that appear less frequently. These counts provide a measure of the stability of the clusterings appearing in the original tree.
- Additionally, from the bootstrap tree we can also compute a consensus tree containing the most stable clusters. This an be viewed as an "ensemble average" of all the bootstrap trees.

A disadvantage of this procedure is that bootstrapping trees is computationally very very expensive, as the original procedure is already time consuming but now needs to be repeated a large number of times.

3.3 K-means clustering

3.3.1 General aims

- Partition the data into K groups, with K given in advance
- The groups are non-overlapping, so each of the n data points / objects $\boldsymbol{x}_i$ is assigned to exactly one of the K groups
- maximise the homogeneity with each group (i.e. each group should contain similar objects)
- maximise the heterogeneity among the different groups (i.e each group should differ from the other groups)

3.3.2 Algorithm

For each group $k \in \{1, \ldots, K\}$ we assume a group mean $\boldsymbol{\mu}_k$.
After running K-means we will get estimates of $\hat{\boldsymbol{\mu}}_k$ of the group means, as well as an allocation of each data point to one of the classes.

Initialisation:

At the start of the algorithm the n observations $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are randomly allocated to one of the K groups. The resulting assignment is given by the function $C(\boldsymbol{x}_i) \in \{1, \ldots, K\}$. With $G_k = \{i | C(\boldsymbol{x}_i) = k\}$ we denote the set of indices of the data points in cluster k, and with $n_k = |G_k|$ the number of samples in cluster k.

Iterative refinement:

1) estimate the group means by

$$\hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i \in G_k} \boldsymbol{x}_i$$

2) update group assignment: each data point $\boldsymbol{x}_i$ is (re)assigned to the group k with the nearest $\hat{\boldsymbol{\mu}}_k$ (in terms of the Euclidean norm). Specifically, the assignment $C(\boldsymbol{x}_i)$ is updated to

$$\begin{aligned} C(\boldsymbol{x}_i) &= \arg\min_k |\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k|_2 \\ &= \arg\min_k (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k) \end{aligned}$$

Steps 1 and 2 are repeated until the algorithm converges (or an upper limit of repeats is reached).

3.3.3 Properties

Despite its simplicity K-means is a surprisingly effective clustering algorithms. The final clustering depends on the initialisation so it is often useful to run K-means several times with different starting allocations of the data points.

As a result of the way the clusters are assigned in K-means this leads to cluster boundaries that form a Voronoi tesselation (cf. https://en.wikipedia.org/wiki/Voronoi_diagram) around the cluster means.

Later we will also discuss the connection of K-means with probabilistic clustering using Gaussian mixture models.

3.3.4 Choosing the number of clusters

Once the K-means clustering has been obtained it is insightful to compute:

a) the total within-group sum of squares SSW (tot.withinss), or total unexplained sum of squares:

$$SSW = \sum_{k=1}^{K} \sum_{i \in G_k} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)$$

This quantity decreases with K and is zero for $K = n$. The K-means algorithm tries to minimise this quantity but it will typically only find a local minimum rather than the global one.

b) the between-group sum of squares SSB (betweenss), or explained sum of squares:

$$SSB = \sum_{k=1}^{K} n_k (\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)^T (\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)$$

where $\hat{\boldsymbol{\mu}}_0 = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i = \frac{1}{n} \sum_{k=1}^{K} n_k \hat{\boldsymbol{\mu}}_k$ is the global mean of the samples. SSB increases with the number of clusters K until for $K = n$ it becomes equal to

c) the total sum of squares

$$SST = \sum_{i=1}^{n} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_0)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_0) \,.$$

By construction $SST = SSB + SSW$ for any K (i.e. SST is a constant independent of K).

If divide the sum of squares by the sample size n we get $T = \frac{SST}{n}$ as the *total variation*, $B = \frac{SSW}{n}$ as the *explained variation* and $W = \frac{SSW}{n}$ as the total *unexplained variation* , with $T = B + W$.

For deciding on the optimal number of clusters we can run K-means for various settings of K and then choose the smallest K for which the explained variation B is not significantly worse compared to a model with substantially larger number of clusters (see example below).

3.3.5 K-medoids aka PAM

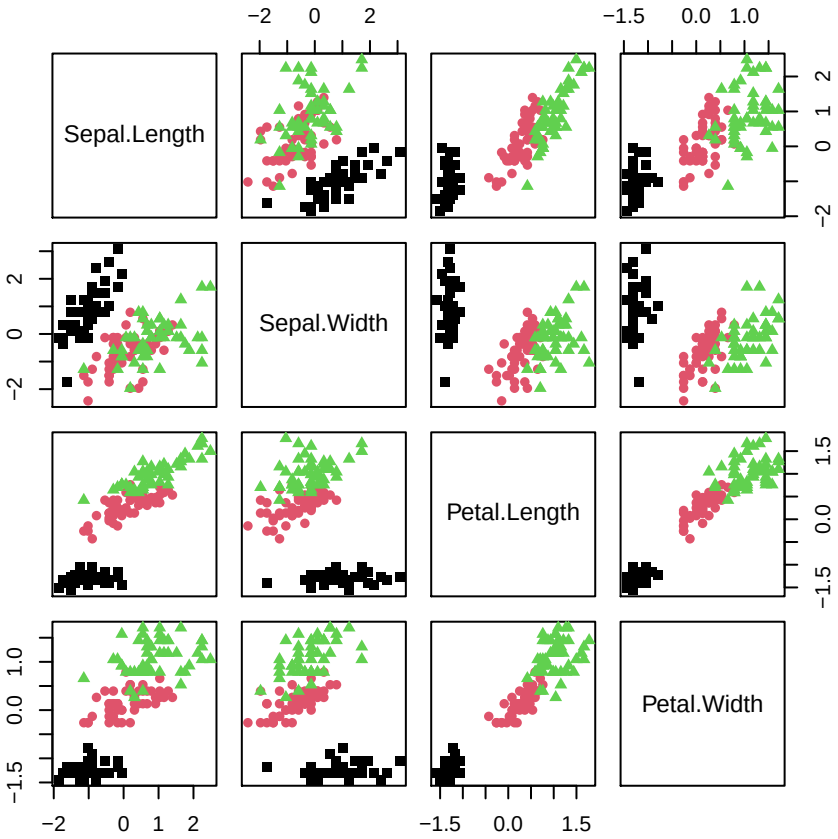
A closely related clustering method is K-medoids or PAM ("Partitioning Around Medoids").

This works exactly like K-means, only that

- instead of the estimated group means $\hat{\boldsymbol{\mu}}_k$ one member of each group is selected as its representative (the socalled "medoid")
- instead of squared Euclidean distance other dissimilarity measures are also allowed.

3.3.6 Application of K-means to Iris data

Scatter plots of Iris data:



The R output from a K-means analysis with true number of clusters specified ($K = 3$) is:

```
## K-means clustering with 3 clusters of sizes 33, 21, 96
##
## Cluster means:
##   Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1   -0.8135055   1.3145538   -1.2825372  -1.2156393
## 2   -1.3232208  -0.3718921   -1.1334386  -1.1111395
## 3    0.5690971  -0.3705265    0.6888118   0.6609378
##
## Clustering vector:
##   [1] 1 2 2 2 1 1 1 1 2 2 1 1 2 2 1 1 1 1 1 1 1 1 1 1 2 1 1 1 2 2 1 1 1 2 2 1
##  [38] 1 2 1 1 2 2 1 1 2 1 2 1 1 3 3 3 3 3 3 3 2 3 3 2 3 3 3 3 3 3 3 3 3 3 3 3
##  [75] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 2 3 3 3 3 2 3 3 3 3 3 3 3 3 3 3 3
## [112] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
## [149] 3 3
##
## Within cluster sum of squares by cluster:
## [1]  17.33362  23.15862 149.25899
##  (between_SS / total_SS =  68.2 %)
##
## Available components:
```

```
##
## [1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
## [6] "betweenss"    "size"         "iter"         "ifault"
```

The corresponding total within-group sum of squares (*SSW*, tot.withinss) is

```
kmeans.out$tot.withinss
```

```
## [1] 189.7512
```

and the between-group sum of squares (*SSB*, betweenss) is

```
kmeans.out$betweenss
```

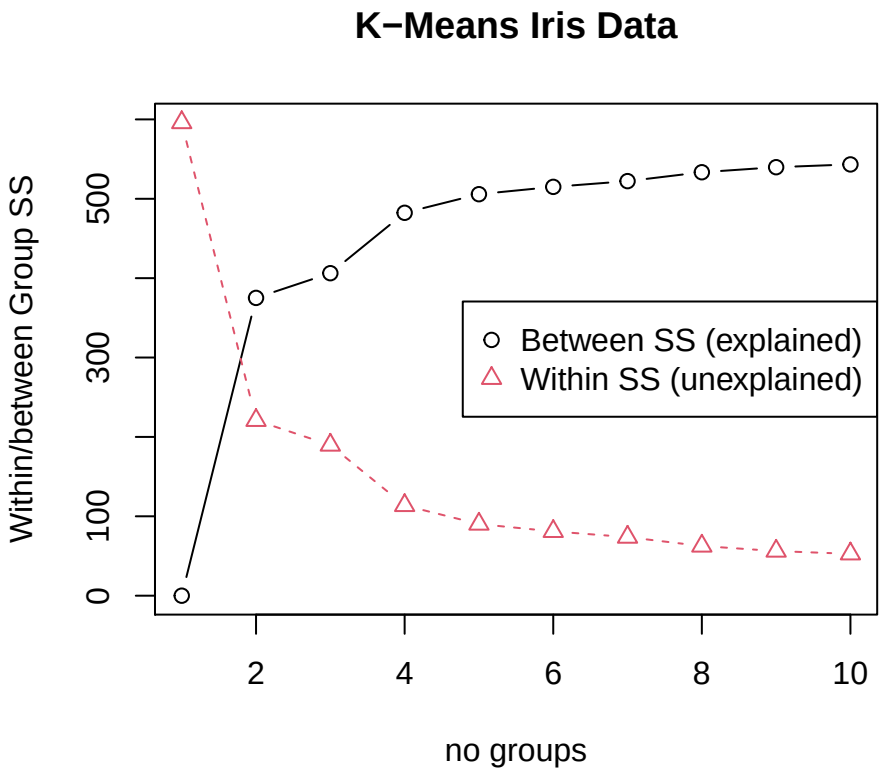
```
## [1] 406.2488
```

By comparing with the known class assignments we can assess the accuracy of *K*-means clustering:

```
table(L.iris, kmeans.out$cluster)
```

```
##
## L.iris         1  2  3
##   setosa      33 17  0
##   versicolor   0  4 46
##   virginica    0  0 50
```

For choosing *K* we run *K*-means several times and compute within and between cluster variation in dependence of *K*:



Thus, $K = 3$ clusters seem appropriate since the the explained variation does not significantly improve (and the unexplained variation does not significantly decrease) with a further increase of the number of clusters.

3.4 Mixture models

3.4.1 Finite mixture model

- K groups / classes / categories, with the number K specified and finite
- each class $k \in \{1, \ldots, K\}$ is modeled by its own distribution F_k with own parameters $\boldsymbol{\theta}_k$.
- density in each class: $f_k(\boldsymbol{x}) = f(\boldsymbol{x}|k)$ with $k \in 1, \ldots, K$
- mixing weight of each class: $\Pr(k) = \pi_k$ with $\sum_{k=1}^{K} \pi_k = 1$
- joint density $f(\boldsymbol{x}, k) = f(\boldsymbol{x}|k)\Pr(k) = f_k(\boldsymbol{x})\pi_k$

This results in the mixture density / marginal density

$$f(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x})$$

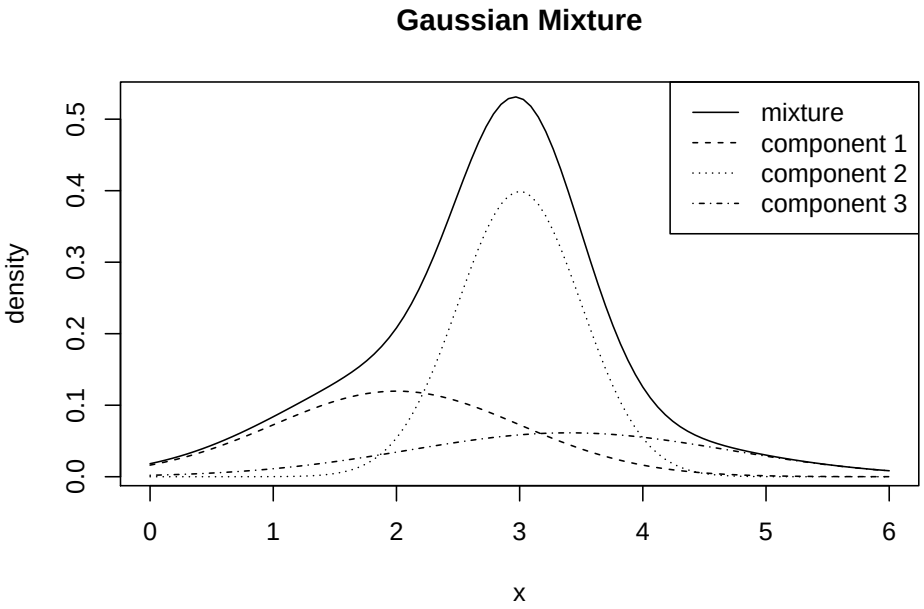
Very often one uses **multivariate normal components** $f_k(\boldsymbol{x}) = N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
$\Longrightarrow$ **Gaussian mixture model** (GMM)

Mixture models are fundamental not just in clustering but for many other applications (e.g. classification).

Note: don't confuse *mixture model* with *mixed model* (=random effects regression model)

3.4.2 Example of mixture of three univariate normal densities:

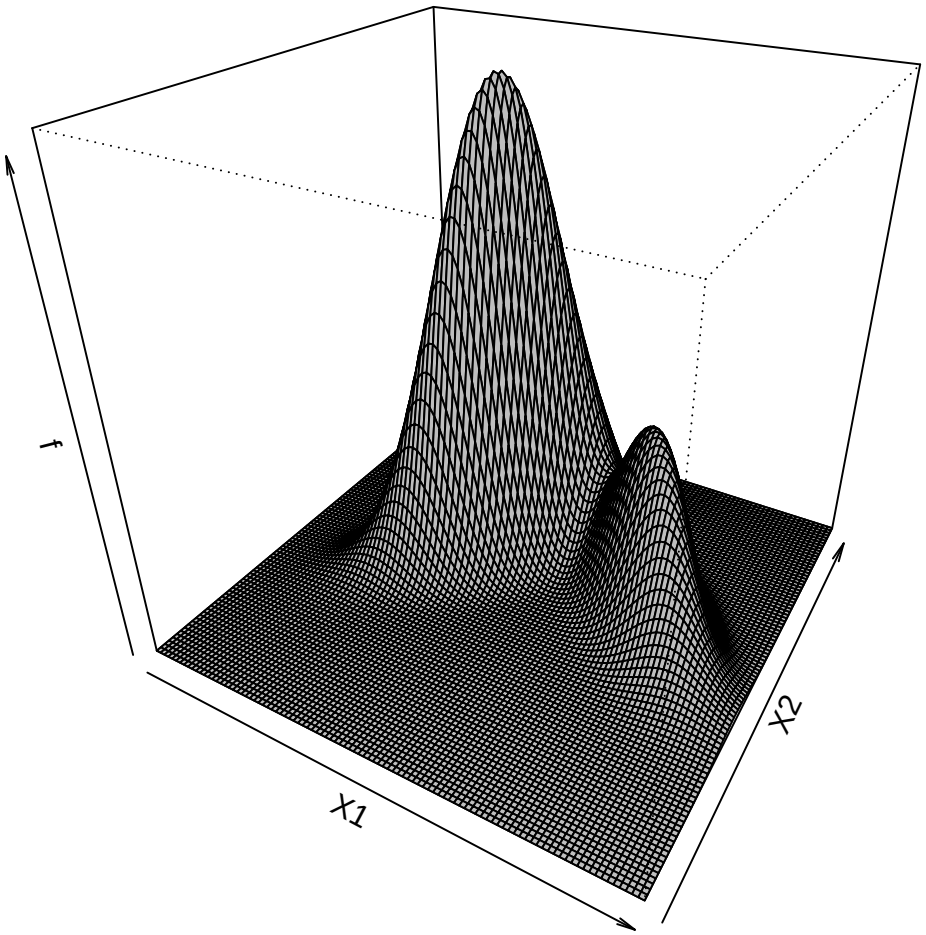
$$f(x) = 0.3\, N(2, 1^2) + 0.5\, N(3, 0.5^2) + 0.2\, N(3.4, 1.3^2)$$



In this case it is clear already by visual inspection that the three subcomponents will not be identifiable.

3.4.3 Example of a mixture of two bivariate normal densities

$$f(\boldsymbol{x}) = 0.7\, N_2\left(\begin{pmatrix}-1\\1\end{pmatrix}, \begin{pmatrix}1 & 0.7\\0.7 & 1\end{pmatrix}\right) + 0.3\, N_2\left(\begin{pmatrix}2.5\\0.5\end{pmatrix}, \begin{pmatrix}1 & -0.7\\-0.7 & 1\end{pmatrix}\right)$$



3.4.4 Sampling from a mixture model and latent allocation variable formulation

Assuming we know how to sample from the components $f_k(\boldsymbol{x})$ of the mixture model it is straightforward to set up a procedure for sampling from the mixture $f(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x})$.

This is done in a two-step generative process:

1. draw from categorical distribution with parameters $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_k)^T$:

$$\boldsymbol{z} \sim \text{Categ}(\boldsymbol{\pi})$$

the vector $\boldsymbol{z} = (z_1, \ldots, z_K)^T$ indicating the group allocation. The group index k is given by $\{k : z_k = 1\}$.

2. Subsequently, sample from the component k selected in step 1:

$$\boldsymbol{x} \sim F_k$$

This two-stage approach is also called *latent allocation variable formulation* of a mixture model, with $\boldsymbol{z}$ (or equivalently k) being the latent variable.

The two-step process needs to repeated for each sample drawn from the mixture (i.e. every time a new latent variable $\boldsymbol{z}$ is generated).

In probabilistic clustering the aim is to infer the state of $\boldsymbol{z}$ for all observed samples.

3.4.5 Predicting the group allocation of a given sample

If we know the mixture model and its components we can predict the probability that an observation $\boldsymbol{x}$ falls in group k using Bayes theorem:

$$z_k = \Pr(k|\boldsymbol{x}) = \frac{\pi_k f_k(\boldsymbol{x})}{f(\boldsymbol{x})}$$

Thus, assuming we can calculate this probability we can **perform probabilistic clustering** by assigning each sample to the class with the largest probability. Unlike in algorithmic clustering, we also get an impression of the uncertainty of the class assignment, since for each sample $\boldsymbol{x}$ get the vector

$$\boldsymbol{z} = (z_1, \ldots, z_K)^T$$

and thus can see if there are several classes with similar assignment probability. This will be the case, e.g., if $\boldsymbol{x}$ lies near the boundary between two classes. Note that $\sum_{k=1}^{K} z_k = 1$.

3.4.6 Decomposition of covariance and total variation

Just like in regression you can decompose the variance into an explained and unexplained part.

The conditional means and variances for each class are $\mathrm{E}(\boldsymbol{x}|k) = \boldsymbol{\mu}_k$ and $\mathrm{Var}(\boldsymbol{x}|k) = \boldsymbol{\Sigma}_k$, and the probability of class k is given by $\Pr(k) = \pi_k$. Using the law of total expectation we can therefore obtain the mean of the mixture density as follows:

$$\begin{aligned}\mathrm{E}(\boldsymbol{x}) &= \mathrm{E}(\mathrm{E}(\boldsymbol{x}|k)) \\ &= \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k \\ &= \boldsymbol{\mu}_0\end{aligned}$$

Similarly, using the law of total variance we compute the marginal variance:

$$\underbrace{\mathrm{Var}(\boldsymbol{x})}_{\text{total}} = \underbrace{\mathrm{Var}(\mathrm{E}(\boldsymbol{x}|k))}_{\text{explained / between-group}} + \underbrace{\mathrm{E}(\mathrm{Var}(\boldsymbol{x}|k))}_{\text{unexplained / within-group}}$$

$$\boldsymbol{\Sigma}_0 = \sum_{k=1}^{K} \pi_k (\boldsymbol{\mu}_k - \boldsymbol{\mu}_0)(\boldsymbol{\mu}_k - \boldsymbol{\mu}_0)^T + \sum_{k=1}^{K} \pi_k \boldsymbol{\Sigma}_k$$

The total variation is given by the trace of the covariance matrix, yielding empirical estimates

$$T = \text{Tr}\left(\hat{\mathbf{\Sigma}}_0\right) = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_0)^T(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_0)$$

$$B = \text{Tr}\left(\sum_{k=1}^{K}\hat{\pi}_k(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)^T\right) = \frac{1}{n}\sum_{k=1}^{K} n_k(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)^T(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)$$

$$W = \text{Tr}\left(\sum_{k=1}^{K}\hat{\pi}_k\hat{\mathbf{\Sigma}}_k\right) = \frac{1}{n}\sum_{k=1}^{K}\sum_{i\in G_k}(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)$$

Compare the above with the $T = B + W$ decomposition of total variation in K-means!

3.4.7 Variation 1: Infinite mixture model

It is possible to construct mixture models with infinitely many components!

Most commonly known example is Dirichlet process mixture model (DPM):

$$\sum_{k=1}^{\infty}\pi_k f_k(\boldsymbol{x})$$

with $\sum_{k=1}^{\infty}\pi_k = 1$ and where the weight π_k are taken from a infinitely dimensional Dirichlet distribution (=Dirichlet process).

DPMs are useful for clustering since with them it is not necessary to determine the number of clusters a priori (since it by definition has infinitely many!). Instead, the number of clusters is a by-product of the fit of the model to observed data.

Related: **"Chinese restaurant process"** - https://en.wikipedia.org/wiki/Chinese_restaurant_process

This describes an algorithm for the allocation process of samples ("persons") to the groups ("restaurant tables") in a DPM.

See also **"stick-breaking process":** https://en.wikipedia.org/wiki/Dirichlet_process#The_stick-breaking_process

3.4.8 Variation 2: Semiparametric mixture model with two classes

A very common model is the following two-component univariate mixture model

$$f(x) = \pi_0 f_0(x) + (1 - \pi_0)f_A(\boldsymbol{x})$$

- f_0: null model, typically parametric such as normal distribution
- f_A: alternative model, typically nonparametric

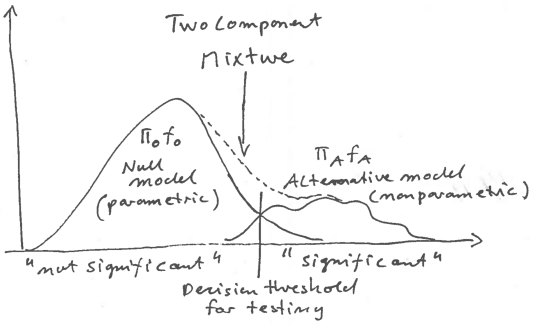
- π_0: prior probability of null model

Using Bayes theorem this allows to compute probability that an observation x belongs to the null model:

$$\Pr(\text{Null}|x) = \frac{\pi_0 f_0(x)}{f(x)}$$

This is called the *local false discovery rate*.

The semi-parametric mixture model is the foundation for statistical testing which is based on defining decision thresholds to separate null model ("not significant") from alternative model ("significant"):



See the lecture notes for Statistical Methods MATH20802 (year 2) for more details.

3.5 Fitting mixture models to data

3.5.1 Direct estimation of mixture model parameters

Given data matrix $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)^T$ with observations from n samples we would like to fit the mixture model $f(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x})$ and learn its parameters $\boldsymbol{\theta}$, for example by maximising the corresponding marginal log-likelihood function with regard to $\boldsymbol{\theta}$:

$$\log L(\boldsymbol{\theta}|\boldsymbol{X}) = \sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x}_i) \right)$$

For a Gaussian mixture model the parameters are $\boldsymbol{\theta} = \{\boldsymbol{\pi}, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K\}$.

However, in practise evaluation of this likelihood function may be difficult, in part due to the form of the log-likelihood function (note the sum inside the logarithm), but also due to its singularities and non-identiability problems.

The above log-likelihood function is also called the *observed data* log-likelihood, or the *incomplete data* log-likelihood, in contrast to the *complete data* log-likelihood described further below.

3.5.2 Estimate mixture model parameters using the EM algorithm

The mixture model may be viewed as an *incomplete* or *missing* data problem: here the missing data are the group allocations $\boldsymbol{k} = (k_1, \ldots, k_n)^T$ belonging to each sample $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$.

If we would know which sample comes from which group the estimation of the parameters $\boldsymbol{\theta}$ would indeed be straightforward using the so-called *complete data log-likelihood* based on the joint distribution $f(\boldsymbol{x}, k) = f_k(\boldsymbol{x})\pi_k$

$$\log L(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{k}) = \sum_{i=1}^{n} \log\left(\pi_{k_i} f_{k_i}(\boldsymbol{x}_i)\right)$$

The idea of the EM algorithm (Dempster et al. 1977) is to exploit the simplicity of the complete data likelihood and to obtain estimates of $\boldsymbol{\theta}$ by first finding the probability distribution z_{ik} of the latent variable k_i, and then using this distribution to compute and optimise the corresponding expected complete-data log-likelihood. Specifically, the z_{ik} contain the *probabilities* of each class for each sample i and thus provide a *soft assignment* of classes rather that a $0/1$ *hard assignment* (as in the K-means algorithm or in the generative latent variable view of mixture models).

In the EM algorithm we iterate between the

1) estimation the probabilistic distribution z_{ik} for the group allocation latent parameters using the current estimate of the parameters $\boldsymbol{\theta}$ (obtained in step 2)
2) maximisation of the expected complete data log-likelihood to estimate the parameters $\boldsymbol{\theta}$. The expectation is taken with regard to the distribution z_{ik} (obtained in step 1).

Specifically, the EM algorithm applied to model-based clustering proceeds as follows:

1) Initialisation: Start with a guess of the parameters $\boldsymbol{\theta}^{(1)}$, then continue with "E" Step, Part A. Alternatively, start with a guess of $z_{ik}^{(1)}$, then continue with "E" Step, Part B. The initialisation may be derived from some prior information, e.g., from running K-means, or simply be at random.

2) **E "expectation" step** — Part A: Use Bayes' theorem to compute new probabilities of allocation for all the samples $\boldsymbol{x}_i$:

$$z_{ik}^{(b+1)} \leftarrow \frac{\pi_k f_k(\boldsymbol{x}_i)}{f(\boldsymbol{x}_i)}$$

Note that to obtain $z_{ik}^{(b+1)}$ the current value $\boldsymbol{\theta}^{(b)}$ of the parameters is required.

— Part B: Construct the expected complete data log-likelihood function using the weights $z_{ik}^{(b+1)}$:

$$Q^{(b+1)}(\boldsymbol{\theta}|\boldsymbol{X}) = \sum_{i=1}^{n}\sum_{k=1}^{k} z_{ik}^{(b+1)} \log\left(\pi_k f_k(\boldsymbol{x}_i)\right)$$

3) **M "maximisation" step** — Maximise the expected complete data log-likelihood to update the mixture model parameters $\boldsymbol{\theta}$:

$$\boldsymbol{\theta}^{(b+1)} \leftarrow \arg\max_{\boldsymbol{\theta}} Q^{(b+1)}(\boldsymbol{\theta}|\boldsymbol{X})$$

4) Repeat with "E" Step until convergence of parameters $\boldsymbol{\theta}^{(b)}$ of the mixture model.

It can be shown that the output $\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \boldsymbol{\theta}^{(3)}, \ldots$ of the EM algorithm converges to the estimate $\hat{\boldsymbol{\theta}}$ found when maximising the marginal log-likelihood. Since maximisation of the expected complete data log-likelihood is often much easier (and analytically tractable) than maximisation of the observed data log-likelihood function the EM algorithm is the preferred approach in this case.

To avoid singularities in the expected log-likelihood function we may wish to adopt a Bayesian approach (or use regularised/penalised ML) for estimating the parameters in the M-step.

3.5.3 EM algorithm for multivariate normal mixture model

For a GMM the EM algorithm can be written down analytically:

E-step:

$$z_{ik} = \frac{\hat{\pi}_k N(\boldsymbol{x}_i|\hat{\boldsymbol{\mu}}_k, \hat{\boldsymbol{\Sigma}}_k)}{f(\boldsymbol{x}_i)}$$

M-step:

$$\hat{n}_k = \sum_{i=1}^{n} z_{ik}$$

$$\hat{\pi}_k = \frac{\hat{n}_k}{n}$$

$$\hat{\boldsymbol{\mu}}_k = \frac{1}{\hat{n}_k} \sum_{i=1}^{n} z_{ik} \boldsymbol{x}_i$$

$$\hat{\boldsymbol{\Sigma}}_k = \frac{1}{\hat{n}_k} \sum_{i=1}^{n} z_{ik} (\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T$$

Note that the estimators $\hat{\boldsymbol{\mu}}_k$ and $\hat{\boldsymbol{\Sigma}}_k$ are weighted versions of the usual empirical estimators (with weights z_{ik} being the soft assignment of classes resulting from the Bayesian updating).

3.5.4 Connection with K-means clustering method

The K-means algorithm is very closely related to probabilistic clustering with a Gaussian mixture models.

Specifically, the class assigment in K-means is

$$C(\boldsymbol{x}_i) = \arg\min_k (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)$$

If in a Gaussian mixture model the probabilities π_k of all classes are asssumed to be identical (i.e. $\pi_k = \frac{1}{K}$) and the covariances $\boldsymbol{\Sigma}_k$ all are assumed to be of the form $\sigma^2 \boldsymbol{I}$, i.e. no dependence on groups, no correlation and identical variance for all variables, then the soft assignment for the class allocation becomes

$$\log(z_{ik}) = -\frac{1}{2\sigma^2} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k) + C$$

where C is a constant depending on $\boldsymbol{x}_i$ but not on k. In order to select a hard class allocation based on z_{ik} we may then use the rule

$$\begin{aligned} C(\boldsymbol{x}_i) &= \arg\max_k \log(z_{ik}) \\ &= \arg\min_k (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k)^T (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}}_k) \end{aligned}$$

Thus, K-means can be viewed as an algorithm to provide hard classifications for a simple restricted Gaussian mixture model.

3.5.5 Choosing the number of classes

Since GMMs operate in a likelihood framework we can use penalised likelihood model selection criteria to choose among different models (i.e. GMMs with different numbers of classes).

The most popular choices are AIC (Akaike Information Criterion) and BIC (Bayesian Information criterion) defined as follows:

$$\text{AIC} = -2 \log L + 2K$$

$$\text{BIC} = -2 \log L + K \log(n)$$

Instead of maximising the log-likehood we minimise AIC and BIC.

Note that in both criteria more complex models with more parameters (in this case groups) are penalised over simpler models in order to prevent overfitting.

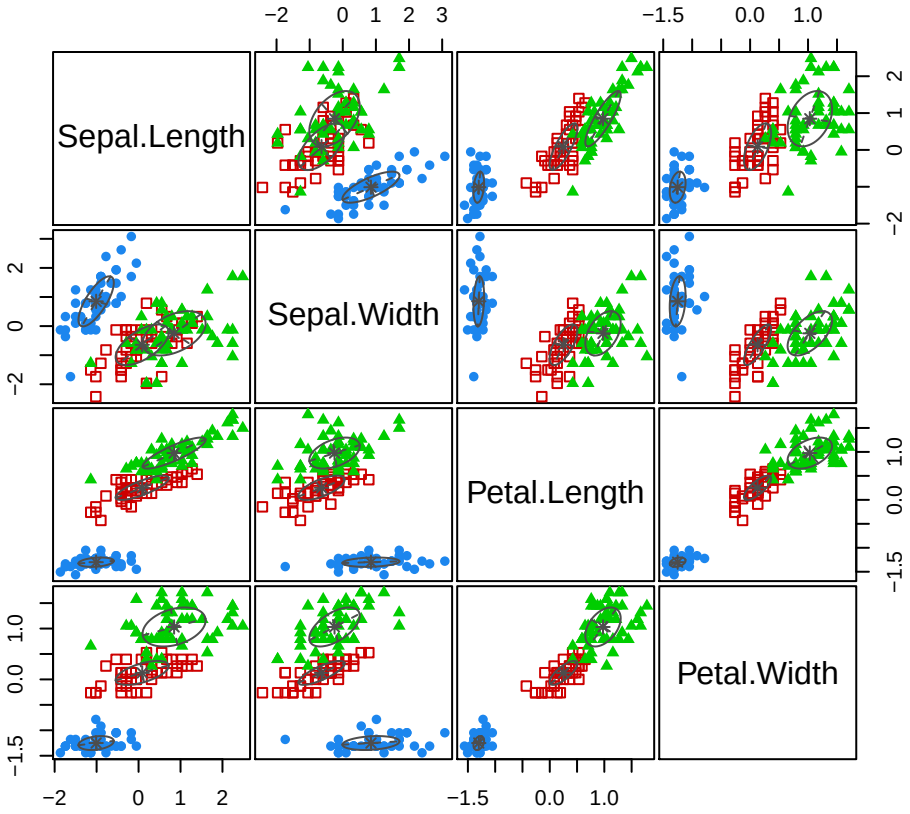
$\Longrightarrow$ find optimal number of groups K.

Another way of choosing optimal numbers of clusters is by cross-validation (see later chapter on supervised learning).

3.5.6 Application of GMMs to Iris flower data

We now explore the application of GMMs to the Iris flower data set we also investigated with PCA and K-means.

First, we run GMM with 3 clusters:



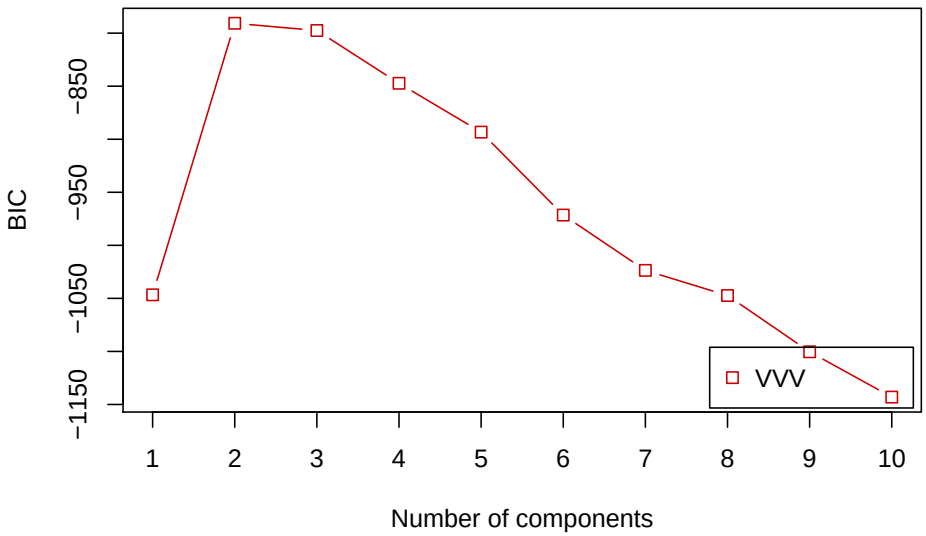
The GMM has a substantially lower misclassification error compared to K-means with the same number of clusters:

```
table(gmm3$classification, L.iris)
```

```
##    L.iris
##      setosa versicolor virginica
##   1     50          0         0
##   2      0         45         0
##   3      0          5        50
```

Note that in the R software "mclust" to analyse GMMs the BIC criterion is defined with the opposite sign ($\text{BIC}_{\text{mclust}} = 2 \log L - K \log(n)$), thus we need to find the *maximum* value rather than the smallest value.

If we compute BIC for various numbers of groups we find that the model with the best $\text{BIC}_{\text{mclust}}$ is a model with 2 clusters but the model with 3 cluster has nearly as good a BIC:



Note that "VVV" is the name of the most general mixture model in "mclust".

Chapter 4

Supervised learning and classification

4.1 Introduction

4.1.1 Supervised learning vs. unsupervised learning

Unsupervised learning:

Starting point:

- unlabeled data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$.

Aim: find labels $y_1, \ldots, y_n$ to attach to each sample $\boldsymbol{x}_i$.

For discrete labels y unsupervised learning is called *clustering*.

Supervised learning:

Starting point:

- labeled *training data*: $\{\boldsymbol{x}_1^{train}, y_1^{train}\}, \ldots, \{\boldsymbol{x}_n^{train}, y_n^{train}\}$
- In addition, we have unlabeled *test data*: $\boldsymbol{x}^{test}$

Aim: use training data to learn a function $f(\boldsymbol{x})$ to predict the label corresponding to the test data. The predictor function may provide a soft (probabilistic) assignment or a hard assignment.

For y discrete supervised learning is called *classification*. For continuous y the label is called response and supervised learning becomes *regression*.

Thus, supervised learning is a two-step procedure:

1) learn predictor function using only the training data
2) predict the label y^{test} for the test data $\boldsymbol{x}^{test}$

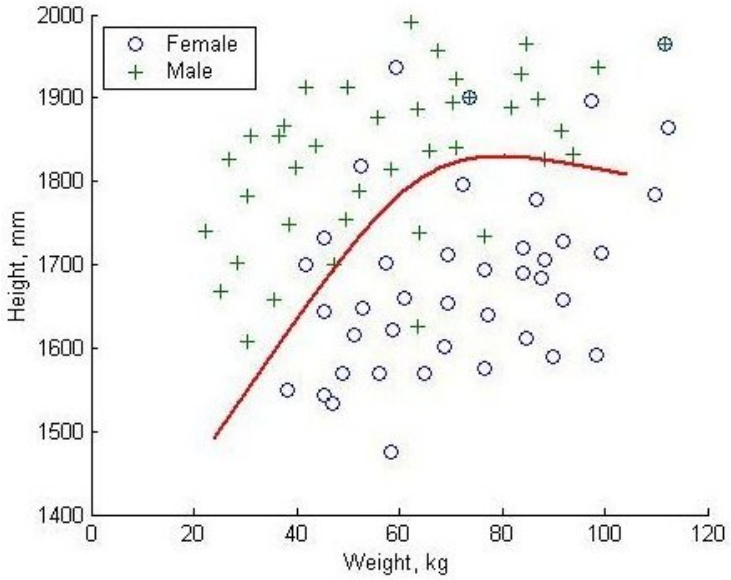
4.1.2 Terminology

The function $f(\boldsymbol{x})$ that predicts the class y is called a *classifier*.

There are many types of classifiers, we focus here primarily on probabilistic classifiers (i.e. those that output the predicted class along with a probability).

The challenge is to find a classifier that explains the current training data well *and* that also generalises well to future unseen data. Note that it is relatively easy to find a predictor that explains the training data but especially in high dimensions (i.e. with many predictors) there is often overfitting and then the predictor does not generalise well!

The classifier function describes the decision boundary between the classes:



In general, simple decision boundaries are preferred over complex decision boundaries to avoid overfitting!

Some commonly used probabilistic methods for classifications:

- QDA (quadratic discriminant analysis)
- LDA (linear discriminant analysis)
- DDA (diagonal discriminant analysis),
- Naive Bayes classification
- logistic regression

Common non-probabilistic methods include:

- SVM (support vector machine),
- random forest
- neural networks

Depending on how the classifiers are trainined there are many variations of the above methods, e.g. Fisher discriminant analysis, regularised LDA, shrinkage disciminant analysis etc.

4.2 Bayesian discriminant rule or Bayes classifier

Same setup as with mixture models:

- K groups with K prespecified
- each group has its own distribution F_k with own parameters $\boldsymbol{\theta}_k$
- the density of each class is $f_k(\boldsymbol{x}) = f(\boldsymbol{x}|k)$.
- prior probability of group k is $\Pr(k) = \pi_k$ with $\sum_{k=1}^{K} \pi_k = 1$
- marginal density is the mixture $f(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k f_k(\boldsymbol{x})$

The posterior probability of group k is then

$$\Pr(k|\boldsymbol{x}) = \frac{\pi_k f_k(\boldsymbol{x})}{f(\boldsymbol{x})}$$

The *discriminant function* is the logarithm of the posterior probability:

$$d_k(\boldsymbol{x}) = \log \Pr(k|\boldsymbol{x}) = \log(\pi_k) + \log(f_k(\boldsymbol{x})) - \log(f(\boldsymbol{x}))$$

Since we use d_k to compare the different classes k we can simplify the discriminant function by dropping all constant terms that do not depend on k — in the above this is the term $\log(f(\boldsymbol{x}))$. Hence we get for the Bayes discriminant function

$$d_k(\boldsymbol{x}) = \log(\pi_k) + \log(f_k(\boldsymbol{x}))$$

This provides us with the probability of each class given the test data $\boldsymbol{x}$. For subsequent "hard" classification we need to use a decision rule, such as selecting the group $\hat{k}$ for that which the group probability / value of discriminant function is maximised

$$\hat{k} = \arg\max_k d_k(\boldsymbol{x})\,.$$

with $d_{\max} = d_{\hat{k}}(\boldsymbol{x})$.

The discriminant functions $d_k(\boldsymbol{x})$ can be mapped back to the probabilistic class assignment by using the softargmax function (also known as softmax function):

$$\Pr(k|\boldsymbol{x}) = \frac{\exp(d_k(\boldsymbol{x}))}{\sum_{c=1}^{K} \exp(d_c(\boldsymbol{x}))} = \frac{\exp(d_k(\boldsymbol{x}) - d_{\max})}{\sum_{c=1}^{K} \exp(d_c(\boldsymbol{x}) - d_{\max})}$$

Note the second form avoids numerical overflow problems when computing the exponential by standardising the maximum of the discriminant functions to zero.

You have already encountered the Bayes classifier in the EM algorithm to predict the state of the latent variables. In a simplied versions it also plays a role in the K-means algorithm (see previous Chapter) and in the likelihood classifier (cf. Worksheet 7).

4.3 Normal Bayes classifier

4.3.1 Quadratic discriminant analysis (QDA) and Gaussian assumption

Quadratic discriminant analysis (QDA) is a special case of the Bayes classifier when all densities are multivariate normal with $f_k(\boldsymbol{x}) = N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$.

This leads to the discriminant function for QDA:

$$d_k^{QDA}(\boldsymbol{x}) = -\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_k) - \frac{1}{2}\log\det(\boldsymbol{\Sigma}_k) + \log(\pi_k)$$

There are a number of noteworthy things here:

- Again terms are dropped that do not depend on k, such as $-\frac{d}{2}\log(2\pi)$.
- Note the appearance of the Mahalanobis distance between $\boldsymbol{x}$ and $\boldsymbol{\mu}_k$ in the last term — recall $d^{Mahalanobis}(\boldsymbol{x}, \boldsymbol{\mu}|\boldsymbol{\Sigma}) = (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu})$.
- The **QDA discriminant function is quadratic in $\boldsymbol{x}$** - hence its name! This implies that the **decision boundaries for QDA classification are quadratic** (i.e. parabolas in two dimensional settings).

For Gaussian models specifically it can useful be to multiply the discriminant function by -2 to get rid of the factor $-\frac{1}{2}$, but note that in that case we then need to find the minimum of the discriminant function rather than the maximum:

$$d_k^{QDA(v2)}(\boldsymbol{x}) = (\boldsymbol{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_k) + \log\det(\boldsymbol{\Sigma}_k) - 2\log(\pi_k)$$

In the literature you will find both versions of Gaussian discriminant functions so you need to check carefully which convention is used. In the following we will use the first version only.

4.3.2 Linear discriminant analysis (LDA)

LDA is a special case of QDA, with the assumption of common overall covariance across all groups: $\boldsymbol{\Sigma}_k = \boldsymbol{\Sigma}$.

This leads to a simplified discriminant function:

$$d_k^{LDA}(\boldsymbol{x}) = -\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_k) + \log(\pi_k)$$

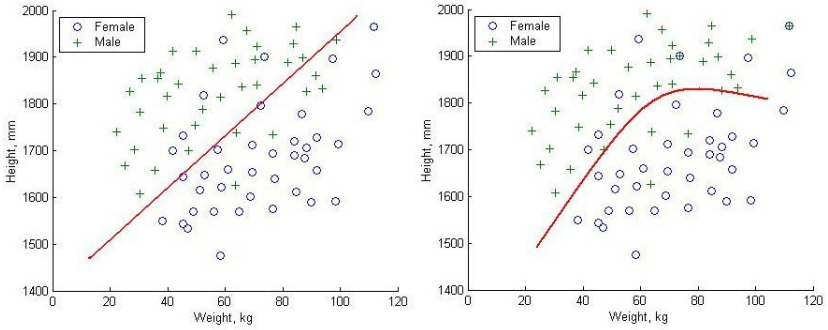
Note that term containing the log-determinant is now gone, and that LDA is essentially now a method that tries to minimize the Mahalanobis distance (while taking also into account the prior class probabilities).

The above function can be further simplified, by noting that the quadratic term $\boldsymbol{x}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{x}$ does not depend on k and hence can be dropped:

$$\begin{aligned} d_k^{LDA}(\boldsymbol{x}) &= \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1} \boldsymbol{x} - \frac{1}{2}\boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k + \log(\pi_k) \\ &= \boldsymbol{b}^T \boldsymbol{x} + a \end{aligned}$$

Thus, the **LDA discriminant function is linear in x, and hence the resulting decision boundaries are linear** as well (i.e. straight lines in two-dimensional settings).

Comparison of decision boundary of LDA (left) compared with QDA (right):



Note that logistic regression (cf. GLM module) takes on exactly the above linear form and is indeed closely linked with the LDA classifier.

4.3.3 Diagonal discriminant analysis (DDA)

In DDA we assume the same setting as LDA, but now we simplify even further by assuming a **diagonal covariance** containing only the variances:

$$\boldsymbol{\Sigma} = \boldsymbol{V} = \begin{pmatrix} \sigma_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_d^2 \end{pmatrix}$$

This simplifies the inversion of $\boldsymbol{\Sigma}$ as

$$\boldsymbol{\Sigma}^{-1} = \boldsymbol{V}^{-1} = \begin{pmatrix} \sigma_1^{-2} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_d^{-2} \end{pmatrix}$$

and leads to the discriminant function

$$\begin{aligned} d_k^{DDA}(\boldsymbol{x}) &= \boldsymbol{\mu}_k^T \boldsymbol{V}^{-1} \boldsymbol{x} - \frac{1}{2} \boldsymbol{\mu}_k^T \boldsymbol{V}^{-1} \boldsymbol{\mu}_k + \log(\pi_k) \\ &= \sum_{j=i}^{d} \frac{\mu_{k,j} x_j - \mu_{k,j}^2 / 2}{\sigma_d^2} + \log(\pi_k) \end{aligned}$$

As special case of LDA, the **DDA classifier is a linear classifier**.

The **Bayes classifier** (using any distribution) **assuming uncorrelated predictors** is also known as the **naive Bayes classifier**.

Hence, **DDA is a naive Bayes classifier** assuming underlying Gaussian distributions.

However, don't let you misguide because of the name "naive": in fact DDA and other "naive" Bayes classfier are often very effective classifiers, especially in high-dimensional settings!

4.4 The training step — learning QDA, LDA and DDA classifiers from data

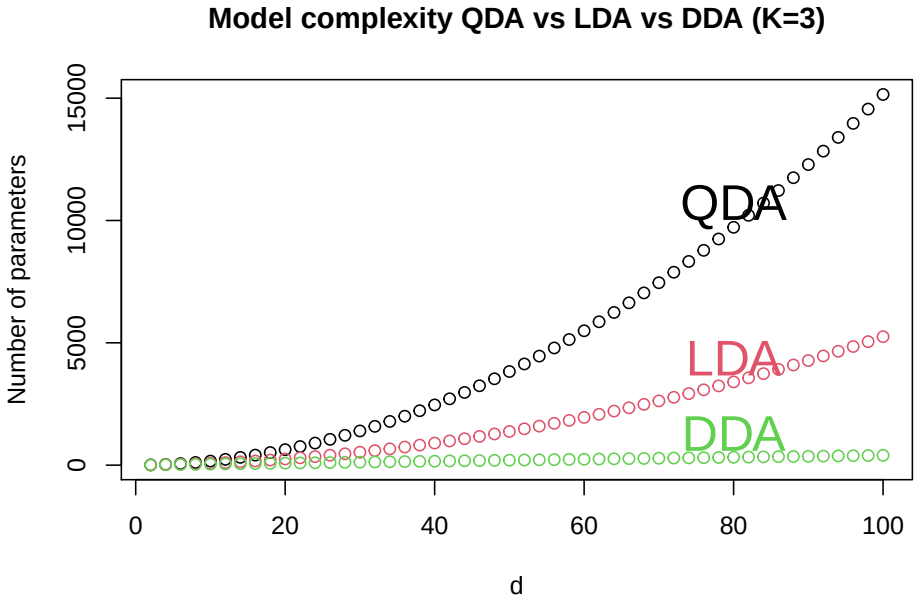
4.4.1 Number of model parameters

In order to predict the class for new data using any of the above discriminant functions we need to first learn the underlying parameters from the training data $\boldsymbol{x}_i^{\text{train}}$ and y_i^{train}:

- For QDA, LDA and DDA we need to learn $\pi_1, \ldots, \pi_K$ with $\sum_{k=1}^{K} \pi_k = 1$ and the mean vectors $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
- For QDA we additionally require $\boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K$
- For LDA we need $\boldsymbol{\Sigma}$
- For DDA we estimate $\sigma_1^2, \ldots, \sigma_d^2$.

Overall, the total number of parameters to be estimated when learning the discriminant functions from training data is as follows:

- QDA: $K - 1 + Kd + K\frac{d(d-1)}{2}$
- LDA: $K - 1 + Kd + \frac{d(d-1)}{2}$
- DDA: $K - 1 + Kd + d$



4.4.2 Estimating the discriminant / predictor function

For QDA, LDA and DDA we learn the predictor by estimating the parameters of the discriminant function from the training data.

4.4.2.1 Large sample size

If the sample size of the training data set is sufficiently large compared to the model dimensions we can use maximum likelihood to estimate the model parameters. To be able use ML we need a larger sample size for QDA and LDA (because full covariances need to be estimated) but for DDA relatively small sample size can be sufficient (which explains why "naive" Bayes methods are very popular in practise).

To obtain the parameters estimates we use the known labels y_i^{train} to sort the samples $\boldsymbol{x}_i^{\text{train}}$ into the corresponding classes, and then apply the standard ML estimators. Let $G_k = \{i : y_i^{\text{train}} = k\}$ be the set of all indices of training sample belonging to group k, n_k the sample size in group k

The ML estimates of the class probabilities are the frequencies

$$\hat{\pi}_k = \frac{n_k}{n}$$

and the ML estimate of the group means $k = 1, \ldots, K$ are

$$\hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i \in g_k} \boldsymbol{x}_i^{\text{train}} .$$

The ML estimate of the global mean $\boldsymbol{\mu}_0$ (i.e. if we assume there is only a single class and ignore the group labels) is

$$\hat{\boldsymbol{\mu}}_0 = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i^{\text{train}} = \sum_{k=1}^{K} \hat{\pi}_k \hat{\boldsymbol{\mu}}_k$$

Note the global mean is identical to the pooled mean (i.e. weighted average of the individual group means).

The ML estimates for the covariances $\boldsymbol{\Sigma}_k$ for QDA are

$$\widehat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k} \sum_{i \in g_k} (\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_k)^T$$

In order to get the ML estimate of the pooled variance $\boldsymbol{\Sigma}$ for use with LDA we compute

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in g_k} (\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_k)(\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_k)^T = \sum_{k=1}^{K} \hat{\pi}_k \widehat{\boldsymbol{\Sigma}}_k$$

Note that the pooled variance $\boldsymbol{\Sigma}$ differs (substantially!) from the global variance Σ_0 that results from simply ignoring class labels and that is computed as

$$\widehat{\boldsymbol{\Sigma}}_0^{ML} = \frac{1}{n} \sum_{i=1}^{n} (\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_0)(\boldsymbol{x}_i^{\text{train}} - \hat{\boldsymbol{\mu}}_0)^T$$

You will recognise the above from the variance decomposion in mixture models, with $\boldsymbol{\Sigma}_0$ being the total variance and the pooled $\boldsymbol{\Sigma}$ the unexplained/with-in group variance.

4.4.2.2 Small sample size

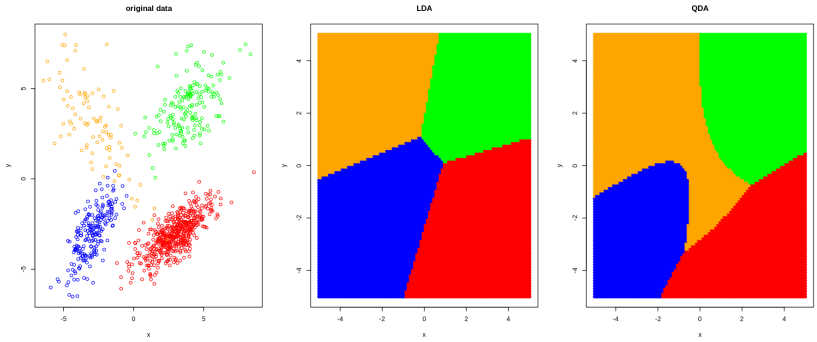
If the dimension d is large compared to the sample size then the number of parameters in the predictor function grows fast. Especially QDA but also LDA is data hungry and ML estimation becomes an ill-posed problem. As discussed in Section 1.5 in this instance we need to use a regularised estimator for the covariance(s) based, e.g., on penalised ML, Bayesian learning, shrinkage estimation. This also ensures that the estimated covariance matrices are positive definite (which is automatically guaranteed only for DDA if all variances are positive). Furthermore, in small sample setting it is advised to reduce the number of parameters, therefore using LDA or DDA is preferred over QDA. This can also prevent overfitting and lead to a predictor that generalises better.

To analyse high-dimensional data in the worksheets we will employ a regularised version of LDA and DDA using Stein-type shrinkage estimation as discussed in Section 1.5 and implemented in the R package "sda".

4.4.3 Comparison of estimated decision boundaries: LDA vs. QDA

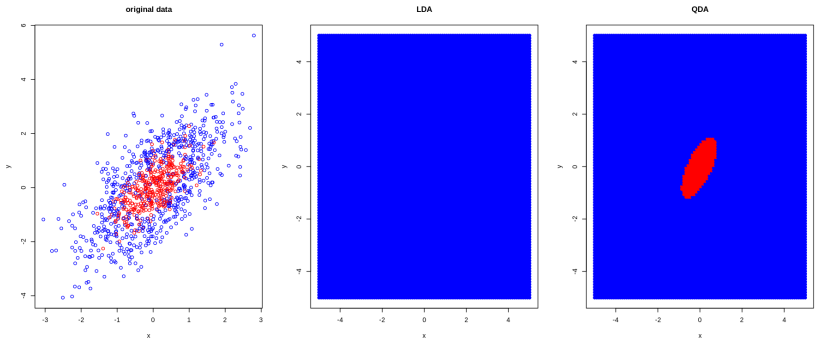
We compare two simple scenarios using simulated data.

Non-nested case ($K = 4$):



Note the linear decision boundaries for LDA!

Nested case ($K = 2$):



There is no linear classifier that can seperate two nested classes!

4.5 Goodness of fit and variable ranking

As in linear regression (cf. "Statistical Methods" module) we are interested in finding out whether the fitted mixture model is an appropriate model, and which particular predictor(s) x_j from $\boldsymbol{x} = (x_1, \ldots, x_d)^T$ are responsible prediction the outcome, i.e. for categorizing a sample into group k.

In order to study these problem it is helpful to rewrite the discriminant function to highlight the influence (or importance) of each predictor.

We focus on linear methods (LDA and DDA) and first look at the simple case $K = 2$ and then generalise to more than two groups.

4.5.1 LDA with $K = 2$ classes

For two classes using the LDA discriminant rule will choose group $k = 1$ if $d_1^{LDA}(\boldsymbol{x}) > d_2^{LDA}(\boldsymbol{x})$, or equivalently, if

$$\Delta_{12}^{LDA} = d_1^{LDA}(\boldsymbol{x}) - d_2^{LDA}(\boldsymbol{x}) > 0$$

Since $d_k(\boldsymbol{x})$ is the log-posterior (plus/minus identical constants) Δ^{LDA} is in fact the **log-posterior odds of class 1 versus class 2** (see Statistical Methods, Bayesian inference).

The difference Δ_{12}^{LDA} is

$$\underbrace{\Delta_{12}^{LDA}}_{\text{log posterior odds}} = \underbrace{(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}^{-1} \left(\boldsymbol{x} - \frac{\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2}{2} \right)}_{\text{log Bayes factor } \log B_{12}} + \underbrace{\log \left(\frac{\pi_1}{\pi_2} \right)}_{\text{log prior odds}}$$

Note that since we only consider simple non-composite models here the log-Bayes factor is identical with the log-likelihood ratio!

The log Bayes factor $\log B_{12}$ is known as the *weight of evidence* in favour of F_1 given $\boldsymbol{x}$. The *expected weight of evidence* assuming $\boldsymbol{x}$ is indeed from F_1 is the Kullback-Leibler discrimination information in favour of group 1, i.e. the KL divergence of from distribution F_2 to F_1:

$$\mathrm{E}_{F_1}(\log B_{12}) = KL(F_1 || F_2) = \frac{1}{2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) = \frac{1}{2}\Omega^2$$

This yields, apart of a scale factor, a population version of the Hotelling T^2 statistic defined as

$$T^2 = c^2 (\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_2)^T \hat{\boldsymbol{\Sigma}}^{-1} (\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_2)$$

where $c = (\frac{1}{n_1} + \frac{1}{n_2})^{-1/2} = \sqrt{n \pi_1 \pi_2}$ is a sample size dependent factor (for $\mathrm{SD}(\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_2)$). T^2 is a measure of fit of the underlying two-component mixture.

Using the whitening transformation with $\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x}$ and $\boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{\Sigma}^{-1}$ we can rewrite the log Bayes factor as

$$\begin{aligned} \log B_{12} &= \left((\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \boldsymbol{W}^T \right) \left(\boldsymbol{W} \left(\boldsymbol{x} - \frac{\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2}{2} \right) \right) \\ &= \boldsymbol{\omega}^T \boldsymbol{\delta}(\boldsymbol{x}) \end{aligned}$$

i.e. as the product of two vectors:

- $\boldsymbol{\delta}(\boldsymbol{x})$ is the whitened $\boldsymbol{x}$ (centered around average means) and
- $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_d)^T = \boldsymbol{W}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$ gives the weight of each whitened component $\boldsymbol{\delta}(\boldsymbol{x})$ in the log Bayes factor.

A large positive or negative value of ω_j indicates that the corresponding whitened predictor is relevant for choosing a class, whereas small values of ω_j close to zero indicate that the corresponding ZCA whitened predictor is unimportant. Furthermore, $\boldsymbol{\omega}^T\boldsymbol{\omega} = \sum_{j=1}^{d} \omega_j^2 = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) = \Omega^2$, i.e. the squared ω_j^2 provide a component-wise decomposition of the overall fit Ω^2.

Choosing ZCA-cor as whitening transformation with $\boldsymbol{W} = \boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}$ we get

$$\boldsymbol{\omega}^{ZCA-cor} = \boldsymbol{P}^{-1/2}\boldsymbol{V}^{-1/2}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

A better understanding of $\boldsymbol{\omega}^{ZCA-cor}$ is provided by comparing with the two-sample t-statistic

$$\hat{\boldsymbol{\tau}} = c\hat{\boldsymbol{V}}^{-1/2}(\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_2)$$

With $\boldsymbol{\tau}$ the population version of $\hat{\boldsymbol{\tau}}$ we can define

$$\boldsymbol{\tau}^{adj} = \boldsymbol{P}^{-1/2}\boldsymbol{\tau} = c\boldsymbol{\omega}^{ZCA-cor}$$

as correlation-adjusted t-scores (cat scores). With $(\hat{\boldsymbol{\tau}}^{adj})^T\hat{\boldsymbol{\tau}}^{adj} = T^2$ we can see that the cat scores offer a component-wise decomposition of Hotelling's T^2.

Note the choice of ZCA-cor whitening is to ensure that the whitened components are interpretable and stay maximally correlated to the original variables. However, you may also choose for example PCA whitening in which case the $\boldsymbol{\omega}^T\boldsymbol{\omega}$ provide the variable importance for the PCA whitened variables.

For DDA, which assumes that correlations among predictors vanish, i.e. $\boldsymbol{P} = \boldsymbol{I}_d$, we get

$$\Delta_{12}^{DDA} = \underbrace{\left((\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T\boldsymbol{V}^{-1/2}\right)}_{c^{-1}\boldsymbol{\tau}^T} \underbrace{\left(\boldsymbol{V}^{-1/2}\left(\boldsymbol{x} - \frac{\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2}{2}\right)\right)}_{\text{centered standardised predictor}} + \log\left(\frac{\pi_1}{\pi_2}\right)$$

Similarly as above, the t-score $\boldsymbol{\tau}$ determines the impact of the standardised predictor in Δ^{DDA}.

Consequently, in DDA we can rank predictors by the squared t-score. Recall that in standard linear regression with uncorrelated predictors we can find the most important predictors by ranking the squared marginal correlations – ranking by (squared) t-scores in DDA is the exact analogy but for discrete response.

4.5.2 Multiple classes

For more than two classes we need to refer to the so-called **pooled centroids formulation** of DDA and LDA (introduced by Tibshirani 2002).

The pooled centroid is given by $\boldsymbol{\mu}_0 = \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k$ — this is the centroid if there would be only a single class. The corresponding probability (for a single class) is $\pi_0 = 1$ and the distribution is called F_0.

The LDA discriminant function for this "group 0" is

$$d_0^{LDA}(\boldsymbol{x}) = \boldsymbol{\mu}_0^T \boldsymbol{\Sigma}^{-1} \boldsymbol{x} - \frac{1}{2} \boldsymbol{\mu}_0^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_0$$

and the log posterior odds for comparison of group k with the pooled group 0 is

$$\begin{aligned} \Delta_k^{LDA} &= d_k^{LDA}(\boldsymbol{x}) - d_0^{LDA}(\boldsymbol{x}) \\ &= \log B_{k0} + \log(\pi_k) \\ &= \boldsymbol{\omega}_k^T \boldsymbol{\delta}_k(\boldsymbol{x}) + \log(\pi_k) \end{aligned}$$

with

$$\boldsymbol{\omega}_k = \boldsymbol{W}(\boldsymbol{\mu}_k - \boldsymbol{\mu}_0)$$

and

$$\boldsymbol{\delta}_k(\boldsymbol{x}) = \boldsymbol{W}(\boldsymbol{x} - \frac{\boldsymbol{\mu}_k + \boldsymbol{\mu}_0}{2})$$

The expected log Bayes factor is

$$\mathrm{E}_{F_k}(\log B_{k0}) = KL(F_k || F_0) = \frac{1}{2}(\boldsymbol{\mu}_k - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_k - \boldsymbol{\mu}_0) = \frac{1}{2} \Omega_k^2$$

With scale factor $c_k = (\frac{1}{n_k} - \frac{1}{n})^{-1/2} = \sqrt{n \frac{\pi_k}{1-\pi_k}}$ (for $\mathrm{SD}(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_0)$, with the minus sign before $\frac{1}{n}$ due to correlation between $\hat{\boldsymbol{\mu}}_k$ and pooled mean $\hat{\boldsymbol{\mu}}_0$) we get as correlation-adjusted t-score for comparing mean of group k with the pooled mean

$$\boldsymbol{\tau}_k^{adj} = c_k \boldsymbol{\omega}_k^{ZCA-cor} .$$

For the two class case ($K = 2$) we get with $\boldsymbol{\mu}_0 = \pi_1 \boldsymbol{\mu}_1 + \pi_2 \boldsymbol{\mu}_2$ for the mean difference $(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) = \pi_2(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$ and with $c_1 = \sqrt{n \frac{\pi_1}{\pi_2}}$ this yields

$$\boldsymbol{\tau}_1^{adj} = \sqrt{n \pi_1 \pi_2} \boldsymbol{P}^{-1/2} \boldsymbol{V}^{-1/2} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2),$$

i.e. the exact same score as in the two-class setting.

4.6 Variable selection and cross-validation

In the previous we saw that in DDA the natural score for **ranking features** with regard to their relevance in separating the classes is the (squared) t-score, and for LDA a whitened version such as the squared correlation-adjusted t-score (based on ZCA-cor whitening) may be used. Once such a ranking has been established the question of a **suitable cutoff** arises, i.e. how many features need (or should) be retained in a model.

For large and high-dimensional models **feature selection can also be viewed as a form of regularisation and also dimension reduction**. Specifically, there

may be many variables/ features that do no contribute to the class prediction. Despite having in principle no effect on the outcome the presence of these "null variables" can nonetheless deterioriate (sometimes dramatically!) the overall predictive accuracy of a trained predictor, because they add noise and increase the model dimension. Therefore, variables that do not contribute to prediction should be filtered out in order to be able to construct good prediction models and classifiers.

4.6.1 Choosing a threshold by multiple testing using false discovery rates

The most simple way to determine a cutoff threshold is to use a standard technique for multiple testing.

For each predictor variable $x_1, \ldots, x_d$ we have a corresponding test statistic measuring the influence of this variable on the response, for example the the t-scores and related statistics discussed in the previous section. In addition to providing an overall ranking the set of all these statistics can be used to determine a suitable cutoff by trying to separate two populations of predictor variables:

- "Null" variables that do not contribute to prediction
- "Alternative" variables that are linked to prediction

As discussed in the "Statistical Methods" module last term (Part 2 - Section 8) this can be done as follows:

- The distribution of the observed test statistics z_i is assumed to follow a two-component mixture where $F_0(z)$ and $F_A(z)$ are the distributions corresponding to the null and the alternative, $f_0(z)$ and $f_a(z)$ the densities, and π_0 and $\pi_A = 1 - \pi_0$ are the weights:

$$f(z) = \pi_0 f_0(z) + (1 - \pi_0) f_a(z)$$

- The null model is typically from a parametric family (e.g. normal around zero and with a free variance parameter) whereas the alternative is often modelled nonparametrically.
- After fitting the mixture model, often assuming some additional constraints to make the mixture identifiable, one can compute false discovery rates (FDR) as follows:

  Local FDR:

$$\widehat{fdr}(z_i) = \hat{\Pr}(\text{null}|z_i) = \frac{\hat{\pi}_0 \hat{f}_0(z_i)}{\hat{f}(z_i)}$$

  Tail-area-based FDR (=q-value):

$$\widehat{Fdr}(z_i) = \hat{\Pr}(\text{null}|Z > z_i) = \frac{\hat{\pi}_0 \hat{F}_0(z_i)}{\hat{F}(z_i)}$$

  Note these are essentially p-values adjusted for multiple testing (by a variant of the Benjamini-Hochberg method).

By thresholding false discovery rates it is possible to identify those variables that clearly belong to each of the two groups but also those features that cannot easily be discriminated to fall into either group:

- "alternative" variables have low local FDR, e.g, $\widehat{fdr}(z_i) \leq 0.2$
- "null" variables have high local FDR, e.g. $\widehat{fdr}(z_i) \geq 0.8$
- features that cannot easily classified as null or alternative, e.g. $0.2 < \widehat{fdr}(z_i) < 0.8$

For feature selection in prediction settings we generally aim to remove only those variable that clearly belong to the null group, leaving all others in the model.

4.6.2 Quantifying prediction error

Another and more direct way to compare models is to compare their predictive performance by quantification of prediction error. Specifically, we are interested in the relative performance of models with diverse sets of predictor. variables.

A measure of predictor error compares the predicted label $\hat{y}$ with the true label y for a validation data set. A validation data set contains both the $\boldsymbol{x}_i$ and the associated label y_i but unlike the training data it has not been used for learning the predictor function.

For continuous response often the squared loss is used:

$$\text{err}(\hat{y}, y) = (\hat{y} - y)^2$$

For binary outcomes one often employs the $0/1$ loss:

$$\text{err}(\hat{y}, y) = \begin{cases} 1, & \text{if } \hat{y} = y \\ 0, & \text{otherwise} \end{cases}$$

Alternatively, any other quantity derived from the confusion matrix (containing TP, TN, FP, FN) can be used.

The mean prediction error is the expectation

$$PE = \text{E}(\text{err}(\hat{y}, y))$$

and thus the empirical mean prediction error is

$$\widehat{PE} = \frac{1}{m} \sum_{i=1}^{m} \text{err}(\hat{y}_i, y_i)$$

where m is the sample size of the validation data set.

More generally, we can also quantify prediction error in the framework of so-called **proper scoring rules**, where the whole probabilistic forecast is taken into account (e.g. the individual probabilities for each class, rather than just the selected most probable class). A commonly used scoring rule is the negative log-probability ("surprise"), and the expected surprise is the cross-entropy

(cf. Statistical Methods module). So this leads back to entropy and likelihood (cf. e.g. MATH20802 lecture notes).

Once we have an estimate of the prediction error of a model we can use it to compare and choose among a set of candiate models, selecting those with a sufficiently low prediction error.

4.6.3 Estimation of prediction error without validation data using cross-validation

Unfortunately, quite often we do not have separate validation data available to evaluate a classifier.

In this case we need to rely on a simple algorithmic procedure called **cross-validation**.

Outline of cross-validation:

1) split the samples in the training data into a number (say K) parts ("folds").
2) use each of the K folds as validation data and the other $K-1$ folds as training data.
3) average over the resulting K individual estimates of prediction error, to get an overall aggregated predictor error, along with an error.

Note that in each case one part of the data is reserved for validation and *not* used for training the predictor.

We choose K such that the folds are not too small (to allow estimation of prediction error) but also not too large (to make sure that we actually are able to train a reliable classifier from the remaining data). A typical value for K is 5 or 10, so that 80% respectively 90% of the samples are used for training and the other 20 % or 10% for validation.

If $K = n$ there are as many folds as there are samples and the validation data set consists only of a single data point. This is called "leave one out" cross-validation (LOOCV). There are analytic approximations for the prediction error obtained by LOOCV so that this approach is computationally inexpensive for some standard models (including regression).

In a number of worksheets cross-validation is employed to evaluate classification models to demonstrate in practise that feature selection is useful to construct compact models with only a small number of variables that nonetheless generalise and predict well.

Further reading:

To study the technical details of cross-validation: read **Section 5.1 Cross-Validation** in James et al. (2013) *An introduction to statistical learning with applications in R*. Springer.

Chapter 5

Multivariate dependencies

5.1 Measuring the linear association between two sets of random variables

5.1.1 Outline

In this section we discuss how to measure the total linear association between two sets of random variables $\boldsymbol{x} = (x_1, \ldots, x_p)^T$ and $\boldsymbol{y} = (y_1, \ldots, y_q)^T$. We assume a joint correlation matrix

$$\boldsymbol{P} = \begin{pmatrix} \boldsymbol{P_x} & \boldsymbol{P_{xy}} \\ \boldsymbol{P_{yx}} & \boldsymbol{P_y} \end{pmatrix}$$

with cross-correlation matrix $\boldsymbol{P_{xy}} = \boldsymbol{P_{yx}^T}$ and the within-group group correlations $\boldsymbol{P_x}$ and $\boldsymbol{P_y}$. If the cross-correlations vanish, $\boldsymbol{P_{xy}} = 0$, then the two random vectors are uncorrelated, and the joint correlation matrix becomes a diagonal block matrix

$$\boldsymbol{P}_{\text{indep}} = \begin{pmatrix} \boldsymbol{P_x} & 0 \\ 0 & \boldsymbol{P_y} \end{pmatrix} .$$

5.1.2 Special cases

In linear regression model the *squared multiple correlation* or *coefficient of determination*

$$\text{Cor}(\boldsymbol{x}, y)^2 = \boldsymbol{P_{yx}} \boldsymbol{P_x^{-1}} \boldsymbol{P_{xy}}$$

is a standard measure to describe the strength of total linear association between the predictors $\boldsymbol{x}$ and the response y. If $\boldsymbol{P_{xy}} = 0$ then $\text{Cor}(\boldsymbol{x}, y)^2 = 0$.

If there is only a single predictor x then $\boldsymbol{P_{xy}} = \rho$ and $\boldsymbol{P_x} = 1$ and therefore the squared multiple correlation reduces to the squared Pearson correlation

$$\text{Cor}(x, y)^2 = \rho^2 .$$

5.1.3 Rozeboom vector correlation

For the general case with two random vectors we are looking for a scalar quantity that quantifies the divergence of the general joint correlation matrix $\boldsymbol{P}$ from the joint correlation matrix $\boldsymbol{P}_{\text{indep}}$ assuming uncorrelated $\boldsymbol{x}$ and $\boldsymbol{y}$.

One such quantity is Hotelling's *vector alienation coefficient* (given in his 1936 CCA paper[1])

$$\begin{aligned} a(\boldsymbol{x}, \boldsymbol{y}) &= \frac{\det(\boldsymbol{P})}{\det(\boldsymbol{P}_{\text{indep}})} \\ &= \frac{\det(\boldsymbol{P})}{\det(\boldsymbol{P}_{\boldsymbol{x}}) \, \det(\boldsymbol{P}_{\boldsymbol{y}})} \end{aligned}$$

With $\boldsymbol{K} = \boldsymbol{P}_{\boldsymbol{x}}^{-1/2} \boldsymbol{P}_{\boldsymbol{xy}} \boldsymbol{P}_{\boldsymbol{y}}^{-1/2}$ (cf. Chapter 2, Canonical correlation analysis) the vector alienation coefficient can be written (using the Weinstein-Aronszajn determinant identity and the formula for the determinant for block-structured matrices, see Appendix) as

$$\begin{aligned} a(\boldsymbol{x}, \boldsymbol{y}) &= \det\left(\boldsymbol{I}_p - \boldsymbol{K}\boldsymbol{K}^T\right) \\ &= \det\left(\boldsymbol{I}_q - \boldsymbol{K}^T\boldsymbol{K}\right) \\ &= \prod_{i=1}^{m} (1 - \lambda_i^2) \end{aligned}$$

where the λ_i are the singular values of $\boldsymbol{K}$, i.e. the canonical correlations for the pair $\boldsymbol{x}$ and $\boldsymbol{y}$.

If $\boldsymbol{P}_{\boldsymbol{xy}} = 0$ und thus $\boldsymbol{x}$ and $\boldsymbol{y}$ are uncorrelated then $\boldsymbol{P} = \boldsymbol{P}_{\text{indep}}$ and thus by construction the vector alienation coefficient $a(\boldsymbol{x}, \boldsymbol{y}) = 1$. Hence, it is itself not a generalisation of the squared multiple correlation.

Instead, Rozeboom (1965) proposed to use as squared *vector correlation* the complement

$$\begin{aligned} \text{Cor}(\boldsymbol{x}, \boldsymbol{y})^2 = \rho_{\boldsymbol{xy}}^2 &= 1 - a(\boldsymbol{x}, \boldsymbol{y}) \\ &= 1 - \det\left(\boldsymbol{I}_p - \boldsymbol{K}\boldsymbol{K}^T\right) \\ &= 1 - \det\left(\boldsymbol{I}_q - \boldsymbol{K}^T\boldsymbol{K}\right) \\ &= 1 - \prod_{i=1}^{m} (1 - \lambda_i^2) \end{aligned}$$

If $\boldsymbol{P}_{\boldsymbol{xy}} = 0$ then $\text{Cor}(\boldsymbol{x}, \boldsymbol{y})^2 = 0$. Moreover, if either $p = 1$ or $q = 1$ the squared vector correlation reduces to the corresponding squared multiple correlation, and for both $p = 1$ and $q = 1$ it becomes squared Pearson correlation.

A more general way to measure multivariate association is mutual information (MI) which not only covers linear but also non-linear association. As we will discuss in a subsequent section the Rozeboom vector correlation arises naturally in MI for the multivariate normal distribution.

[1] Hotelling, H. 1936. Relations between two sets of variates. Biometrika **28**:321–377.

5.1.4 RV coefficient

Another common approach to measure association between two random vectors is the RV coefficient introduced by Robert and Escoufier (1976) as

$$RV(\boldsymbol{x},\boldsymbol{y}) = \frac{\mathrm{Tr}(\boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yx})}{\mathrm{Tr}(\boldsymbol{\Sigma}_x^2)\mathrm{Tr}(\boldsymbol{\Sigma}_y^2)}$$

It is easier to compute than the Rozeboom vector correlation since it is based on the matrix trace rather than matrix determinant.

For $q = p = 1$ the RV coefficient reduces to the squared correlation. However, the RV coefficient does *not* reduce to the multiple correlation coefficient for $q = 1$ and $p > 1$, and therefore the RV coefficient cannot be considered a coherent generalisation of Pearson and multiple correlation to the case of two random vectors.

5.2 Mutual information as generalisation of correlation

5.2.1 Definition of mutual information

Recall the definition of Kullback-Leibler divergence, or relative entropy, between two distributions:

$$I^{KL}(F||G) := \mathrm{E}_F \log\left(\frac{f(\boldsymbol{x})}{g(\boldsymbol{x})}\right)$$

Here F plays the role of the true distribution and G is an approximating distribution, with f and g being the corresponding densities.

The *Mutual Information* (MI) between two random variables $\boldsymbol{x}$ and $\boldsymbol{y}$ is defined as the KL divergence between the corresponding joint distribution and the product distribution:

$$\mathrm{MI}(\boldsymbol{x},\boldsymbol{y}) = I^{KL}(F_{\boldsymbol{x},\boldsymbol{y}}||F_{\boldsymbol{x}}F_{\boldsymbol{y}}) = \mathrm{E}_{F_{\boldsymbol{x},\boldsymbol{y}}} \log\left(\frac{f(\boldsymbol{x},\boldsymbol{y})}{f(\boldsymbol{x})\,f(\boldsymbol{y})}\right).$$

Thus, MI measures how well the joint distribution can be approximated by the product distribution (which would be the appropriate joint distribution if $\boldsymbol{x}$ and $\boldsymbol{y}$ are independent). Since MI is an application of KL divergence is shares all its properties. In particular, $\mathrm{MI}(\boldsymbol{x},\boldsymbol{y}) = 0$ implies that the joint distribution and product distributions are the same. Hence the two random variables $\boldsymbol{x}$ and $\boldsymbol{y}$ are independent if the mutual information vanishes.

5.2.2 Mutual information between two normal variables

The KL divergence between two multivariate normal distributions F_0 and F is

$$I^{KL}(F_0||F) = \frac{1}{2}\left\{(\boldsymbol{\mu}-\boldsymbol{\mu}_0)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_0) + \mathrm{Tr}\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}_0\right) - \log\det\left(\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}_0\right) - d\right\}$$

This allows compute the mutual information $\mathrm{MI}_{\mathrm{norm}}(x,y)$ between two univariate random variables x and y that are are correlated and assumed to be jointly

bivariate normal. Let $\boldsymbol{z} = (x, y)^T$. The joint bivariate normal distribution is characterised by the mean $\mathrm{E}(\boldsymbol{z}) = \boldsymbol{\mu} = (\mu_x, \mu_y)^T$ and the covariance matrix

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_x^2 & \rho\,\sigma_x\sigma_y \\ \rho\,\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix}$$

where $\mathrm{Cor}(x, y) = \rho$. If x and y are independent then $\rho = 0$ and

$$\boldsymbol{\Sigma}_{\text{indep}} = \begin{pmatrix} \sigma_x^2 & 0 \\ 0 & \sigma_y^2 \end{pmatrix}.$$

The product

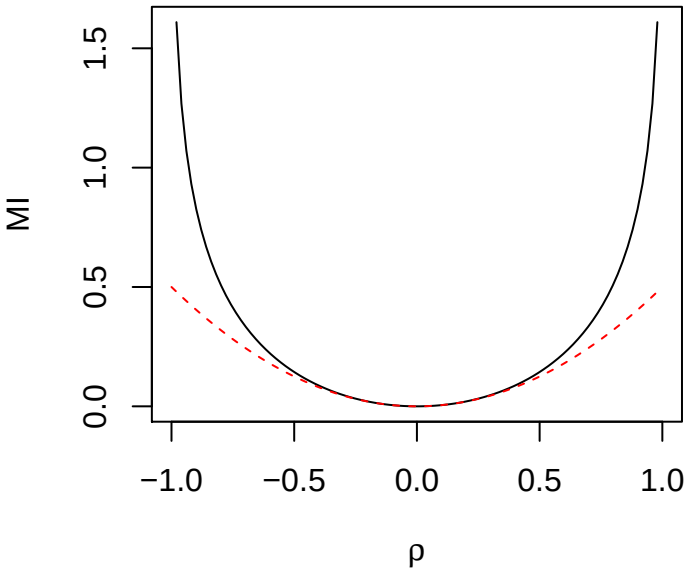
$$\boldsymbol{A} = \boldsymbol{\Sigma}_{\text{indep}}^{-1}\boldsymbol{\Sigma} = \begin{pmatrix} 1 & \rho\frac{\sigma_y}{\sigma_x} \\ \rho\frac{\sigma_x}{\sigma_y} & 1 \end{pmatrix}$$

has trace $\mathrm{Tr}(\boldsymbol{A}) = 2$ and determinant $\det(\boldsymbol{A}) = 1 - \rho^2$.

With this the mutual information between x and y can be computed as

$$\begin{aligned} \mathrm{MI}_{\text{norm}}(x, y) &= I^{KL}(N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) || N(\boldsymbol{\mu}, \boldsymbol{\Sigma}_{\text{indep}})) \\ &= \frac{1}{2}\left\{ \mathrm{Tr}\left(\boldsymbol{\Sigma}_{\text{indep}}^{-1}\boldsymbol{\Sigma}\right) - \log\det\left(\boldsymbol{\Sigma}_{\text{indep}}^{-1}\boldsymbol{\Sigma}\right) - 2 \right\} \\ &= -\frac{1}{2}\log(1 - \rho^2) \\ &\approx \frac{\rho^2}{2} \end{aligned}$$

Thus $\mathrm{MI}_{\text{norm}}(x, y)$ is is a one-to-one function of the squared correlation ρ^2 between x and y:



For small values of correlation $2\mathrm{MI}_{\text{norm}}(x, y) \approx \rho^2$.

5.2.3 Mutual information between two normally distributed random vectors

The mutual information $\mathrm{MI}_{\mathrm{norm}}(\boldsymbol{x},\boldsymbol{y})$ between two multivariate normal random vector $\boldsymbol{x}$ and $\boldsymbol{y}$ can be computed in a similar fashion as in the bivariate case.

Let $\boldsymbol{z} = (\boldsymbol{x},\boldsymbol{y})^T$ with dimension $d = p + q$. The joint multivariate normal distribution is characterised by the mean $\mathrm{E}(\boldsymbol{z}) = \boldsymbol{\mu} = (\boldsymbol{\mu}_x^T, \boldsymbol{\mu}_y^T)^T$ and the covariance matrix

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_x & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{xy}^T & \boldsymbol{\Sigma}_y \end{pmatrix} .$$

If $\boldsymbol{x}$ and $\boldsymbol{y}$ are independent then $\boldsymbol{\Sigma}_{xy} = 0$ and

$$\boldsymbol{\Sigma}_{\mathrm{indep}} = \begin{pmatrix} \boldsymbol{\Sigma}_x & 0 \\ 0 & \boldsymbol{\Sigma}_y \end{pmatrix} .$$

The product

$$\begin{aligned} \boldsymbol{A} = \boldsymbol{\Sigma}_{\mathrm{indep}}^{-1}\boldsymbol{\Sigma} &= \begin{pmatrix} \boldsymbol{I}_p & \boldsymbol{\Sigma}_x^{-1}\boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_y^{-1}\boldsymbol{\Sigma}_{yx} & \boldsymbol{I}_q \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{I}_p & \boldsymbol{V}_x^{-1/2}\boldsymbol{P}_x^{-1}\boldsymbol{P}_{xy}\boldsymbol{V}_y^{1/2} \\ \boldsymbol{V}_y^{-1/2}\boldsymbol{P}_y^{-1}\boldsymbol{P}_{yx}\boldsymbol{V}_x^{1/2} & \boldsymbol{I}_q \end{pmatrix} \end{aligned}$$

has trace $\mathrm{Tr}(\boldsymbol{A}) = d$ and determinant

$$\begin{aligned} \det(\boldsymbol{A}) &= \det(\boldsymbol{I}_p - \boldsymbol{K}\boldsymbol{K}^T) \\ &= \det(\boldsymbol{I}_q - \boldsymbol{K}^T\boldsymbol{K}) \end{aligned}$$

with $\boldsymbol{K} = \boldsymbol{P}_x^{-1/2}\boldsymbol{P}_{xy}\boldsymbol{P}_y^{-1/2}$. With $\lambda_1, \ldots, \lambda_m$ the singular values of $\boldsymbol{K}$ (i.e. the canonical correlations between $\boldsymbol{x}$ and $\boldsymbol{y}$) we get

$$\det(\boldsymbol{A}) = \prod_{i=1}^{m}(1 - \lambda_i^2)$$

The mutual information between $\boldsymbol{x}$ and $\boldsymbol{y}$ is then

$$\begin{aligned} \mathrm{MI}_{\mathrm{norm}}(\boldsymbol{x},\boldsymbol{y}) &= I^{KL}(N(\boldsymbol{\mu},\boldsymbol{\Sigma})||N(\boldsymbol{\mu},\boldsymbol{\Sigma}_{\mathrm{indep}})) \\ &= \frac{1}{2}\left\{ \mathrm{Tr}\left(\boldsymbol{\Sigma}_{\mathrm{indep}}^{-1}\boldsymbol{\Sigma}\right) - \log\det\left(\boldsymbol{\Sigma}_{\mathrm{indep}}^{-1}\boldsymbol{\Sigma}\right) - d \right\} \\ &= -\frac{1}{2}\sum_{i=1}^{m}\log(1 - \lambda_i^2) \end{aligned}$$

Note that $\mathrm{MI}_{\mathrm{norm}}(\boldsymbol{x},\boldsymbol{y})$ is the sum of the MIs resulting from the individual canonical correlations λ_i with the same functional form as in the bivariate normal case.

By comparison with the squared Rozeboom vector correlation coefficient ρ_{xy}^2 we recognize that

$$\mathrm{MI}_{\mathrm{norm}}(\boldsymbol{x},\boldsymbol{y}) = -\frac{1}{2}\log(1 - \rho_{xy}^2) \approx \frac{1}{2}\rho_{xy}^2$$

Thus, in the multivariate case $\mathrm{MI}_{\mathrm{norm}}(\boldsymbol{xy})$ has again exactly the same functional relationship with the vector correlation $\rho^2_{\boldsymbol{x},\boldsymbol{y}}$ as
as the $\mathrm{MI}_{\mathrm{norm}}(x, y)$ for two univariate variables with squared Pearson correlation ρ^2.

Thus, Rozebooms vector correlation is derived via mutual information for jointly multivariate normal distributed variables.

5.2.4 Using MI for variable selection

In principle, MI can be computed for any distribution and model and thus applies to both normal and non-normal models, and to both linear and nonlinear relationships.

In very general way we may denote by $F_{\boldsymbol{y}|\boldsymbol{x}}$ we denote a predictive model for $\boldsymbol{y}$ conditioned on $\boldsymbol{x}$ and $F_{\boldsymbol{y}}$ is the marginal distribution of $\boldsymbol{y}$ without predictors. Note that the predictive model can assume any form (incl. nonlinear). Typically $F_{\boldsymbol{y}|\boldsymbol{x}}$ is a complex model and $F_{\boldsymbol{y}}$ a simple model (no predictors).

Then mutual information between $\boldsymbol{x}$ and $\boldsymbol{y}$ can be also understood as expectated KL divergence between the conditional and marginal distributions:

$$\mathrm{E}_{F_{\boldsymbol{x}}}\, I^{KL}(F_{\boldsymbol{y}|\boldsymbol{x}}||F_{\boldsymbol{y}}) = \mathrm{MI}(\boldsymbol{x}, \boldsymbol{y})$$

This can be shown as follows. The KL divergence between $F_{\boldsymbol{y}|\boldsymbol{x}}$ and $F_{\boldsymbol{y}}$ is given by

$$I^{KL}(F_{\boldsymbol{y}|\boldsymbol{x}}, F_{\boldsymbol{y}}) = \mathrm{E}_{F_{\boldsymbol{y}|\boldsymbol{x}}} \log\left(\frac{f(\boldsymbol{y}|\boldsymbol{x})}{f(\boldsymbol{y})}\right),$$

which is a random variable since it depends on $\boldsymbol{x}$. Taking the expectation with regard to $F_{\boldsymbol{x}}$ (the distribution of $\boldsymbol{x}$) we get

$$\mathrm{E}_{F_{\boldsymbol{x}}} I^{KL}(F_{\boldsymbol{y}|\boldsymbol{x}}, F_{\boldsymbol{y}}) = \mathrm{E}_{F_{\boldsymbol{x}}}\mathrm{E}_{F_{\boldsymbol{y}|\boldsymbol{x}}} \log\left(\frac{f(\boldsymbol{y}|\boldsymbol{x})f(\boldsymbol{x})}{f(\boldsymbol{y})f(\boldsymbol{x})}\right) = \mathrm{E}_{F_{\boldsymbol{x},\boldsymbol{y}}} \log\left(\frac{f(\boldsymbol{x},\boldsymbol{y})}{f(\boldsymbol{y})f(\boldsymbol{x})}\right) = \mathrm{MI}(\boldsymbol{x}, \boldsymbol{y})\,.$$

Because of this link of MI with conditioning the MI between response and predictor variables is often used for variable and feature selection in general models.

5.2.5 Other measures of general dependence

Besides mutual information there are others measures of general dependence between multivariate random variables.

The two most important ones that have been proposed in the recent literatur are i) distance correlation and ii) the maximal information coefficient (MIC and MIC_e).

5.3 Graphical models

5.3.1 Purpose

Graphical models combine features from

- graph theory
- probability
- statistical inference

The literature on graphical models is huge, we focus here only on two commonly used models:

- DAGs (directed acyclic graphs), all edges are directed, no directed loops (i.e. no cycles, hence "acyclic")
- GGM (Gaussian graphical models), all edges are undirected

Graphical models provide probabilistic models for trees and for networks, with random variables represented by nodes in the graphs, and branches representing conditional dependencies. In this regard they generalise both the tree-based clustering approaches as well as the probabilistic non-hierarchical methods (GMMs).

However, the class of graphical models goes much beyond simple unsupervised learning models. It also includes regression, classification, time series models etc. See e.g. the reference book by Murphy (2012).

5.3.2 Basic notions from graph theory

- Mathematically, a graph $G = (V, E)$ consists of a a set of vertices or nodes $V = \{v_1, v_2, \ldots\}$ and a set of branches or edges $E = \{e_1, e_2, \ldots\}$.
- Edges can be undirected or directed.
- Graphs containing only directed edges are directed graphs, and likewise graphs containing only undirected edges are called undirected graphs. Graphs containing both directed and undirected edges are called partially directed graphs.
- A path is a sequence of of vertices such that from each of its vertices there is an edge to the next vertex in the sequence.
- A graph is connected when there is a path between every pair of vertices.
- A cycle is a path in a graph that connects a node with itself.
- A connected graph with no cycles is a called a tree.
- The degree of a node is the number of edges it connects with. If edges are all directed the degree of a node is the sum of the in-degree and out-degree, which counts the incoming and outgoing edges, respectively.
- External nodes are nodes with degree 1. In a tree-structed graph these are also called leafs.

Some notions are only relevant for graphs with directed edges:

- In a directed graph the parent node(s) of vertex v is the set of nodes $\text{pa}(v)$ directly connected to v via edges directed from the parent node(s) towards v.

- Conversely, v is called a child node of $\text{pa}(v)$. Note that a parent node can have several child nodes, so v may not be the only child of $\text{pa}(v)$.
- In a directed tree graph, each node has only a single parent, except for one particular node that has no parent at all (this node is called the root node).
- A DAG, or directed acyclic graph, is a directed graph with no directed cycles. A (directed) tree is a special version of a DAG.

5.3.3 Probabilistic graphical models

A graphical model uses a graph to describe the relationship between random variables $x_1, \ldots, x_d$. The variables are assumed to have a joint distribution with density/mass function $\Pr(x_1, x_2, \ldots, x_d)$. Each random variable is placed in a node of the graph.

The structure of the graph and the type of the edges connecting (or not connecting) any pair of nodes/variables is used to describe the conditional dependencies, and to simplify the joint distribution.

Thus, a graphical model is in essence a visualisation of the joint distribution using structural information from the graph helping to understand the mutual relationship among the variables.

5.3.4 Directed graphical models

In a **directed graphical model** the graph structure is assumed to be a DAG (or a directed tree, which is also a DAG).

Then the joint probability distribution can be factorised into a *product of conditional probabilities* as follows:

$$\Pr(x_1, x_2, \ldots, x_d) = \prod_i \Pr(x_i | \text{pa}(x_i))$$

Thus, the overall joint probability distribution is specified by local conditional distributions and the graph structure, with the directions of the edges providing the information about parent-child node relationships.

Probabilistic DAGs are also known as "Bayesian networks".

Idea: by trying out all possible trees/graphs and fitting them to the data using maximum likelihood (or Bayesian inference) we hope to be able identify the graph structure of the data-generating process.

Challenges

1) in the tree/network the internal nodes are usually not known, and thus have to be treated as *latent* variables.

Answer: To impute the states at these nodes we may use the EM algorithm as in GMMs (which in fact can be viewed as graphical models, too!).

2) If we treat the internal nodes as unknowns we need to marginalise over the internal nodes, i.e. we need to sum / integrate over all possible set of states of the internal nodes!

Answer: This can be handled very effectively using the **Viterbi algorithm** which is essentially an application of the generalised distributive law. In particular for tree graphs this means that the summations occurs locally at each nodes and propagates recursively accross the tree.

3) In order to infer the tree or network structure the space of all trees or networks need to be explored. This is not possible in an exhaustive fashion unless the number of variables in the tree is very small.

Answer: Solution: use heuristic approaches for tree and network search!

4) Furthermore, there exist so-called "equivalence classes" of graphical models, i.e. sets of graphical models that share the same joint probability distribution. Thus, all graphical models within the same equivalence class cannot be distinguished from observational data, even with infinite sample size!

Answer: this is a fundamental mathematical problem of identifiability so there is now way around this issue. However, on the positive side, this also implies that the search through all graphical models can be restricted to finding the so-called "essential graph" (e.g. https://projecteuclid.org/euclid.aos/1031833662)

Conclusion: using directed graphical models for structure discovery is very time consuming and computationally demanding for anything but small toy data sets.

This also explains why heuristic and non-model based approaches (such as hierarchical clustering) are so popular even though full statistical modelling is in principle possible.

5.3.5 Undirected graphical models

Another class of graphical models are models that contain only undirected edges. These **undirected graphical models** are used to represent the pairwise conditional (in)dependencies among the variables in the graph, and the resulting model is therefore also called **conditional independence graph**.

If x_i and x_j two selected random variables/nodes, and the set $\{x_k\}$ represents all other variables/nodes with $k \neq i$ and $k \neq j$. We say that variables x_i and x_j are conditionally independent given all the other variables $\{x_k\}$

$$x_i \perp\!\!\!\perp x_j | \{x_k\}$$

if the joint probability density of x_i, x_j and x_k factorises as

$$\Pr(x_1, x_2, \ldots, x_d) = \Pr(x_i|\{x_k\})\Pr(x_j|\{x_k\})\Pr(\{x_k\})\,.$$

or equivalently

$$\Pr(x_i, x_j|\{x_k\}) = \Pr(x_i|\{x_k\})\Pr(x_j|\{x_k\})\,.$$

In a corresponding conditional independence graph, there is no edge between x_i and x_j, as in such a graph *missing edges correspond to conditional independencies* between the respective non-connected nodes.

5.3.5.1 Gaussian graphical model

Assuming that $x_1, \ldots, x_d$ are jointly normal distributed, i.e. $\boldsymbol{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, it turns out that it is straightforward to identify the pairwise conditional independencies. From $\boldsymbol{\Sigma}$ we first obtain the precision matrix

$$\boldsymbol{\Omega} = (\omega_{ij}) = \boldsymbol{\Sigma}^{-1}.$$

Crucially, it can be shown that $\omega_{ij} = 0$ implies $x_i \perp\!\!\!\perp x_j | \{x_k\}$! Hence, from the precision matrix $\boldsymbol{\Omega}$ we can directly read off all the pairwise conditional independencies among the variables $x_1, x_2, \ldots, x_d$!

Often, the covariance matrix $\boldsymbol{\Sigma}$ is dense (few zeros) but the corresponding precision matrix $\boldsymbol{\Omega}$ is sparse (many zeros).

The conditional independence graph computed for normally distributed variables is called a **Gaussian graphical model**, or **GGM**. A further alternative name is **covariance selection model**.

5.3.5.2 Related quantity: partial correlation

From the precision matrix $\boldsymbol{\Omega}$ we can also compute the matrix of pairwise full conditional *partial correlations*:

$$\rho_{ij|\text{rest}} = -\frac{\omega_{ij}}{\sqrt{\omega_{ii}\omega_{jj}}}$$

which is essentially the standardised precision matrix (similar to correlation but with an extra minus sign!)

The partial correlations lie in the range between -1 and +1, $\rho_{ij|\text{rest}} \in [-1, 1]$, just like standard correlations.

If $\boldsymbol{x}$ is multivariate normal then $\rho_{ij|\text{rest}} = 0$ indicates conditional independence between x_i and x_j.

Regression interpretation: partial correlation is the correlation that remains between the two variables if the effect of the other variables is "regressed away". In other words, the partial correlation is exactly equivalent to the correlation between the residuals that remain after regressing x_i on the variables $\{x_k\}$ and x_j on $\{x_k\}$.

5.3.6 Algorithm for learning GGMs

From the above we can devise a simple algorithm to to learn Gaussian graphical model (GGM) from data:

1. Estimate covariance $\hat{\boldsymbol{\Sigma}}$ (in such a way that it is invertible!)
2. Compute corresponding partial correlations
3. If $\hat{\rho}_{ij|\text{rest}} \approx 0$ then there is (approx). conditional independence between x_i and x_j.
   In practise this is done by statistical testing for vanishing partial correlations. If there are many edges we also need adjustment for simultaneous multiple testing since all edges are tested in parallel.

5.3.7 Example: exam score data (Mardia et al 1979:)

Correlations (rounded to 2 digits):

```
##            mechanics vectors algebra analysis statistics
## mechanics       1.00    0.55    0.55     0.41       0.39
## vectors         0.55    1.00    0.61     0.49       0.44
## algebra         0.55    0.61    1.00     0.71       0.66
## analysis        0.41    0.49    0.71     1.00       0.61
## statistics      0.39    0.44    0.66     0.61       1.00
```

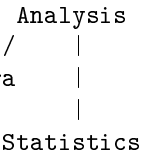
Partial correlations (rounded to 2 digits):

```
##            mechanics vectors algebra analysis statistics
## mechanics       1.00    0.33    0.23     0.00       0.02
## vectors         0.33    1.00    0.28     0.08       0.02
## algebra         0.23    0.28    1.00     0.43       0.36
## analysis        0.00    0.08    0.43     1.00       0.25
## statistics      0.02    0.02    0.36     0.25       1.00
```

Note that that there are no zero correlations but there are **four partial correlations close to 0**, indicating **conditional independencies** between:

- analysis and mechanics,
- statistics and mechanics,
- analysis and vectors, and
- statistics and vectors.

Thus, of 10 possible edges four are missing, and thus the conditional independence graph looks as follows:



Chapter 6

Nonlinear and nonparametric models

In the last part of the module we discuss methods that go beyond the linear methods prevalent in classical multivariate statistics.

Relevant textbooks:

The lectures for much of this part of the module follow selected chapters from the following three text books:

- James et al. (2013) *An introduction to statistical learning with applications in R*. Springer.
- Hastie et al. (2009) *The elements of statistical learning: data mining, inference, and prediction*. Springer.
- Rogers and Girolami (2017) *A first course in machine learning (2nd edition)*. CRC Press.

Please study the relevant section and chapters as indicated below in each subsection!

6.1 Limits of linear models and correlation

Linear models are very effective tools. However, it is important to recognise their limits especially when modelling complex nonlinear relationships.

6.1.1 Correlation only measures linear dependence

A very simple demonstration of this is given by the following example. Assume x is a normal distributed random variable with $x \sim N(0,1)$. From x we construct a second random variable $y = x^2$ — thus y fully depends on x with no added extra noise. What is the correlation between x and y?

Let's ansers this question by running a small computer simulation:

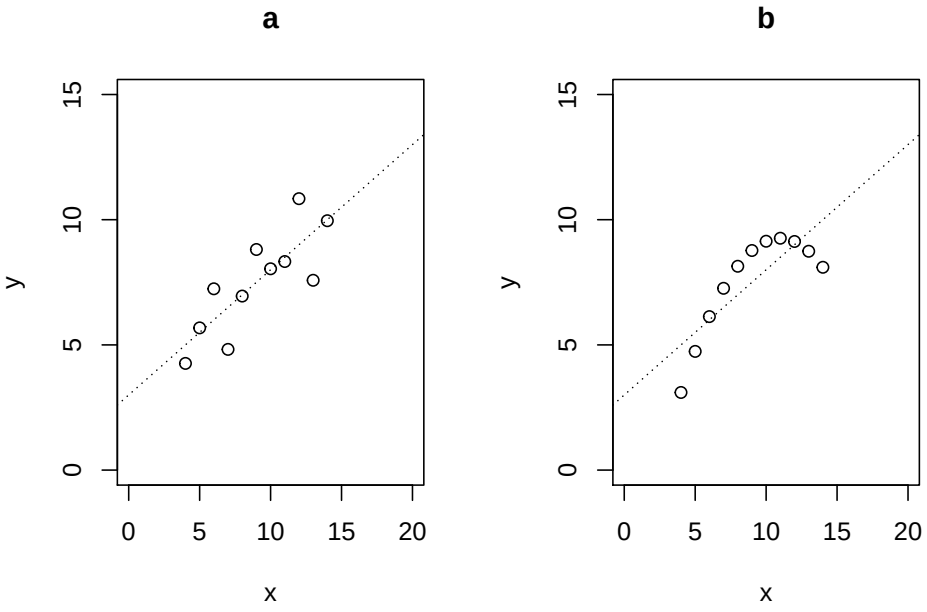
```
x=rnorm(10000)
y = x^2
cor(x,y)
```

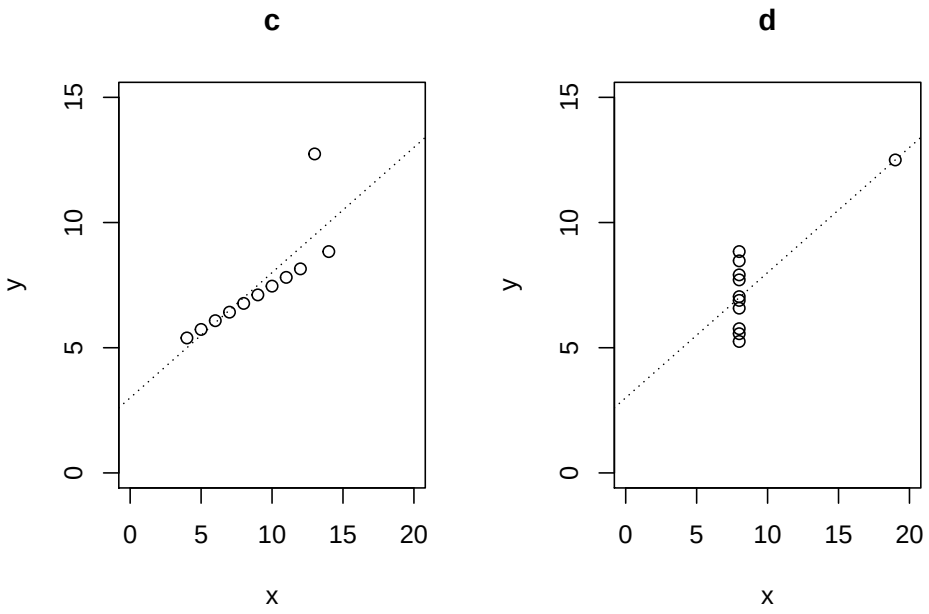
```
## [1] -0.01589823
```

Thus, correlation is (almost) zero even though x and y are fully dependent! This is because correlation only measures linear association!

6.1.2 Anscombe data sets

Using correlation, and more generally linear models, blindly can thus hide the underlying complexity of the analysed data. This is demonstrated by the classic "Anscombe quartet" of data sets (F. J. Anscombe. 1973. Graphs in statistical analysis. The American Statistician 27:17-21, http://dx.doi.org/10.1080/00031305.1973.10478966):





As evident from the scatter plots the relationship between the two variables x and y is very different in the four cases! However, intriguingly all four data sets share exactly the same linear characteristics and summary statistics:

- Means $m_x = 9$ and $m_y = 7.5$
- Variances $s_x^2 = 11$ and $s_y^2 = 4.13$
- Correlation $r = 0.8162$
- Linear model fit with intercept $a = 3.0$ and slope $b = 0.5$

Thus, in actual data analysis it is always a **good idea to inspect the data visually** to get a first impression whether using a linear model makes sense.

In the above only data "a" follows a linear model. Data "b" represents a quadratic relationship. Data "c" is linear but with an outlier that disturbs the linear relationship. Finally data "d" also contains an outlier but also represent a case where y is (apart from the outlier) is not dependent on x.

In the Worksheet 10 a more recent version of the Anscombe quartet will be analysed in the form of the "datasauRus" dozen - 13 highly nonlinear datasets that all share the same linear characteristics.

6.2 Random forests

Another widely used approach for prediction in nonlinear settings is the method of random forests.

Relevant reading:

Please read: James et al. (2013) **Chapter 8 "Tree-Based Methods"**

Specifically:

- Section 8.1 The Basics of Decision Trees
- Section 8.2.1 Bagging
- Section 8.2.2 Random Forests

6.2.1 Stochastic vs. algorithmic models

Two cultures in statistical modelling: stochastic vs. algorithmic models

Classic discussion paper by Leo Breiman (2001): Statistical modeling: the two cultures. Statistical Science. Vol 16, pages 199-231. https://projecteuclid.org/euclid.ss/1009213726

6.2.2 Random forests

Invented by Breimann in 1996.

Basic idea:

- A single decision tree is unreliable and unstable (weak predictor/classifier).
- Use boostrap to generate multiple decision trees (="forest")
- Average over predictions from all tree (="bagging", bootstrap aggregation)

The averaging procedure has the effect of variance stabilisation. Intringuingly, averaging across all decision trees dramatically improves the overall prediction accuracy!

The Random Forests approach is an example of an **ensemble method** (since it is based on using an "ensemble" of trees).

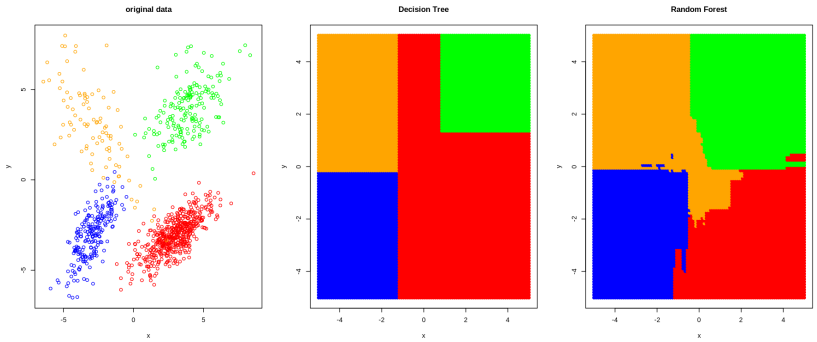
Variations: boosting, XGBoost (https://xgboost.ai/)

Random forests will be applied in Worksheet 10.

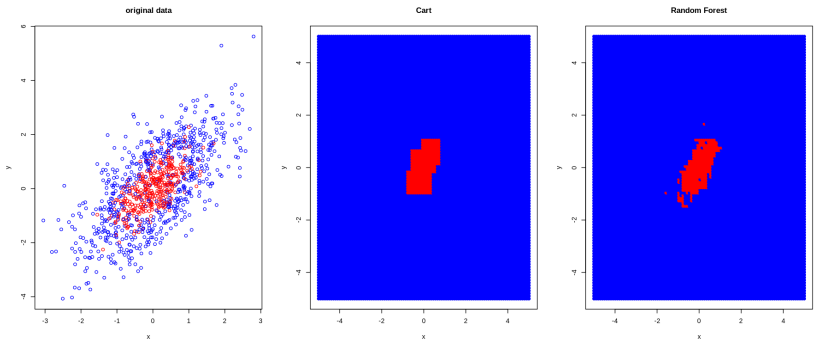
They are computationally expensive but typically perform very well!

6.2.3 Comparison of decision boundaries: decision tree vs. random forest

Non-nested case:



Nested case:



Compare also with the decision boundaries for LDA and QDA (previous chapter).

6.3 Gaussian processes

Gaussian processes offer another nonparametric approach to model nonlinear dependencies. They provide a probabilistic model for the unknown nonlinear function.

Relevant reading

Please read: Rogers and Girolami (2017) **Chapter 8: Gaussian processes.**

6.3.1 Main concepts

- Gaussian processes (GPs) belong the the family of **Bayesian nonparametric models**
- Idea:
  - start with prior over a function (!),
  - then condition on observed data to get posterior distribution (again over all functions)
  - use an infinitely dimensional multivariate normal distribution as prior

6.3.2 Technical background:

GPs make use of the fact that marginal and conditional distributions of a multivariate normal are also multivariate normal.

Multivariate normal distribution:

$$\boldsymbol{z} \sim N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Assume:

$$\boldsymbol{z} = \begin{pmatrix} \boldsymbol{z}_1 \\ \boldsymbol{z}_2 \end{pmatrix}$$

with

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}$$

and

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{12}^T & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

with corresponding dimensions d_1 and d_2 and $d_1 + d_2 = d$.

Marginal distributions:

Any subset of $\boldsymbol{z}$ is also multivariate normal distributed:

$$\boldsymbol{z}_i \sim N_{d_i}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_{ii})$$

Conditional multivariate normal:

The conditional distribution is also multivariate normal:

$$\boldsymbol{z}_i | \boldsymbol{z}_j = \boldsymbol{z}_{i|j} \sim N_{d_i}(\boldsymbol{\mu}_{i|j}, \boldsymbol{\Sigma}_{i|j})$$

with

$$\boldsymbol{\mu}_{i|j} = \boldsymbol{\mu}_i + \boldsymbol{\Sigma}_{ij}\boldsymbol{\Sigma}_{jj}^{-1}(\boldsymbol{z}_j - \boldsymbol{\mu}_j)$$

and

$$\boldsymbol{\Sigma}_{i|j} = \boldsymbol{\Sigma}_{ii} - \boldsymbol{\Sigma}_{ij}\boldsymbol{\Sigma}_{jj}^{-1}\boldsymbol{\Sigma}_{ij}^T$$

$\boldsymbol{z}_{i|j}$ and $\boldsymbol{\mu}_{i|j}$ have dimension $d_i \times 1$ and $\boldsymbol{\Sigma}_{i|j}$ has dimension $d_i \times d_i$

6.3.3 Covariance functions and kernel

The GP prior is a infinitely dimensional multivariate normal with mean zero and the **covariance specified by a function**:

A widely used covariance function is

$$\text{Cov}(x, x') = \sigma^2 e^{-\frac{(x-x')^2}{2l^2}}$$

This is known as the **squared-exponential kernel** or **Radial-basis function (RBF) kernel**.

Note that $(x, x) = \sigma^2$ and the autocorrelation $\text{Cor}(x, x') = e^{-\frac{(x-x')^2}{2l^2}}$.

The parameter l is the length scale parameter and describes the wigglyness or smoothness of the resulting function. Small values of l mean more complex, more wiggly functions, and low autocorrelation.

There are many other kernel functions, including periodic, polynomial and linear kernels.

6.3.4 GP model

Nonlinear regression in the GP approach is conceptually very simple:

- start with GP prior over all x
- then condition on the observed $x_1, \ldots, x_n$
- the resulting conditional multivariate normal can used to predict the function values at any unobserved values of x
- automatically provides credible intervals for predictions.

GP regression also provides a direct link with Bayesian linear regression (using a linear kernel).

Drawbacks: computationally expensive (n^3 because of the matrix inversion)

6.4 Neural networks

Another highly important class of models for nonlinear prediction (and nonlinear function approximation) are neural networks.

Relevant reading:

Please read: Hastie et al. (2009) **Chapter 11 "Neural networks"**

6.4.1 History

Neural networks are actually relatively old models, going back to the 1950s!

Three phases of neural networks (NN)

- 1950/60: replicating functions of neurons in the brain (perceptron)
- 1980/90: neural networks as universal function approximators
- 2010—today: deep learning

The first phase was biologically inspired, the second phase focused on mathematical properties, and the current phase is pushed forward by advances in computer science and numerical optimisation:

- backpropagation algorithm
- auto-differentiation,
- stochastic gradient descent
- use of GPUs and TPUs,
- availability and devlopment of software packages by major internet companies:
  - TensorFlow/Keras (Google),
  - MXNet (Amazon),
  - PyTorch (Facebook),
  - PaddlePaddle (Baidu) etc.

6.4.2 Neural networks

Neural networks are essentially stacked systems of linear regressions, mapping input nodes (random variables) to outputs (response nodes). Each internal layer corresponds to internal latent variables. Each layer is connected with the next layer by **non-linear activation functions**.

- feedforward single layer NN
- stacked nonlinear multiple regression with hidden variables
- optimise by empirical risk minimisation

It can be shown that NN can approximate any arbitrary non-linear function mapping input and output.

"Deep" neural networks have many layers, and their optimisation requires advanced techniques (see above).

Neural networks are very highly parameterised models and require typically a lot of data for training.

Some of the statistical aspects of NN are not well understood: in particular it is known that NN overfit the data but can still generalise well. On the other hand, it is also know that NN can also be "fooled", i.e. prediction can be unstable (adversarial examples).

Current statistical research on NN focuses on interpretability and on links with Bayesian inference and models (e.g. GPs). For example:

- https://link.springer.com/book/10.1007/978-3-030-28954-6
- https://arxiv.org/abs/1910.12478

6.4.3 Learning more about deep learning

A good place to to learn more about deep learning and about the actual implementations in computer code on various platforms is the book "Dive into deep learning" by Zhang et al. (2020) available online at https://d2l.ai/

Appendix A

Brief refresher on matrices

This is intended a very short recap of some essentials you need to know about matrices. We will frequently make use of matrix calculations. Matrix notation helps to make multivariate equations simpler and to understand them better.

For more details please consult the lecture notes of earlier modules (e.g. linear algebra).

In this course we only work with **real matrices**, i.e. we assume all matrix elements are real numbers.

A.1 Matrix basics

A.1.1 Matrix notation

In matrix notation we distinguish between scalars, vectors, and matrices:

Scalar: x, X, lower or upper case, plain type.

Vector: $\boldsymbol{x}$, lower case, bold type. In handwriting an arrow $\vec{x}$ indicates a vector.

In component notation we write $\boldsymbol{x} = (x_1, \ldots, x_d)^T = (x_i)^T$. By convention, a vector is a column vector, i.e. the elements are arranged in a column and the index (here i) refers to the row of the column. If you transpose a column vector it becomes a row vector $\boldsymbol{x}^T = (x_1, \ldots, x_d) = (x_i)$ and the index now refers to the column.

Matrix: $\boldsymbol{X}$, upper case, bold type. In handwriting an underscore $\underline{X}$ indicates a matrix.

In component notation we write $\boldsymbol{X} = (x_{ij})$. By convention, the first index (here i) of the scalar elements x_{ij} denotes the row and the second index (here j) the column of the matrix. Assuming that n is the number of rows and d is the number of columns you can also view the matrix $\boldsymbol{X} = (\boldsymbol{x}_j) = (\boldsymbol{z}_i)^T$ as being composed of column vectors $\boldsymbol{x}_j = (x_{1j}, \ldots, x_{nj})^T$ or of row vectors $\boldsymbol{z}_i^T = (x_{i1}, \ldots, x_{id})$.

A (column) vector is a matrix of size $d \times 1$. A row vector is a matrix of size $1 \times d$. A scalar is a matrix of size 1×1.

A.1.2 Random matrix

A **random matrix** (vector) is a matrix (vector) whose elements are random variables.

Note that the standard notation used in univariate statistics to distinguish random variables and their realisations (i.e. upper versus lower case) does not work in multivariate statistics. Therefore, you need to determine from the context whether a quantity represents a random variable, or whether it is a constant.

A.1.3 Special matrices

$\boldsymbol{I}_d$ is the identity matrix. It is a square matrix of size $d \times d$ with the diagonal filled with 1 and off-diagonals filled with 0.

$$\boldsymbol{I}_d = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & 0 & & 1 \end{pmatrix}$$

$\mathbf{1}$ is a matrix that contains only 1s. Most often it is used in the form of a column vector with d rows:

$$\mathbf{1}_d = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

A diagonal matrix is a matrix where all off-diagonal elements are zero.

A triangular matrix is a square matrix whose elements either below or above the diagonal are all zero (upper vs. lower triangular matrix).

A.2 Simple matrix operations

A.2.1 Matrix addition and multiplication

Matrices behave much like common numbers. For example, there exist matrix addition $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ and matrix multiplication $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{B}$.

Matrix addition is simply the result of the addition of the corresponding elements in $\boldsymbol{A}$ and $\boldsymbol{B}$, i.e $c_{ij} = a_{ij} + b_{ij}$. For matrix addition $\boldsymbol{A}$ and $\boldsymbol{B}$ must have the same size, i.e. the same number of rows and columns.

The dot product between two vectors is $\boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{a}^T\boldsymbol{b} = \boldsymbol{a}\boldsymbol{b}^T = \sum_{i=1}^{d} a_i b_i$.

Matrix multiplication is defined as $c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$ where m is the number of columns of $\boldsymbol{A}$ and the number of rows in $\boldsymbol{B}$. Thus, $\boldsymbol{C}$ contains all possible dot products of the row vectors in $\boldsymbol{A}$ with the column vectors in $\boldsymbol{B}$. For matrix multiplication the number of columns in $\boldsymbol{A}$ must match the number of rows in $\boldsymbol{B}$. Note that matrix multiplication is in general not commutative, i.e. $\boldsymbol{AB} \neq \boldsymbol{BA}$.

A.2.2 Matrix transpose

The matrix transpose $t(\boldsymbol{A}) = \boldsymbol{A}^T$ interchanges rows and columns. The transpose is a linear operator $(\boldsymbol{A} + \boldsymbol{B})^T = \boldsymbol{A}^T + \boldsymbol{B}^T$ and applied to a matrix product it reverses the ordering, i.e. $(\boldsymbol{AB})^T = \boldsymbol{B}^T \boldsymbol{A}^T$.

If $\boldsymbol{A} = \boldsymbol{A}^T$ then $\boldsymbol{A}$ is symmetric (and square).

By construction given a rectangular $\boldsymbol{A}$ the matrices $\boldsymbol{A}^T \boldsymbol{A}$ and $\boldsymbol{A}\boldsymbol{A}^T$ are symmetric with non-negative diagonal.

A.3 Matrix summaries

A.3.1 Matrix trace

The trace of the matrix is the sum of the diagonal elements $\mathrm{Tr}(\boldsymbol{A}) = \sum a_{ii}$.

A useful identity for the matrix trace is

$$\mathrm{Tr}(\boldsymbol{AB}) = \mathrm{Tr}(\boldsymbol{BA})$$

with for two vectors becomes

$$\boldsymbol{a}^T \boldsymbol{b} = \mathrm{Tr}(\boldsymbol{b}\boldsymbol{a}^T)\,.$$

The squared Frobenius norm, i.e. the sum of the squares of all entries of a rectangular matrix $\boldsymbol{A} = (a_{ij})$, can be written using the trace as follows:

$$\begin{aligned} ||\boldsymbol{A}||_F^2 &= \sum_{i,j} a_{ij}^2 \\ &= \mathrm{Tr}(\boldsymbol{A}^T \boldsymbol{A}) = \mathrm{Tr}(\boldsymbol{A}\boldsymbol{A}^T)\,. \end{aligned}$$

A.3.2 Determinant of a matrix

If $\boldsymbol{A}$ is a square matrix the determinant $\det(\boldsymbol{A})$ is a scalar measuring the volume spanned by the column vectors in $\boldsymbol{A}$ with the sign determined by the orientation of the vectors.

If $\det(\boldsymbol{A}) \neq 0$ the matrix $\boldsymbol{A}$ is non-singular or non-degenerate. Conversely, if $\det(\boldsymbol{A}) = 0$ the matrix $\boldsymbol{A}$ is singular or degenerate.

One way to compute the determinant of a matrix $\boldsymbol{A}$ is the Laplace cofactor expansion approach that proceeds recursively based on the determinants of the submatrices $\boldsymbol{A}_{-i,-j}$ obtained by deleting row i and column j from $\boldsymbol{A}$. Specifically, at each level we compute the

1) cofactor expansion either
   a) along the i-th row — pick any row i:

$$\det(\boldsymbol{A}) = \sum_{j=1}^{d} a_{ij}(-1)^{i+j} \det(\boldsymbol{A}_{-i,-j}) \text{ , or}$$

   b) along the j-th column — pick any j:

$$\det(\boldsymbol{A}) = \sum_{i=1}^{d} a_{ij}(-1)^{i+j} \det(\boldsymbol{A}_{-i,-j})$$

.

2) Then repeat until the submatrix is a scalar a and $\det(a) = a$.

The recursive nature of this algorithm leads to a complexity of order $O(d!)$ so it is not practical except for very small d. Therefore, in practice other more efficient algorithms for computing determinants are used but these still have algorithmic complexity in the order of $O(d^3)$ so for large dimensions obtaining determinants is very expensive.

However, some specially structured matrices do allow for very fast calculation. In particular, it turns out that the determinant of a triangular matrix (which includes diagonal matrices) is simply the product of the diagonal elements.

For a two-dimensional matrix $\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ the determinant is $\det(A) = a_{11}a_{22} - a_{12}a_{21}$.

The determinant of a block-structured matrix

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12} \\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22} \end{pmatrix}$$

is

$$\det(\boldsymbol{A}) = \det(\boldsymbol{A}_{22}) \det(\boldsymbol{C}_1) = \det(\boldsymbol{A}_{11}) \det(\boldsymbol{C}_2)$$

with (Schur complement of $\boldsymbol{A}_{22}$)

$$\boldsymbol{C}_1 = \boldsymbol{A}_{11} - \boldsymbol{A}_{12}\boldsymbol{A}_{22}^{-1}\boldsymbol{A}_{21}$$

and (Schur complement of $\boldsymbol{A}_{11}$)

$$\boldsymbol{C}_2 = \boldsymbol{A}_{22} - \boldsymbol{A}_{21}\boldsymbol{A}_{11}^{-1}\boldsymbol{A}_{12}$$

For a block-diagonal matrix $\boldsymbol{A}$ with $\boldsymbol{A}_{12} = 0$ and $\boldsymbol{A}_{21} = 0$ the determinant is $\det(\boldsymbol{A}) = \det(\boldsymbol{A}_{11}) \det(\boldsymbol{A}_{22})$.

Determinants have a multiplicative property,

$$\det(\boldsymbol{AB}) = \det(\boldsymbol{BA}) = \det(\boldsymbol{A}) \det(\boldsymbol{B}) .$$

Another important identity is

$$\det(\boldsymbol{I}_n + \boldsymbol{AB}) = \det(\boldsymbol{I}_m + \boldsymbol{BA})$$

where $\boldsymbol{A}$ is a $n \times m$ and $\boldsymbol{B}$ is a $m \times n$ matrix. This is called the Weinstein-Aronszajn determinant identity (also credited to Sylvester).

A.4 Matrix inverse

A.4.1 Inversion of square matrix

If $\boldsymbol{A}$ is a square matrix then the inverse matrix $\boldsymbol{A}^{-1}$ is a matrix such that

$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I}\,.$$

Only non-singular matrices with $\det(\boldsymbol{A}) \neq 0$ are invertible.

As $\det(\boldsymbol{A}^{-1}\boldsymbol{A}) = \det(\boldsymbol{I}) = 1$ the determinant of the inverse matrix equals the inverse determinant,

$$\det(\boldsymbol{A}^{-1}) = \det(\boldsymbol{A})^{-1}\,.$$

The transpose of the inverse is the inverse of the transpose as

$$\begin{aligned}(\boldsymbol{A}^{-1})^T &= (\boldsymbol{A}^{-1})^T\,\boldsymbol{A}^T(\boldsymbol{A}^T)^{-1} \\ &= (\boldsymbol{A}\boldsymbol{A}^{-1})^T\,(\boldsymbol{A}^T)^{-1} = (\boldsymbol{A}^T)^{-1}\,.\end{aligned}$$

The inverse of a matrix product $(\boldsymbol{A}\boldsymbol{B})^{-1} = \boldsymbol{B}^{-1}\boldsymbol{A}^{-1}$ is the product of the indivdual matrix inverses in reverse order.

There are many different algorithms to compute the inverse of a matrix (which is essentially a problem of solving a system of equations). The computational complexity of matrix inversion is of the order $O(d^3)$ where d is the dimension of $\boldsymbol{A}$. Therefore matrix inversion is very costly in higher dimensions.

However, for specially structured matrices inversion can be done effectively regardless of dimension. For example, the inverse of a diagonal matrix is another diagonal matrix obtained by inverting the diagonal elements. Another example are orthogonal matrices.

A.4.2 Orthogonal matrices

An orthogonal matrix $\boldsymbol{Q}$ is a square matrix with the property that $\boldsymbol{Q}^T = \boldsymbol{Q}^{-1}$, i.e. the transpose is also the inverse. This implies that $\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{I}$.

The identity matrix $\boldsymbol{I}$ is the simplest example of an orthogonal matrix.

An orthogonal matrix $\boldsymbol{Q}$ can be interpreted geometrically as an operator performing rotation, reflection and/or permutation. Multiplication of $\boldsymbol{Q}$ with a vector will result in a new vector of the same length but with a change in direction (unless $\boldsymbol{Q} = \boldsymbol{I}$).

Multiplication of two orthogonal matrices yields another orthogonal matrix. All orthogonal matrices of dimension d form a group with respect to multiplication called the orthogonal group $O(d)$.

The determinant $\det(\boldsymbol{Q})$ of an orthogonal matrix is either +1 or -1. The individual eigenvalues λ_i of an orthogonal matrix are typically complex but all lie on the complex unit circle (hence $|\lambda_i| = 1$). The subset of orthogonal matrices with $\det(\boldsymbol{Q}) = 1$ are called rotation matrices and form the special orthogonal group $SO(d)$.

A.5 Eigenvalues and eigenvectors

A.5.1 Definition

Assume a square symmetric matrix $\boldsymbol{A}$ of size $d \times d$. A vector $\boldsymbol{u} \neq 0$ is called an eigenvector of the matrix $\boldsymbol{A}$ and λ the corresponding eigenvalue if

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{u}\lambda\,.$$

A.5.2 Finding eigenvalues and vectors

To find the eigenvalues and eigenvector the *eigenequation* is rewritten as

$$(\boldsymbol{A} - \boldsymbol{I}\lambda)\boldsymbol{u} = 0\,.$$

For any solution $\boldsymbol{u} \neq 0$ the corresponding eigenvalue λ must make the matrix $\boldsymbol{A} - \boldsymbol{I}\lambda$ singular, i.e. the determinant must vanish

$$\det(\boldsymbol{A} - \boldsymbol{I}\lambda) = 0\,.$$

This is the *characteristic equation* of the matrix $\boldsymbol{A}$, and its solution yields d not necessarily distinct and also potentially complex eigenvalues $\lambda_1, \ldots, \lambda_d$.

Given the eigenvalues we then solve the eigenequation for the corresponding non-zero eigenvectors $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_d$. Note that the eigenvector is only defined by the eigenequation up to a scalar, and eigenvectors of real matrices can also have complex components (a common example are rotation matrices). By convention eigenvectors are typically standardised to unit length which leaves a sign ambiguity for real eigenvectors and complex eigenvectors fixed only up to a factor with modulus 1).

A.5.3 Eigenequation in matrix notation

With the matrix

$$\boldsymbol{U} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_d)$$

containing the standardised eigenvectors in the columns and the diagonal matrix

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \lambda_d \end{pmatrix}$$

containing the eigenvalues (typically sorted in order of magnitude) the eigenvalue equation can be written as

$$\boldsymbol{A}\boldsymbol{U} = \boldsymbol{U}\boldsymbol{\Lambda}\,.$$

A.5.4 Defective matrix

in most cases the eigenvectors $\boldsymbol{u}_i$ will be linearly independent so that they form a basis to span a d dimensional space.

However, if this is not the case and the matrix $\boldsymbol{A}$ does not have a complete basis of eigenvectors, then the matrix is called defective. In this case the matrix $\boldsymbol{U}$ containing the eigenvectors is singular and $\det(\boldsymbol{U}) = 0$.

An example of a defective matrix is $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ which has determinant 1 so that it can be inverted and its column vectors do form a complete basis but has only one distinct eigenvector $(1, 0)^T$ so that the eigenvector basis is incomplete.

A.5.5 Eigenvalues of a diagonal or triangular matrix

In the special case that $\boldsymbol{A}$ is diagonal or a triangular matrix the eigenvalues are easily determined. This follows from the simple form of their determinants as the product of the diagonal elements. Hence for these matrices the characteristic equation becomes $\prod_i^d (a_{ii} - \lambda) = 0$ and has solution $\lambda_i = a_{ii}$, i.e. the eigenvalues are equal to the diagonal elements.

A.5.6 Eigenvalues and vectors of a symmetric matrix

If $\boldsymbol{A}$ is symmetric, i.e. $\boldsymbol{A} = \boldsymbol{A}^T$, then its eigenvalues and eigenvectors have special properties:

i) all eigenvalues of $\boldsymbol{A}$ are real,
ii) the eigenvectors are orthogonal, i.e $\boldsymbol{u}_i^T \boldsymbol{u}_j = 0$ for $i \neq j$, and real. Thus, the matrix $\boldsymbol{U}$ containing the standardised orthonormal eigenvectors is orthogonal.
iii) $\boldsymbol{A}$ is never defective as $\boldsymbol{U}$ forms a complete basis.

A.5.7 Positive definite matrices

If all eigenvalues of a square matrix $\boldsymbol{A}$ are real and $\lambda_i \geq 0$ then $\boldsymbol{A}$ is called *positive semi-definite*. If all eigenvalues are strictly positive $\lambda_i > 0$ then $\boldsymbol{A}$ is called *positive definite*.

Note that a matrix does not need to be symmetric to be positive definite, e.g. $\begin{pmatrix} 2 & 3 \\ 1 & 4 \end{pmatrix}$ has positive eigenvalues 5 and 1. It also has a complete set of eigenvectors and is diagonisable.

A symmetric matrix $\boldsymbol{A}$ is positive definite if the quadratic form $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} > 0$ for any non-zero $\boldsymbol{x}$, and it is positive semi-definite if $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \geq 0$. This holds also the other way around: a symmetric positive definite matrix (with positive eigenvalues) has a positive quadratic form, and a symmetric positive semi-definite matrix (with non-negative eigenvalues) a non-negative quadratic form.

A symmetric positive definite matrix always has a positive diagonal (this can be seen by setting $\boldsymbol{x}$ above to a unit vector with 1 at a single position, and 0 at all other elements). However, just requiring a positive diagonal is too weak to ensure positive definiteness of a symmetric matrix, for example $\begin{pmatrix} 1 & 10 \\ 10 & 1 \end{pmatrix}$ has a negative eigenvalue of -9. On the other hand, a symmetric matrix is indeed positive definite if it is strictly diagonally dominant, i.e. if all its diagonal

elements are positive and are larger than the absolute value of any of the corresponding row or column elements. However, diagonal dominance is too restrictive as criterion to characterise all symmetric positive definite matrices, since there are many symmetric matrices that are positive definite but not diagonally dominant, such as $\begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$.

Finally, the sum of a symmetric positive semi-definite matrix $\boldsymbol{A}$ and a symmetric positive definite matrix $\boldsymbol{B}$ is itself symmetric positive definite because the corresponding quadratic form $\boldsymbol{x}^T(\boldsymbol{A}+\boldsymbol{B})\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{B}\boldsymbol{x} > 0$ is positive. Similarly, the sum of two symmetric positive (semi)-definite matrices is itself symmetric positive (semi)-definite.

A.6 Matrix decompositions

A.6.1 Diagonalisation and eigenvalue decomposition

If $\boldsymbol{A}$ is a square non-defective matrix then $\boldsymbol{U}$ is invertible and we can rewrite the eigenvalue equation to

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{-1}.$$

This is called the eigendecomposition, or spectral decomposition, of $\boldsymbol{A}$ and equivalently

$$\boldsymbol{\Lambda} = \boldsymbol{U}^{-1}\boldsymbol{A}\boldsymbol{U}$$

is the diagonalisation of $\boldsymbol{A}$. Thus any matrix $\boldsymbol{A}$ that is not defective is diagonalisable using eigenvalue decomposition.

A.6.2 Orthogonal eigenvalue decomposition

For symmetric $\boldsymbol{A}$ this becomes

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$

with real eigenvalues and orthogonal matrix $\boldsymbol{U}$ and

$$\boldsymbol{\Lambda} = \boldsymbol{U}^T\boldsymbol{A}\boldsymbol{U}.$$

This special case is known as the orthogonal diagonalisation of $\boldsymbol{A}$.

The orthogonal decomposition for symmetric $\boldsymbol{A}$ is unique apart from the signs of the eigenvectors. In order to make it fully unique one needs to impose further restrictions (e.g. require a positive diagonal of $\boldsymbol{U}$). Note that this can be particularly important in computer application where the sign can vary depending on the specific implementation of the underlying numerical algorithms.

A.6.3 Singular value decomposition

The **singular value decomposition** (SVD) is a generalisation of the orthogonal eigenvalue decomposition for symmetric matrices.

Any (!) rectangular matrix $\boldsymbol{A}$ of size $n \times d$ can be factored into the product

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T$$

where $\boldsymbol{U}$ is a $n \times n$ orthogonal matrix, $\boldsymbol{V}$ is a second $d \times d$ orthogonal matrix and $\boldsymbol{D}$ is a diagonal but rectangular matrix of size $n \times d$ with $m = min(n, d)$ real diagonal elements $d_1, \ldots d_m$. The d_i are called singular values, and appear along the diagonal in $\boldsymbol{D}$ by order of magnitude.

The SVD is unique apart from the signs of the columns vectors in $\boldsymbol{U}$, $\boldsymbol{V}$ and $\boldsymbol{D}$ (you can freely specify the column signs of any two of the three matrices). By convention the signs are chosen such that the singular values in $\boldsymbol{D}$ are all non-negative, which leaves ambiguity in columns signs of $\boldsymbol{U}$ and $\boldsymbol{V}$. Alternatively, one may fix the columns signs of $\boldsymbol{U}$ and $\boldsymbol{V}$, e.g. by requiring a positive diagonal, which then determines the sign of the singular values (thus allowing for negative singular values as well).

If $\boldsymbol{A}$ is symmetric then the SVD and the orthogonal eigenvalue decomposition coincide (apart from different sign conventions for singular values, eigenvalues and eigenvectors).

Since $\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{V}\boldsymbol{D}^T\boldsymbol{D}\boldsymbol{V}^T$ and $\boldsymbol{A}\boldsymbol{A}^T = \boldsymbol{U}\boldsymbol{D}\boldsymbol{D}^T\boldsymbol{U}^T$ the squared singular values correspond to the eigenvalues of $\boldsymbol{A}^T\boldsymbol{A}$ and $\boldsymbol{A}\boldsymbol{A}^T$. It also follows that $\boldsymbol{A}^T\boldsymbol{A}$ and $\boldsymbol{A}\boldsymbol{A}^T$ are both positive semi-definite symmetric matrices, and that $\boldsymbol{V}$ and $\boldsymbol{U}$ contain the respective sets of eigenvectors.

A.6.4 Polar decomposition

Any square matrix $\boldsymbol{A}$ can be factored into the product

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{B}$$

of an orthogonal matrix $\boldsymbol{Q}$ and a symmetric positive semi-definite matrix $\boldsymbol{B}$.

This follows from the SVD of $\boldsymbol{A}$ given as

$$\begin{aligned}\boldsymbol{A} &= \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T \\ &= (\boldsymbol{U}\boldsymbol{V}^T)(\boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^T) \\ &= \boldsymbol{Q}\boldsymbol{B}\end{aligned}$$

with non-negative $\boldsymbol{D}$. Note that this decomposition is unique as the sign ambiguities in the columns of $\boldsymbol{U}$ and $\boldsymbol{V}$ cancel out in $\boldsymbol{Q}$ and $\boldsymbol{B}$.

A.6.5 Cholesky decomposition

A symmetric positive definite matrix $\boldsymbol{A}$ can be decomposed into a product of a triangular matrix $\boldsymbol{L}$ with its transpose

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^T .$$

Here, $\boldsymbol{L}$ is a lower triangular matrix with positive diagonal.

This decomposition is unique and is called **Cholesky factorisation**. It is often used to check whether a symmetric matrix is positive definite as it is algorithmically less demanding than eigenvalue decomposition.

A.7 Matrix summaries based on eigenvalues and singular values

A.7.1 Trace and determinant computed from eigenvalues

The eigendecomposition $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{-1}$ allows to establish a link between trace and determinant and eigenvalues.

Specifically,

$$\begin{aligned}\mathrm{Tr}(\boldsymbol{A}) &= \mathrm{Tr}(\boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{-1}) = \mathrm{Tr}(\boldsymbol{\Lambda}\boldsymbol{U}^{-1}\boldsymbol{U}) \\ &= \mathrm{Tr}(\boldsymbol{\Lambda}) = \sum_{i=1}^{d} \lambda_i\end{aligned}$$

thus the trace of a square matrix $\boldsymbol{A}$ is equal to the *sum* of its eigenvalues. Likewise,

$$\begin{aligned}\det(\boldsymbol{A}) &= \det(\boldsymbol{U}) \det(\boldsymbol{\Lambda}) \det(\boldsymbol{U}^{-1}) \\ &= \det(\boldsymbol{\Lambda}) = \prod_{i=1}^{d} \lambda_i\end{aligned}$$

therefore the determinant of $\boldsymbol{A}$ is the *product* of the eigenvalues.

The relationship between eigenvalues and the trace and the determinant is demonstrated here for diagonisable non-defective matrices. However, it does hold also in general for any matrix. This can be shown by using certain non-diagonal matrix decompositions (e.g. Jordan decomposition).

As a result, if any of the eigenvalues is equal to zero then $\det(\boldsymbol{A}) = 0$ and as hence $\boldsymbol{A}$ is singular and not invertible.

The trace and determinant of a real matrix are always real even though the individual eigenvalues may be complex.

A.7.2 Rank and condition number

The rank is the dimension of the space spanned by both the column and row vectors. A rectangular matrix of dimension $n \times d$ will have rank of at most $m = \min(n, d)$, and if the maximum is indeed achieved then it has full rank.

The condition number describes how well- or ill-conditioned a full rank matrix is. For example, for a square matrix a large condition number implies that the matrix is close to being singular and thus ill-conditioned. If the condition number is infinite then the matrix is not full rank.

The rank and condition of a matrix can both be determined from the m singular values $d_1, \ldots, d_m$ of a matrix obtained by SVD:

i) The rank is number of non-zero singular values.
ii) The condition number is the ratio of the largest singular value divided by the smallest singular value (absolute values if signs are allowed).

If a square matrix $\boldsymbol{A}$ is singular then the condition number is infinite, and it will not have full rank. On the other hand, a non-singular square matrix, such as a positive definite matrix, has full rank.

A.8 Functions of symmetric matrices

We focus on symmetric square matrices $\boldsymbol{A}$ which are always diagonisable with real eigenvalues and orthogonal eigenvectors.

A matrix function $f(\boldsymbol{A})$, generalising from a simple function $f(a)$ can then be defined via the orthogonal eigenvalue decomposition as

$$f(\boldsymbol{A}) = \boldsymbol{U} f(\boldsymbol{\Lambda}) \boldsymbol{U}^T = \boldsymbol{U} \begin{pmatrix} f(\lambda_1) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & f(\lambda_d) \end{pmatrix} \boldsymbol{U}^T$$

Therefore, in order to obtain the corresponding matrix function, the function is simply applied on the level of eigenvalues. By construction $f(\boldsymbol{A})$ will also be symmetric and and real-valued as long as the transformed eigenvalues $f(\lambda_i)$ are real.

Examples:

Example A.1. matrix power: $f(a) = a^p$ (with p real number)

Special cases of matrix power include :

- matrix inversion: $f(a) = a^{-1}$
- the matrix square root: $f(a) = a^{1/2}$
  (since there are multiple solutions to the square root there are also multiple matrix square roots. The principal matrix square root is given by using the positive square roots of all the eigenvalues. Thus the **principal matrix square root** of a positive semidefinite matrix is also positive semidefinite and it is unique).

Example A.2. matrix exponential: $f(a) = \exp(a)$

Example A.3. matrix logarithm: $f(a) = \log(a)$

For a positive definite matrix $\boldsymbol{A}$ computing the trace of the matrix logarithm of $\boldsymbol{A}$ is the same as taking the log of the determinant of $\boldsymbol{A}$:

$$\mathrm{Tr}(\log(\boldsymbol{A})) = \log\det(\boldsymbol{A})$$

because $\sum \log(\lambda_i) = \log(\prod \lambda_i)$.

A.9 Matrix calculus

A.9.1 First order vector derivatives

A.9.1.1 Gradient

The **nabla operator** (also known as **del operator**) is the *row* vector

$$\nabla = (\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_d}) = \frac{\partial}{\partial \boldsymbol{x}}$$

containing the first order partial derivative operators.

The **gradient** of a scalar-valued function $f(\boldsymbol{x})$ with vector argument $\boldsymbol{x} = (x_1, \ldots, x_d)^T$ is also a *row* vector (with d columns) and can be expressed using the nabla operator

$$\begin{aligned} \nabla f(\boldsymbol{x}) &= \left(\frac{\partial f(\boldsymbol{x})}{\partial x_1}, \ldots, \frac{\partial f(\boldsymbol{x})}{\partial x_d} \right) \\ &= \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = \text{grad} f(\boldsymbol{x}) \,. \end{aligned}$$

Note the various notations for the gradient.

Example A.4. $f(\boldsymbol{x}) = \boldsymbol{a}^T \boldsymbol{x} + b$. Then $\nabla f(\boldsymbol{x}) = \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = \boldsymbol{a}^T$.

Example A.5. $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{x}$. Then $\nabla f(\boldsymbol{x}) = \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = 2\boldsymbol{x}^T$.

Example A.6. $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$. Then $\nabla f(\boldsymbol{x}) = \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} = \boldsymbol{x}^T (\boldsymbol{A} + \boldsymbol{A}^T)$.

A.9.1.2 Jacobian matrix

For a vector-valued function

$$\boldsymbol{f}(\boldsymbol{x}) = (f_1(\boldsymbol{x}), \ldots, f_m(\boldsymbol{x}))^T \,.$$

the computation of the gradient of each component yields the **Jacobian matrix** (with m rows and d columns)

$$\begin{aligned} \boldsymbol{J}_f(\boldsymbol{x}) &= \begin{pmatrix} \nabla f_1(\boldsymbol{x}) \\ \vdots \\ \nabla f_m(\boldsymbol{x}) \end{pmatrix} = \left(\frac{\partial f_i(\boldsymbol{x})}{\partial x_j} \right) \\ &= \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} = D\boldsymbol{f}(\boldsymbol{x}) \end{aligned}$$

Again, note the various notations for the Jacobian matrix!

Example A.7. $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$. Then $\boldsymbol{J}_f(\boldsymbol{x}) = \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} = \boldsymbol{A}$.

If $m = d$ then the Jacobian matrix is a square matrix and this allows to compute the **Jacobian determinant**

$$\det \boldsymbol{J}_f(\boldsymbol{x}) = \det \left(\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right)$$

If $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x})$ is an invertible function with $\boldsymbol{x} = \boldsymbol{f}^{-1}(\boldsymbol{y})$ then the Jacobian matrix is invertible and the inverted matrix is in fact the Jacobian of the inverse function!

This allows to compute the Jacobian determinant of the backtransformation as as the inverse of the Jacobian determinant the original function:

$$\det D\boldsymbol{f}^{-1}(\boldsymbol{y}) = (\det D\boldsymbol{f}(\boldsymbol{x}))^{-1}$$

or in alternative notation

$$\det D\boldsymbol{x}(\boldsymbol{y}) = \frac{1}{\det D\boldsymbol{y}(\boldsymbol{x})}$$

.

A.9.2 Second order vector derivatives

The matrix of all second order partial derivates of scalar-valued function with vector-valued argument is called the **Hessian matrix** and is computed by double application of the nabla operator:

$$\begin{aligned}\nabla^T \nabla f(\boldsymbol{x}) &= \begin{pmatrix} \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1^2} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2^2} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\boldsymbol{x})}{\partial x_d \partial x_1} & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f(\boldsymbol{x})}{\partial x_d^2} \end{pmatrix} \\ &= \left(\frac{\partial f(\boldsymbol{x})}{\partial x_i \partial x_j} \right) = \left(\frac{\partial}{\partial \boldsymbol{x}} \right)^T \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}}.\end{aligned}$$

By construction it is square and symmetric.

A.9.3 First order matrix derivatives

The derivative of a scalar-valued function $f(\boldsymbol{X})$ with regard to a matrix argument $\boldsymbol{X}$ can also be defined and results in a matrix with transposed dimensions compared to $\boldsymbol{X}$.

Two important specific examples are:

Example A.8. $\frac{\partial \mathrm{Tr}(\boldsymbol{AX})}{\partial \boldsymbol{X}} = \boldsymbol{A}$

Example A.9. $\frac{\partial \log\det(\boldsymbol{X})}{\partial \boldsymbol{X}} = \frac{\partial \mathrm{Tr}(\log \boldsymbol{X})}{\partial \boldsymbol{X}} = \boldsymbol{X}^{-1}$

Appendix B

Further study

In this module we can only touch the surface of the field of multivariate statistics and machine learning. If you would like to study further I recommend the following books below as a starting point.

B.1 Recommended reading

For multivariate statistics and machine learning:

- Härdle and Simar (2015) *Applied multivariate statistical analysis. 4th edition*. Springer.
- Hastie et al. (2009) *The elements of statistical learning: data mining, inference, and prediction*. Springer.
- James et al. (2013) *An introduction to statistical learning with applications in R*. Springer.
- Marden (2015) *Multivariate Statistics: Old School*
- Rogers and Girolami (2017) *A first course in machine learning (2nd Edition)*. Chapman and Hall / CRC.

B.2 Advanced reading

Additional (advanced) reference books for probabilistic machine learning are:

- Murphy (2012) *Machine learning: a probabilistic perspective*. MIT Press.
- Bishop (2006) *Pattern recognition and machine learning*. Springer.

Bibliography

Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer. https://www.microsoft.com/en-us/research/people/cmbishop/prml-book/.

Härdle, W. K. and Simar, L. (2015). *Applied Multivariate Statistical Analysis*. Springer, Berlin.

Hastie, T., Tibshirani, R., and Friedman, J. (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer, 2nd edition. https://web.stanford.edu/~hastie/ElemStatLearn/.

James, G., Witten, D., Hastie, T., and Tibshirani, R. (2013). *An Introduction to Statistical Learning with Applications in R*. Springer. http://faculty.marshall.usc.edu/gareth-james/ISL/.

Marden, J. I. (2015). *Multivariate Statistics: Old School*. CreateSpace. http://stat.istics.net/Multivariate.

Murphy, K. P. (2012). *Machine Learning: A Probabilistic Perspective*. MIT Press.

Rogers, S. and Girolami, M. (2017). *A first course in machine learning*. Chapman and Hall / CRC, 2nd edition.

Zhang, A., Lipton, Z. C., Li, M., and Smola, A. J. (2020). *Dive into Deep Learning*. https://d2l.ai.