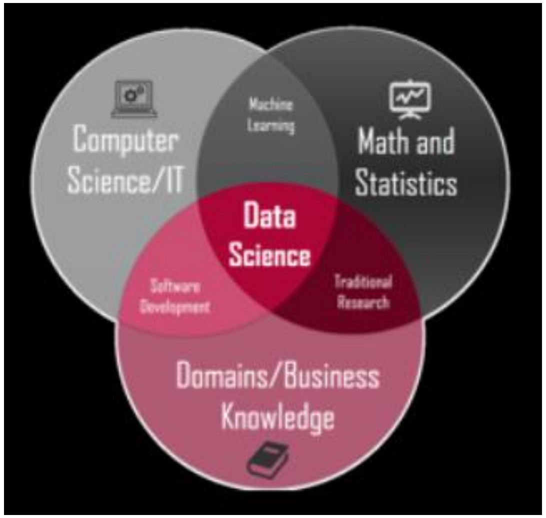
DAT200 - Applied machine learning

Subspace analysis

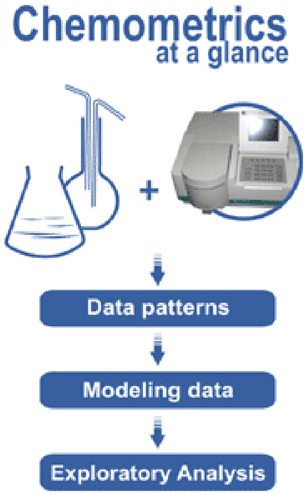
PCA, PCR, PLSR

Why Chemometrics in addition to ML?

- Wikipedia on **Data Science**
  - Data-driven science
  - Techniques and theories from mathematics, statistics, information science, and computer science



- Wikipedia on **Chemometrics**
  - Data-driven science
  - Methods from applied mathematics, multivariate statistics, and computer science



Why Chemometrics in addition to ML?

Chemometrics

- Languages
  - MATLAB, R
- Repositories
  - MATLAB file exchange, models.life.ku.dk, CRAN, …

Data Science

- Languages
  - Python, R, Java, Perl, C/C++
- Repositories
  - GitHub, CRAN, …

Why Chemometrics in addition to ML?

- Campus Ås has long and strong tradition in chemometrics
- Chemometrics has many similarities with ML
- Important **additional value** of using chemometrics
  - ML is mainly concerned with building good models for **prediction** of outcomes
  - ML is often considered as a **black box** (usually little interest in interpretation of variation in data)
  - Chemometrics is concerned with building good models that can be used for **interpretation** of the data and **prediction** of outcomes
  - Chemometrics handles well situations where data has many more (often highly correlated) variables than observations ($n << k$)

Why Chemometrics in addition to ML?

- Methods used in both chemometrics and ML
  - Principal component analysis (PCA)
  - Partial least squares regression (PLSR)
- Chemometrics methods we will discuss here
  - PCA, PLSR
  - Principal component regression (PCR)

Summary

- Subspace methods
  - Principal directions in data
  - Orthogonal components
  - Visualisation
  - Compression
- Predictor driven:
  - Principal component analysis (PCA)
  - Principal component regression (PCR)
- Response driven:
  - Partial least squares regression (PLSR)

Multivariate data – how to extract information?

OECD data: most frequent types (%) of cancer found in men from participating countries (Organisation for Economic Cooperation and Development)

	A	B	C	D	E	F	G	H	I	J	K
1	**MEN**	**Trachea-bronchus-lung**	**Colon, rectum and anus**	**Stomach**	**Pancreas**	**Prostate**	**Liver**	**Hodgkins disease**	**Leukemia**	**Bladder**	**Skin**
2	**Australia**	20.49342921	9.290023969	2.954789652	5.033473841	13.61269526	4.049921481	0.157037772	3.855690553	3.107694851	4.425985619
3	**Austria**	22.28692919	10.94472176	4.584951008	6.627842485	10.57496765	5.66648179	0.147901645	3.780735811	3.031983731	1.941209096
4	**Belgium**	30.09070593	10.45090049	3.253582227	5.179439989	9.162613382	3.450769029	0.144603655	3.56908111	4.719337452	1.018798475
5	**Canada**	27.73162434	11.44341588	3.011841654	5.419732574	9.739694596	3.863702297	0.195163119	3.789856792	3.534034866	1.5375689
6	**Chile**	13.304823	8.022491486	17.27251129	4.165676724	16.19545419	5.044745387	0.22174705	3.00942425	2.162033737	0.554367625
7	**Czech Rep.**	24.87532416	13.97034377	4.45508345	6.742469579	9.455415919	3.464326086	0.279273888	3.37123479	3.557417381	1.522707627
8	**Denmark**	24.31158521	12.16819648	3.212602332	6.375589184	14.30166212	3.162986852	0.21086579	3.100967502	4.366162243	2.245100471
9	**Estonia**	26.37195122	10.26422764	8.333333333	5.43699187	13.00813008	2.388211382	0.101626016	3.861788618	3.506097561	1.016260163
10	**Finland**	23.9178867	9.818586887	4.169318905	7.940802037	13.57415659	4.232972629	0.159134309	2.737110121	2.928071292	2.418841502
11	**France**	25.12575792	10.16168875	3.360655738	5.335728722	9.885470469	6.466427128	0.143723333	3.535818549	4.350999326	1.112732989
12	**Germany**	24.4012222	11.17718566	4.592272563	6.795183494	11.01291192	4.106843644	0.151953215	3.609915563	3.19840983	1.467785918
13	**Greece**	31.66724517	8.50399167	4.830498669	5.229665625	9.013074164	1.237996066	0.792548883	3.823903737	5.582552355	0.76940877
14	**Hungary**	30.41257367	16.08195341	5.287678922	5.29329217	6.797642436	3.104125737	0.117878193	2.559640752	3.575638507	1.044063991
15	**Iceland**	20.32258065	13.22580645	4.193548387	3.870967742	17.09677419	0.967741935	0.64516129	2.903225806	5.806451613	0.967741935
16	**Ireland**	22.95747731	12.32680363	4.395604396	5.805064501	12.4462494	3.511705686	0.238891543	3.057811753	2.866698519	1.887243192
17	**Israel**	21.82289737	12.67135976	5.446461652	8.725453872	7.725083364	3.501296777	0.351982216	5.094479437	4.890700259	2.278621712
18	**Italy**	26.06741808	10.90044415	6.087111372	5.398893824	7.628006369	6.95340652	0.250356155	3.660018436	4.687630939	1.131316517
19	**Japan**	23.99056121	11.97177581	14.73796762	7.315521922	5.327753633	9.132765224	0.051157496	2.214981311	2.426985349	0.151168096
20	**Korea**	26.20420989	10.09857518	13.10748569	5.630407645	3.142352891	18.28160647	0.094701046	1.977960484	1.975808187	0.271189359
21	**Luxembourg**	25.18382353	11.94852941	4.044117647	6.066176471	7.720588235	6.066176471	0.183823529	4.779411765	4.044117647	1.838235294
22	**Mexico**	11.49597401	6.91058059	8.227150728	5.088289306	16.32151434	7.591467721	0.740217545	6.260771295	1.873145925	0.802373217
23	**Netherlands**	27.15515358	11.46939311	3.543496308	5.334906279	11.07615677	2.127845502	0.157294534	3.062874121	3.700790842	2.154061257
24	**New Zealand**	19.7737655	13.09549706	4.198390255	4.763976506	12.72569067	3.56754405	0.195779856	4.15488362	2.74091799	5.286056124
25	**Norway**	21.39823009	13.45132743	3.203539823	6.194690265	17.48672566	2.566371681	0.17699115	3.221238938	4.247787611	3.309734513
26	**Poland**	30.65693431	11.9202253	6.439067379	4.550069927	8.201620783	2.0863268	0.19541353	2.927371305	5.145889611	1.41579018
27	**Portugal**	20.39060984	14.4667917	8.730518011	4.733880877	11.1039255	4.695078575	0.155209209	3.000711376	4.416995408	0.821315398
28	**Slovak Rep.**	22.66305123	15.09918653	6.108177537	5.651491366	7.606679035	3.11117454	0.285428857	2.554588269	3.125445983	1.541315827
29	**Slovenia**	24.94577007	13.72792067	7.468236752	5.11310815	11.09389526	3.997520917	0.154942671	2.479082739	4.09048652	2.169197397
30	**Spain**	26.77706347	14.07025989	5.245117455	4.827701776	8.81600195	5.138478413	0.19652052	2.953901466	6.384631791	0.885104049
31	**Sweden**	16.05304484	12.34514046	3.350200663	6.962135753	20.44145873	3.577037166	0.157040656	3.568312685	4.240097714	2.748211481
32	**Switzerland**	21.6075388	10.18847007	3.680709534	6.241685144	14.16851441	5.365853659	0	3.359201774	4.257206208	2.372505543
33	**Turkey**	38.97165809	7.623419473	8.846855339	5.211385946	7.225854048	3.723589565	0.219275775	3.612927024	3.397749862	0.57175646
34	**United Kingdom**	22.80308077	10.26261351	3.447751949	4.946063135	12.70759557	3.427883548	0.191671634	3.22335589	4.037960333	1.521685775
35	**United States**	29.1412459	9.06313206	2.226842334	6.211578252	9.487245059	4.537710188	0.237131309	4.268031445	3.463644848	1.993364309
36	**OECD**	25.99183401	10.69682199	6.27003433	5.933305685	9.235450758	5.686093446	0.194011091	3.432922396	3.617678042	1.304311271

PRINCIPAL COMPONENT ANALYSIS

Principal Component Analysis (PCA)

What is it and for which situations can I use it for?

- Analysis of **one** data table $\boldsymbol{X}$
- Versatile method for almost all types of data to obtain an **overview** (for example in an early phase of investigation)
- **Explorative multivariate** statistical method
- Particularly suitable in situations …
  - With **lots** of data
  - Where **little** prior information is available
- Other names for PCA
  - Singular value decomposition (SVD)
  - Eigenvector decomposition

Principal Component Analysis (PCA)

How does it work and what kind of information do I get?

- Idea behind PCA – find the **most interesting** dimensions or directions of variability, so-called principal components
- Extracts **main information** (**systematic variation**) in the data
- Visualisation: present results graphically for interpretation
  - Information on **objects**
  - Information on **variables**
  - Other results

Principal Component Analysis (PCA)

What can I do with it / use it for?

- **Interpretation** of the **variance** in the data
  - Gain knowledge on how **objects** are distributed (patterns using background information)
  - Gain knowledge on how **variables** contribute to variance in the data
  - Generate hypotheses and ideas for further experimentation
- **Data pre-processing** and **data compression**
  - Use PCA as **filter** to get rid of **noise**
  - Use components **instead of** original data in subsequent analysis
  - **Dimensionality reduction** (as often used in ML) – use components as input in *classifiers*, *regression*, *clustering*, not original data
- **Classification** (not part of syllabus)
  - **SIMCA** method where PCA is applied for computations

PCA – data structure

1 $\longrightarrow$ K

1 ... N

	A	B	C	D	E	F	G	H	I	J	K
1	MEN	Trachea-bronchus-lung	Colon, rectum and anus	Stomach	Pancreas	Prostate	Liver	Hodgkins disease	Leukemia	Bladder	Skin
2	Australia	20.49342921	9.290023969	2.954789652	5.033473841	13.61269526	4.049921481	0.157037772	3.855690553	3.107694851	4.425985619
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$\boldsymbol{X}$

- Number of **objects (rows)**:
  - $n = 1 \ldots N$
- Number of **variables (columns)**:
  - $k = 1 \ldots K$
- Observed value x_{nk} for
  - n'th object
  - k'th variable

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1K} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NK} \end{pmatrix}$$

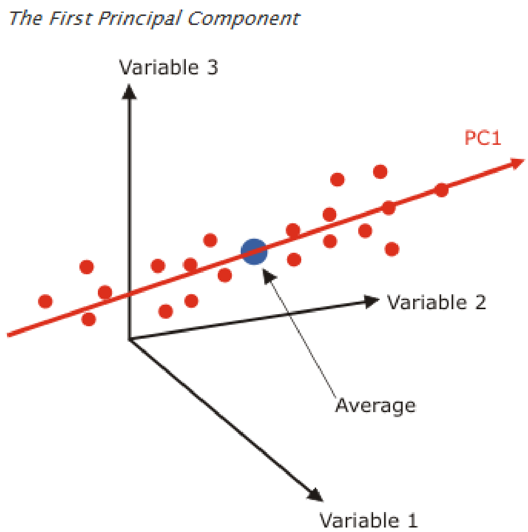
DEMO: OECD data – cancer in men

Concept behind PCA

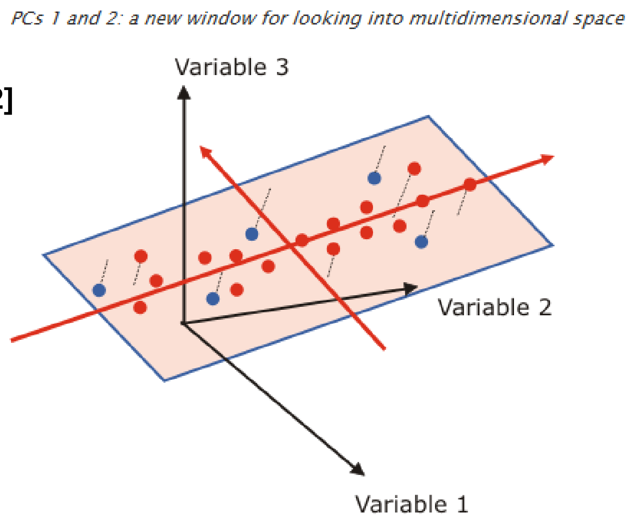
PCA basics – description of method

- Figures below: data with 3 variables and a number of objects
- Each row is represented as a point in three-dimensional coordinate system
- **Note**: not typical situation for use of PCA, since only 3 variables in data set.
  - However, appropriate for illustration
  - For matrices for more than 3 variables PCA cannot be visualised graphically, but mathematics are identical

[1]



[2]



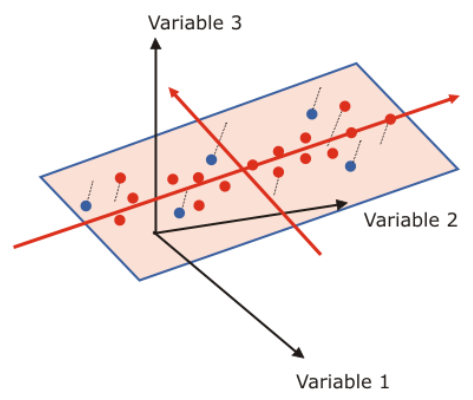
[1] & [2] Figures from CAMO Unscrambler software help documentation

PCA basics – description of method

- **Step 1**: compute averages of all variables (large point in plot below)
- **Step 2**: subtract averages from their corresponding variables. This is often called "*data centering*". This corresponds to moving the origin of coordinate system or vector space to average data point $\overline{x}$
- **Step 3**: search for direction in space that has **largest** variance ➔ component 1
- **Step 4**: search for direction in space that has **largest** variance **AND** is **orthogonal** to component 1 ➔ component 2
- **Step 5**: search for direction in space that has **largest** variance **AND** is **orthogonal** to component 1 **and** component 2 ➔ component 3
- **Step 6**: etc.

- **Maximum** possible number of components
  - $min(K, N-1)$

PCs 1 and 2: a new window for looking into multidimensional space **[1]**



[1] Figure from T. Næs, P.B. Brockhoff, O. Tomic, *Statistics for Sensory and Consumer Science*, (2010)

PCA basics

Data → Systematic variation + Residuals

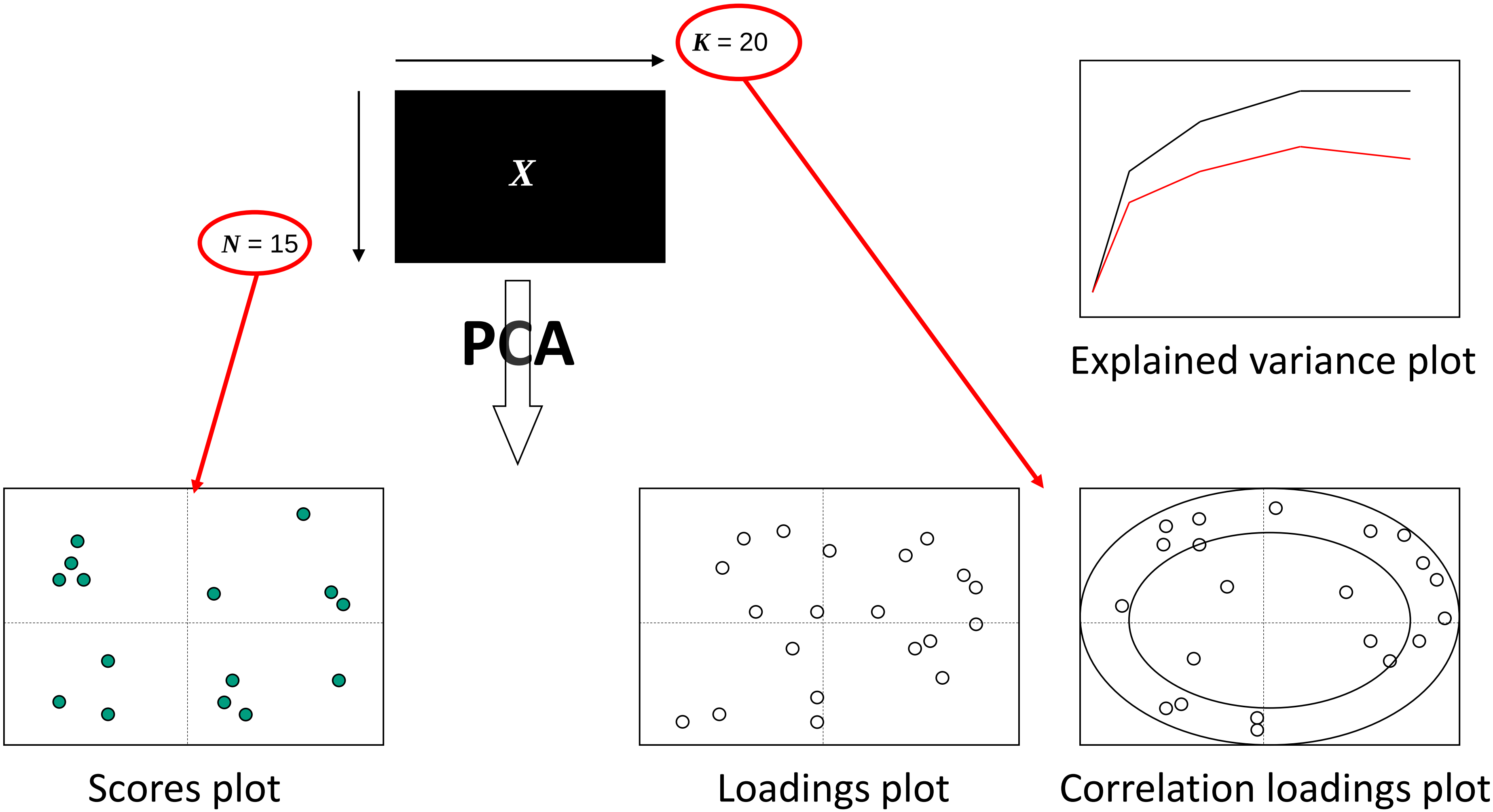
$$X = TP' + E$$

X: data matrix
T: PCA scores matrix
P: PCA loadings matrix
E: residuals / noise

Principal Components (PC's) describing the systematic variation in the data

PCA basics

Data in this illustration consists of 15 observations and 20 variables ➔ data matrix $\boldsymbol{X}$ of dimension (15×20)



PCA – scores and **loadings**

PCA basics – scores and loadings

- **Score plot**
  - is a scatter plot of columns of $\boldsymbol{T}$
  - objects close to each other have similar overall properties
  - objects far apart are very different
  - New coordinate system in a more compact subspace which spans the major variations

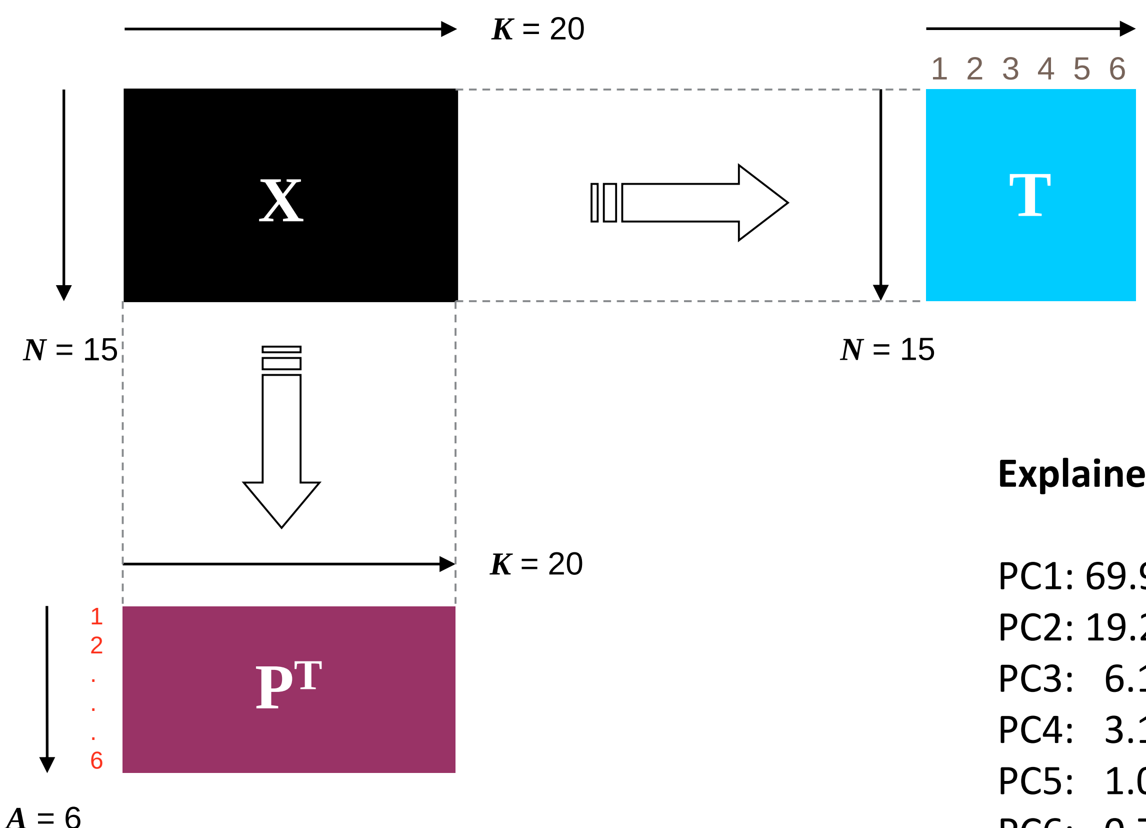
- **Loading plot**
  - is a scatter plot of rows of $\boldsymbol{P}^T$ (or columns of $\boldsymbol{P}$)
  - variables close to each other are highly correlated
  - Variables on opposite side of each other are highly negatively correlated

PCA basics – scores and loadings

- **Score plot** and **loading plot** together (so-called **bi-plot**)
  - Samples to the **right** in the scores plot are dominated by (have large values of) variables to the **right** in the loadings plot; objects at the **top** of the scores plot are dominated by variables at the **top** in the loadings plot; etc.

- Usually, **two-dimensional** plots with the **first two** components are used
- **Three-dimensional** plots of **first three** components are also possible (on screen with rotation)
- It is also possible to plot component 1 vs. component 2 in one plot and components 2 vs. component 3 in another plot, etc.

PCA basics – scores and loadings



T: PCA scores matrix

P: PCA loadings matrix
A: number of components computed

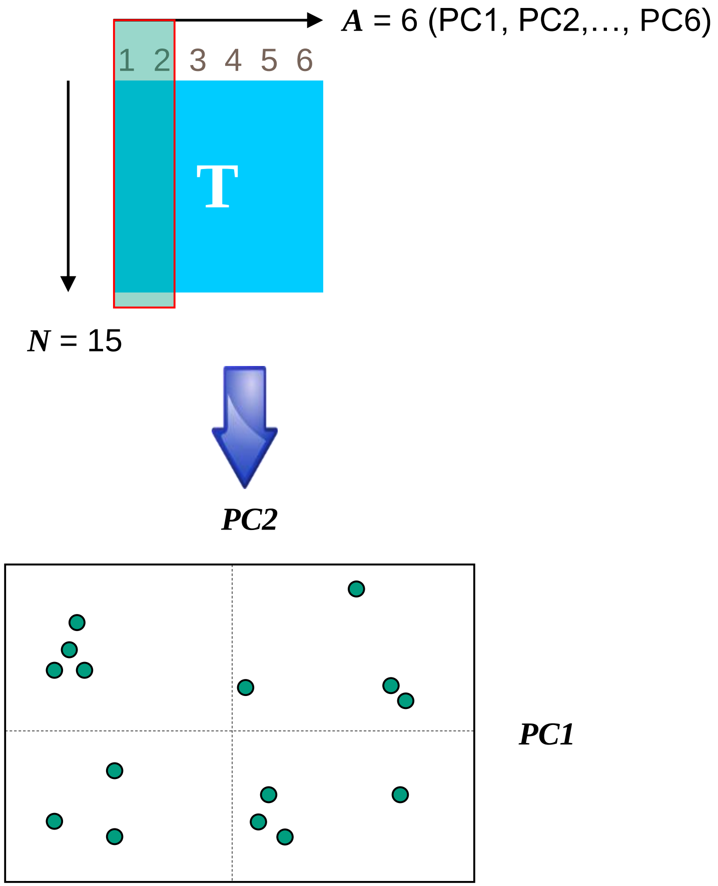
Explained variance in each component

PC1: 69.9%
PC2: 19.2%
PC3: 6.1%
PC4: 3.1%
PC5: 1.0%
PC6: 0.7%

Total: 100%

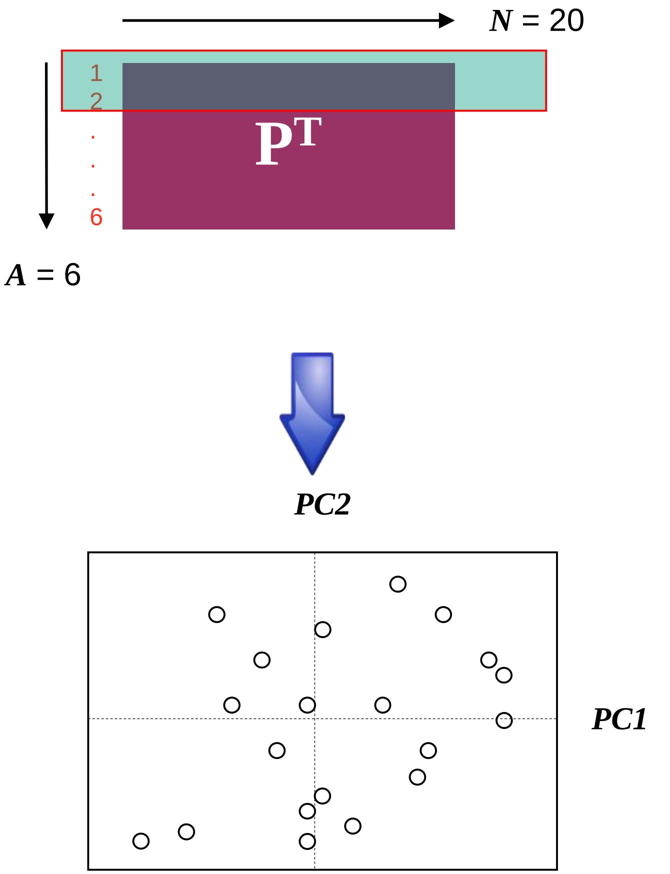
PCA basics – plotting scores and loadings

T: PCA scores matrix



Scores plot

P: PCA loadings matrix



Loadings plot

PCA – explained variance

PCA basics – explained variance

- Important information on **how much** variance (%) each component explains of the **total variance** in $\boldsymbol{X}$
- Explained variance by each component
  - **Highest** explained variance for **first** component
  - **Second**-highest explained variance for **second** component
  - **Third**-highest explained variance for **third** component
  - Etc.
- The higher the component, the higher the chance that it is unstable (since based on very small variances)

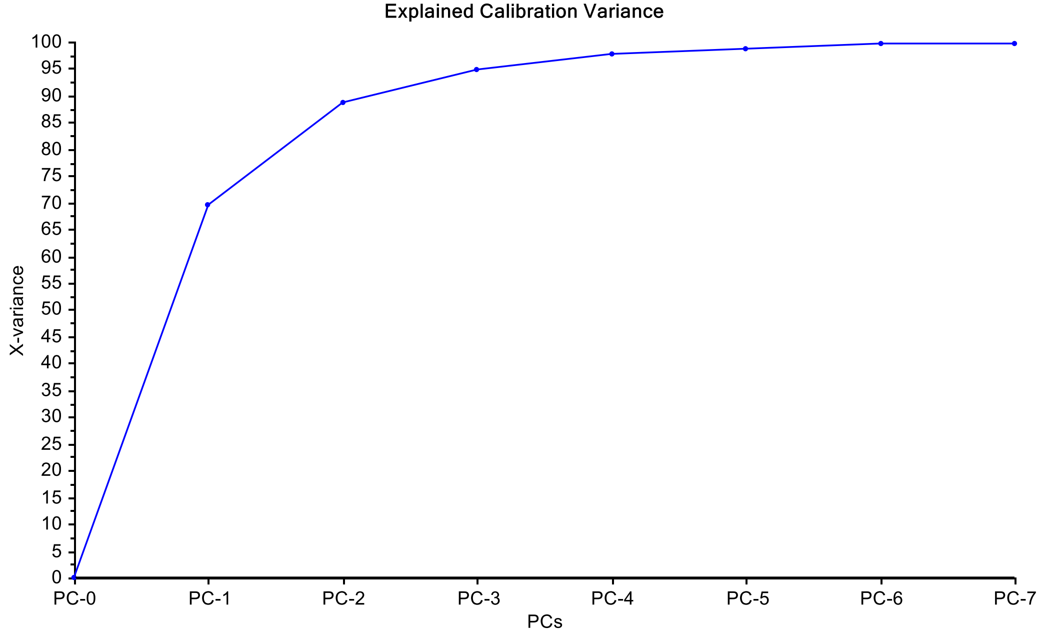
PCA basics – explained variance

Calibrated explained variance at each component

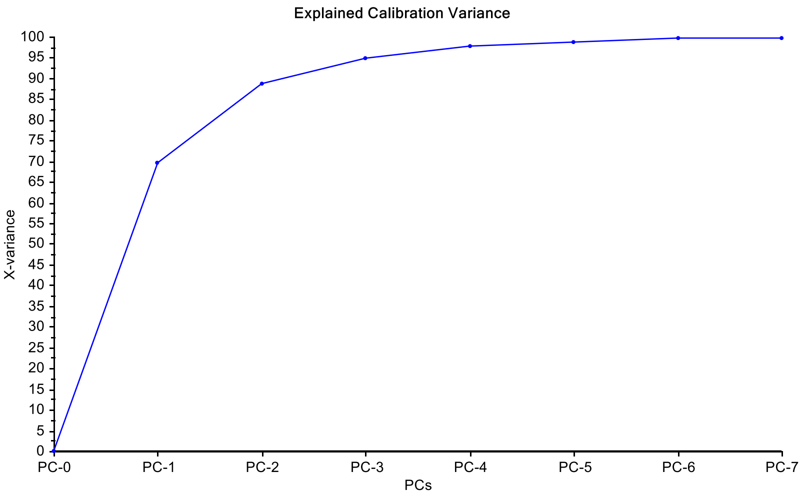
PC1: 69.9%
PC2: 19.2%
PC3: 6.1%
PC4: 3.1%
PC5: 1.0%
PC6: 0.7%

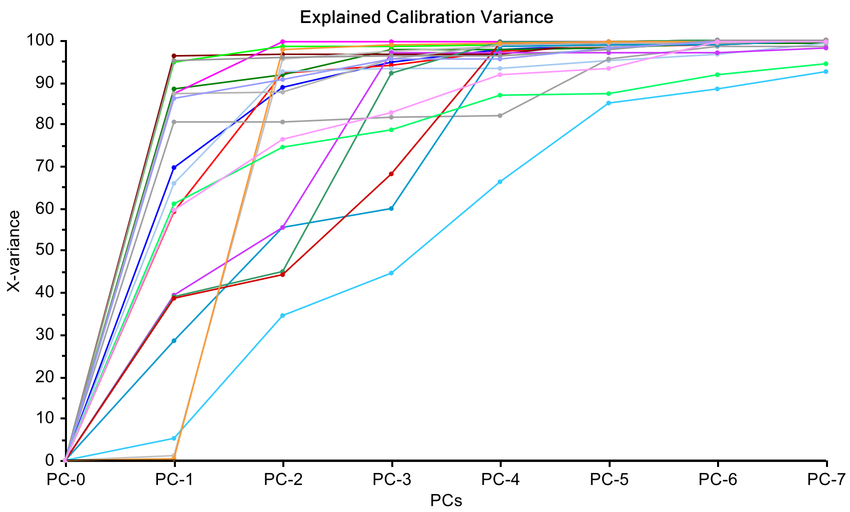
Total: 100%

Calibrated cumulative explained variance at each component



PCA basics – explained variance





Calibrated cumulative explained variance at each component across **all variables**

Calibrated cumulative explained variance for **each variable indivdually**

More on **validated** explained variance below in «PCA - validation»

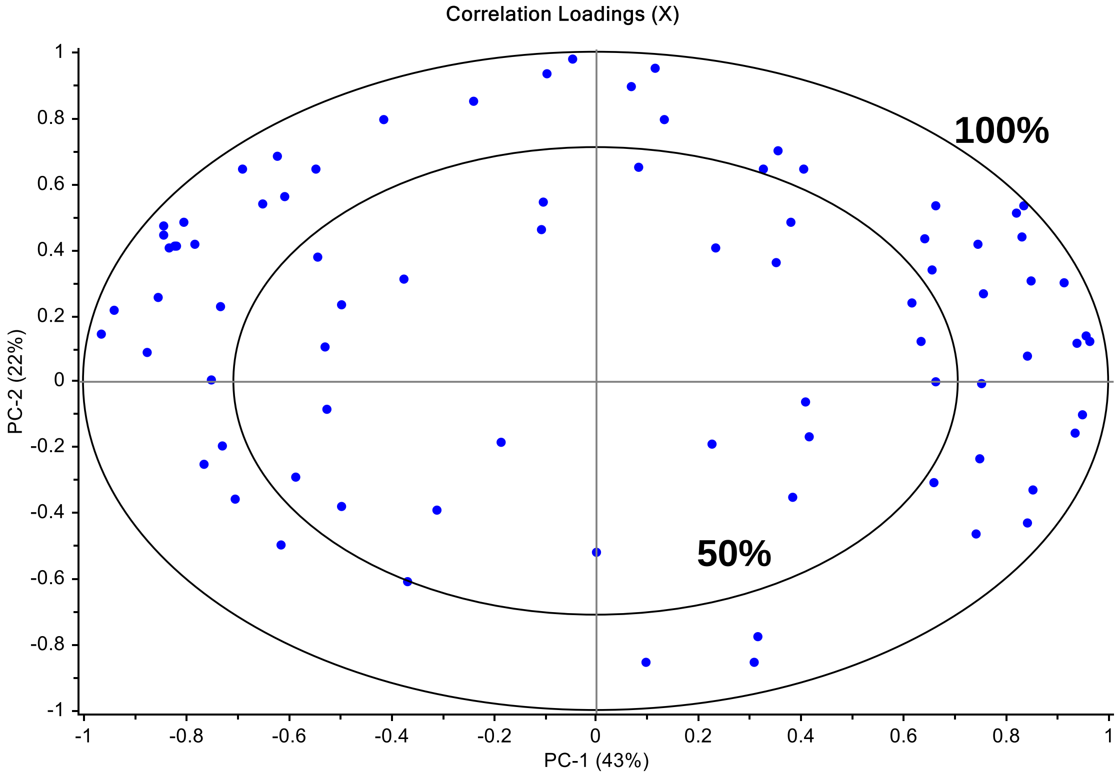
PCA – correlation loadings

PCA basics – correlation loadings

- Correlation loadings are a **modification** of the regular loadings ($\boldsymbol{P}$)
- Computed from **principal components** ($\boldsymbol{T}$) and **original variables** ($\boldsymbol{X}$)
- Graphical description of correlation loadings computation follows below
- **Advantage** of correlation loading plot
    - Provides direct information about on much the different variables are **correlated with** or **explained by** the different components
    - In particular, when the units of the variables are different, this may give additional and useful information
    - When variables are already **standardised**, the differences between the loadings and the correlation loadings plots will generally be **smaller**

PCA basics – correlation loadings

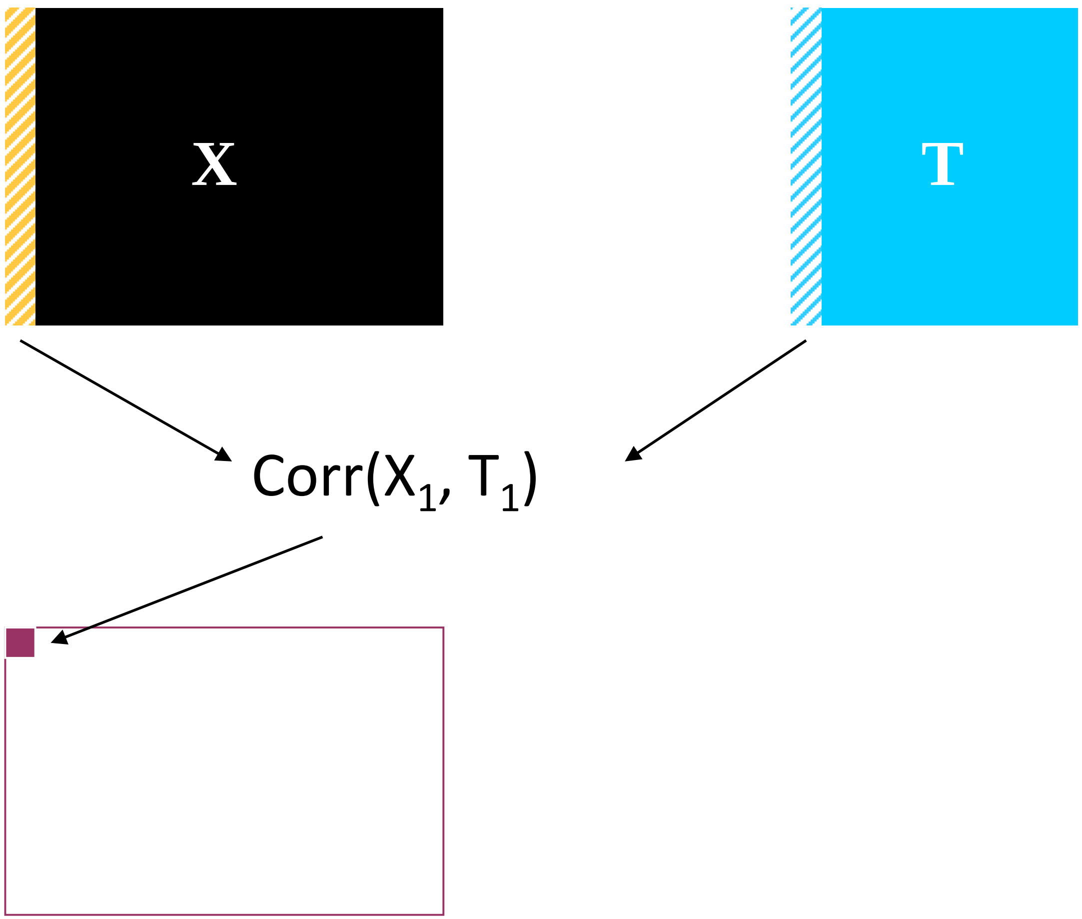
- Circles in the plot corresponding to various degrees of explained variances
- Typically one will present a circle for **100%** explained and for **50%** explained variance by the **two** components



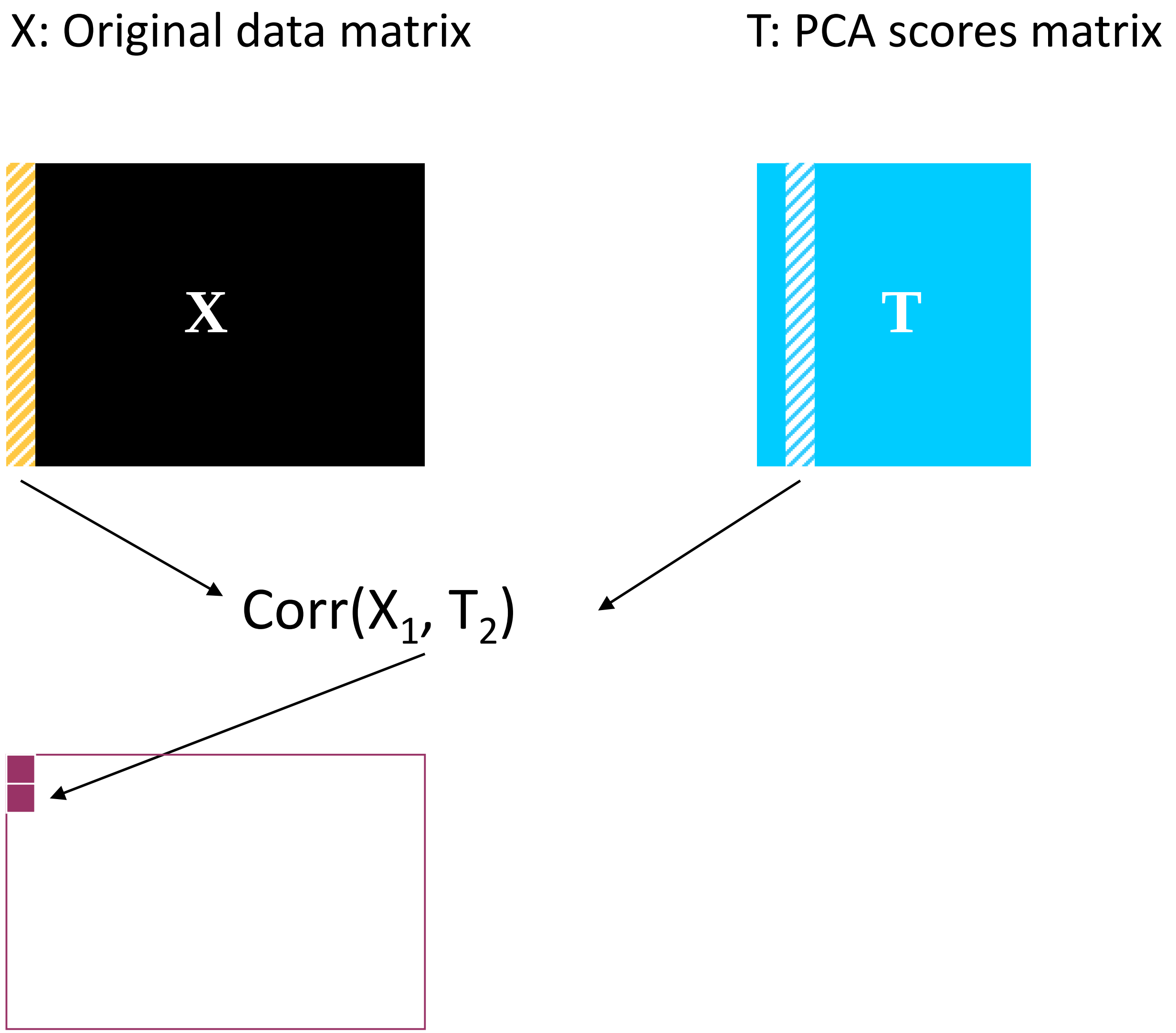
PCA basics – computation of correlation loadings

X: Original data matrix

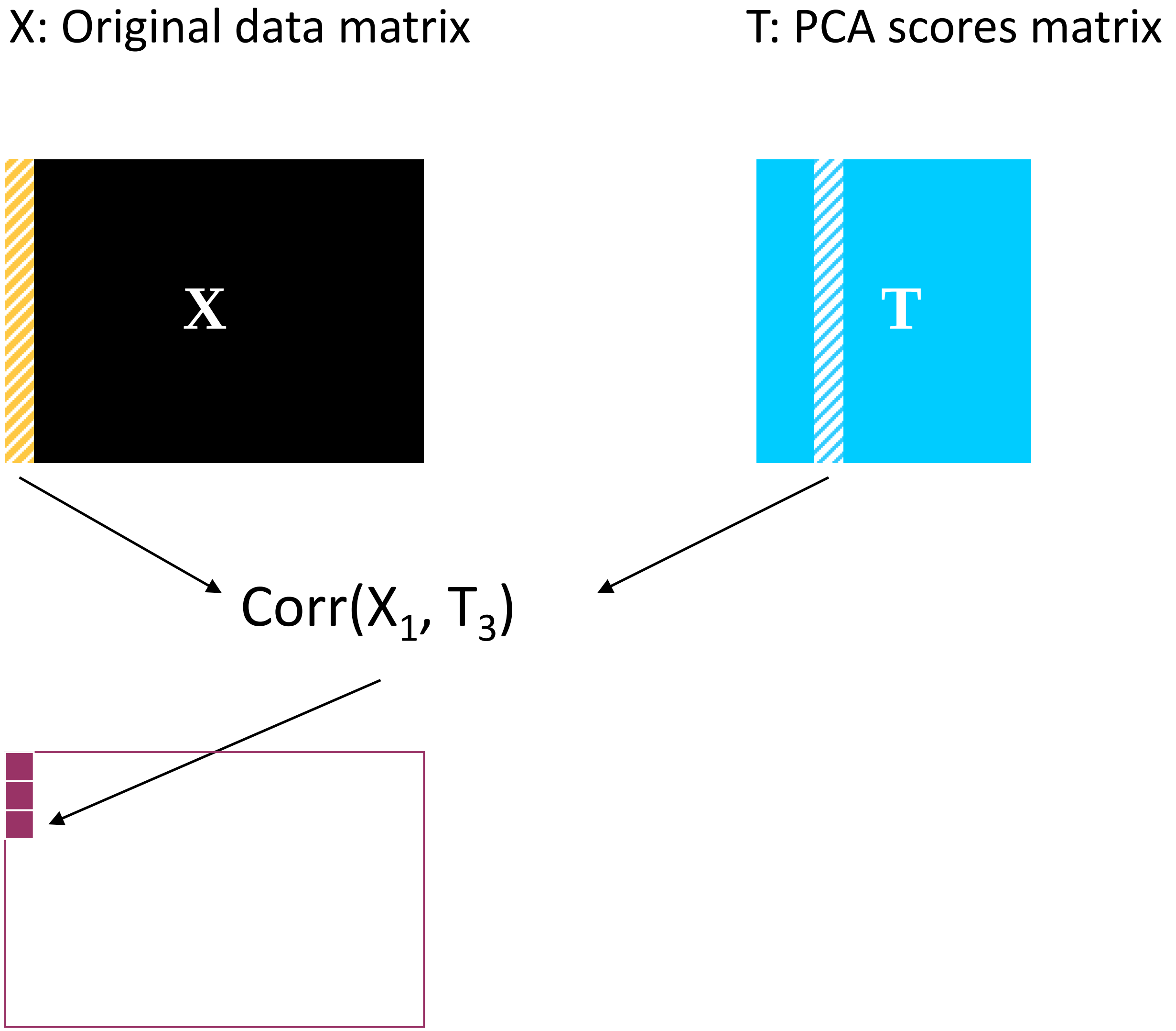
T: PCA scores matrix



PCA basics – computation of correlation loadings



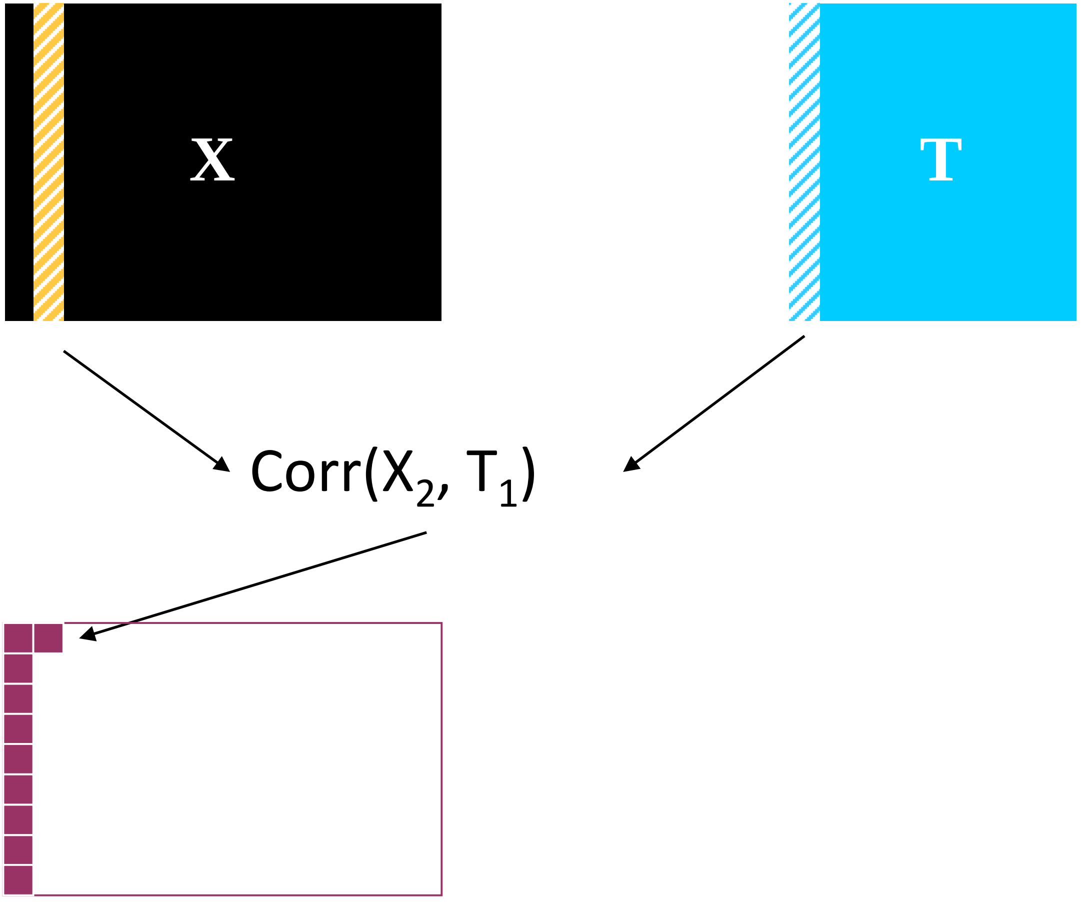
PCA basics – computation of correlation loadings



PCA basics – computation of correlation loadings

X: Original data matrix

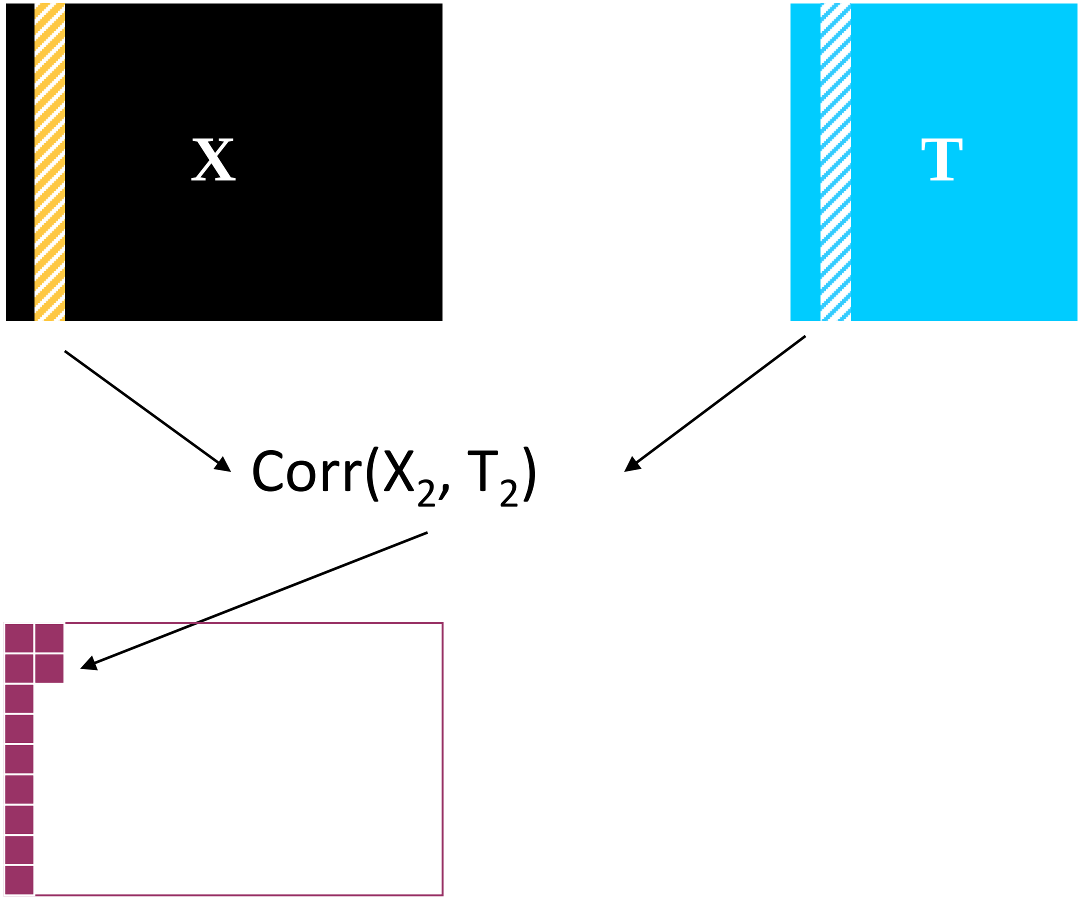
T: PCA scores matrix



PCA basics – computation of correlation loadings

X: Original data matrix

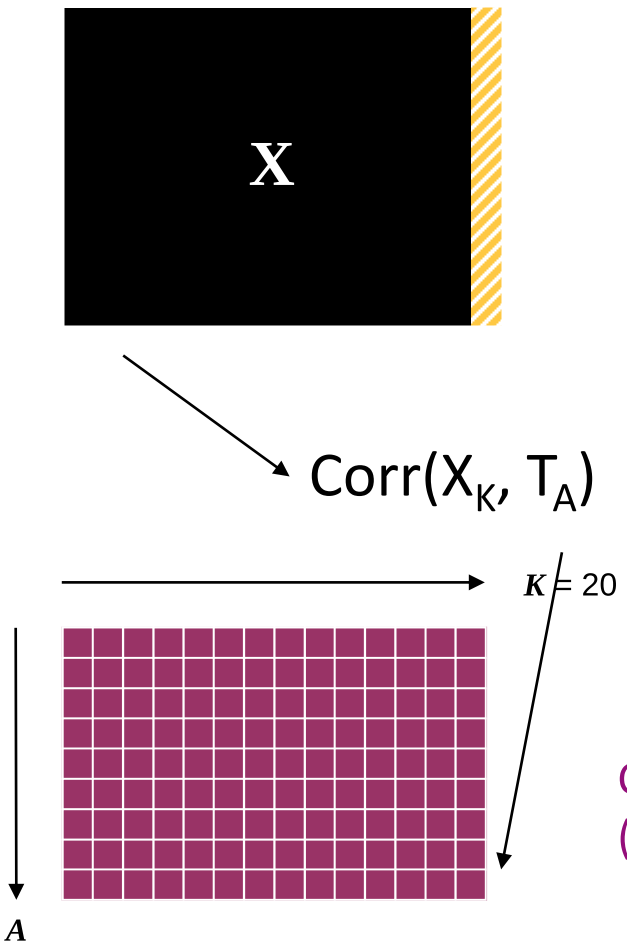
T: PCA scores matrix



PCA basics – computation of correlation loadings

X: Original data matrix

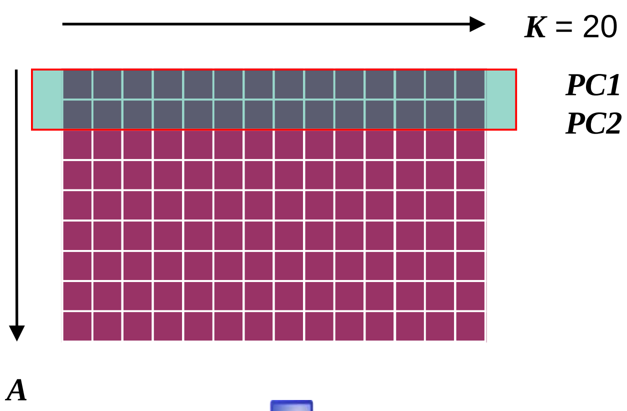
T: PCA scores matrix

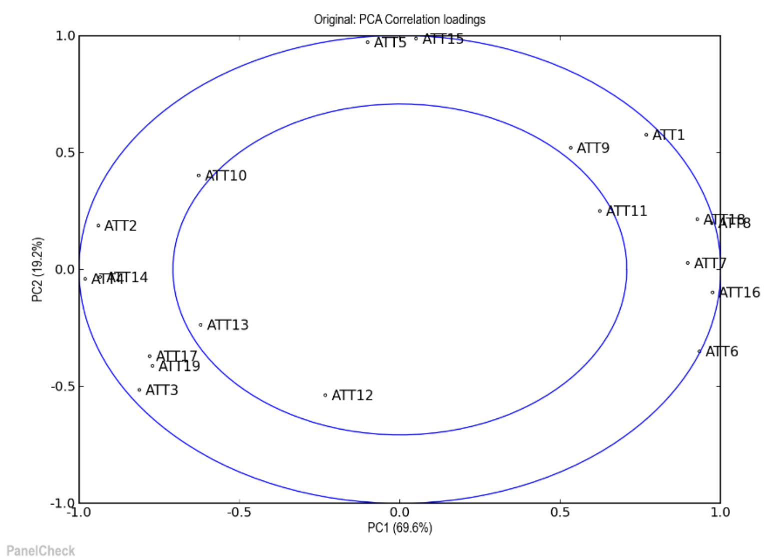


Correlation loadings matrix
(same dimension as loadings matrix ***P***)

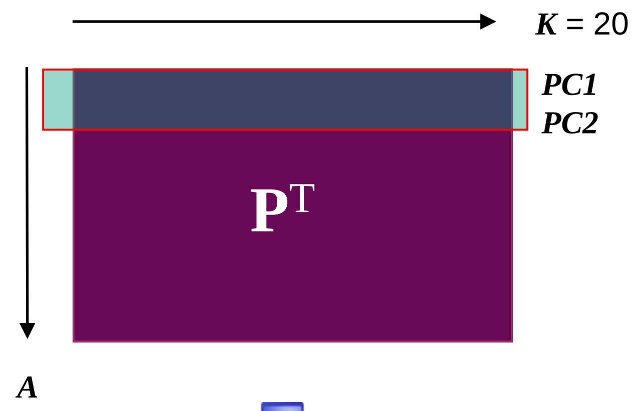
PCA basics – plotting correlation loadings

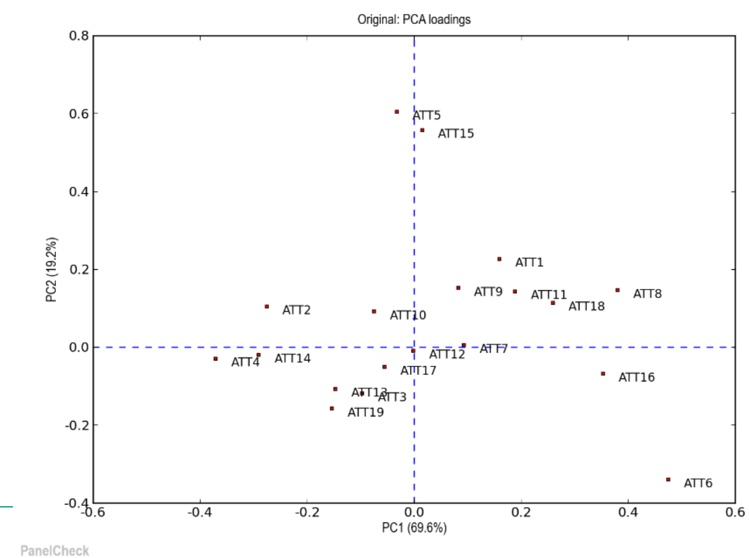
Correlation loadings matrix





Loadings matrix





PCA – centring and **standardisation**

PCA basics – centring and standardisation

- Only purpose of PCA is to look for directions with **high variance**
- This implies: if there are variables $\boldsymbol{x}_k$ in $\boldsymbol{X}$ that have a **larger variance** than others …
  - they will be given **most** attention
  - ➔ They will **dominate** the extracted components
  - ➔ They will **dominate** the plots
- Generally one is interested in letting all variables play a role in the estimation of components (there are exceptions) ➔ standardise variables $\boldsymbol{x}_k$ in $\boldsymbol{X}$
- Matrices in multivariate statistics are always **either** *centered* or *standardised*

PCA basics – centring and standardisation

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1K} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NK} \end{pmatrix}$$

- Number of **objects (rows)**:
  - $n = 1 \ldots N$
- Number of **variables (columns)**:
  - $k = 1 \ldots K$
- Observed value x_{nk} for
  - n'th object
  - k'th variable

center

$$\boxed{x_{nk,cent} = x_{nk} - \bar{x}_k}$$

$$\bar{x}_k = \frac{1}{N}\sum_{n=1}^{N} x_{nk}$$

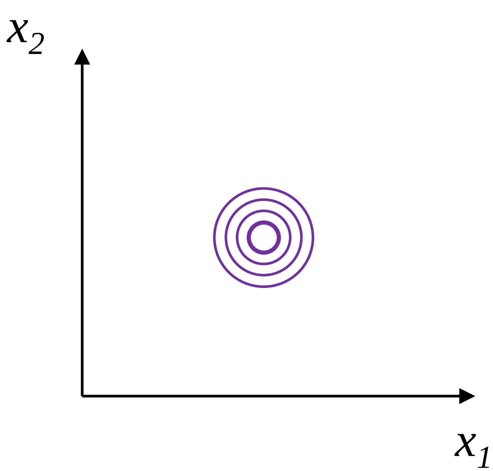
where

standardise

$$\boxed{x_{nk,stand} = \frac{x_{nk} - \bar{x}_k}{\sigma_k}}$$

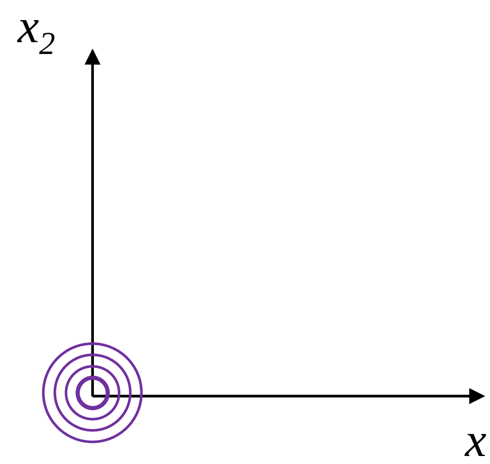
$$\sigma_k = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(x_{nk} - \bar{x}_k)^2}$$

PCA basics – centring and standardisation



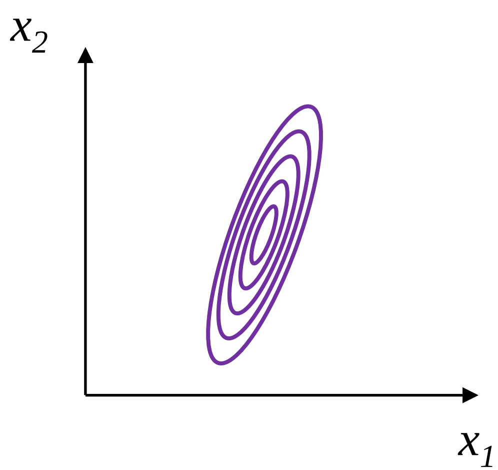
center data

$$\boxed{x_{nk,cent} = x_{nk} - \bar{x}_k}$$



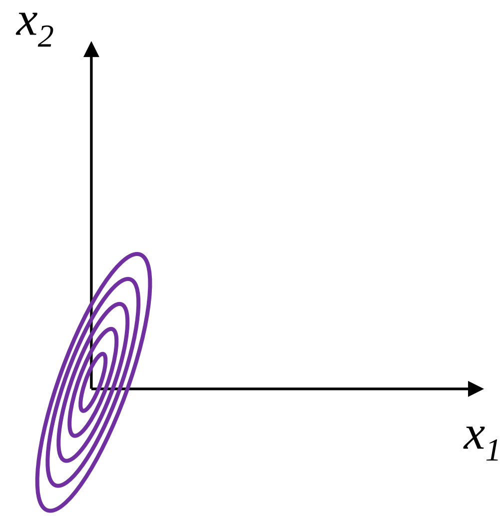
Equal variance of
x_1 and x_2

PCA basics – centring and standardisation



center data

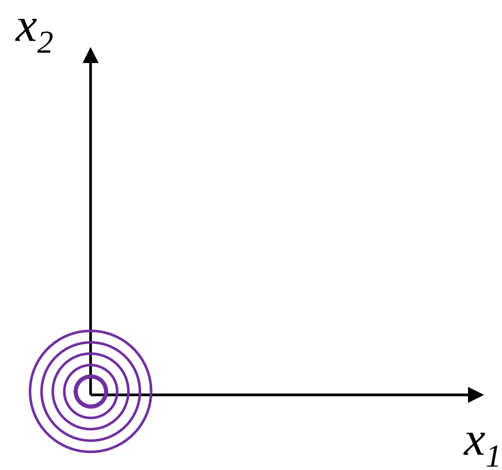
$$x_{nk,cent} = x_{nk} - \bar{x}_k$$



Variance of x_2 is larger than variance of x_1

standardise data

$$x_{nk,stand} = \frac{x_{nk} - \bar{x}_k}{\sigma_k}$$



malahanobis

PCA basics – centring and standardisation

Person	Height (cm)	Weight (kg)	Shoe size
Person A	174	55	46
Person B	188	92	45
Person C	158	65	42
Person D	202	110	49
Person E	171	96	44
Person F	193	79	48
Mean	181	82.833333	45.6667
STD	16.198765	20.507722	2.58199

Original data

Person	Height (cm)	Weight (kg)	Shoe size
Person A	-7	-27.833333	0.33333
Person B	7	9.1666667	-0.66667
Person C	-23	-17.833333	-3.66667
Person D	21	27.166667	3.33333
Person E	-10	13.166667	-1.66667
Person F	12	-3.8333333	2.33333
Mean	0.00	0.00	0.00
STD	16.198765	20.507722	2.58199

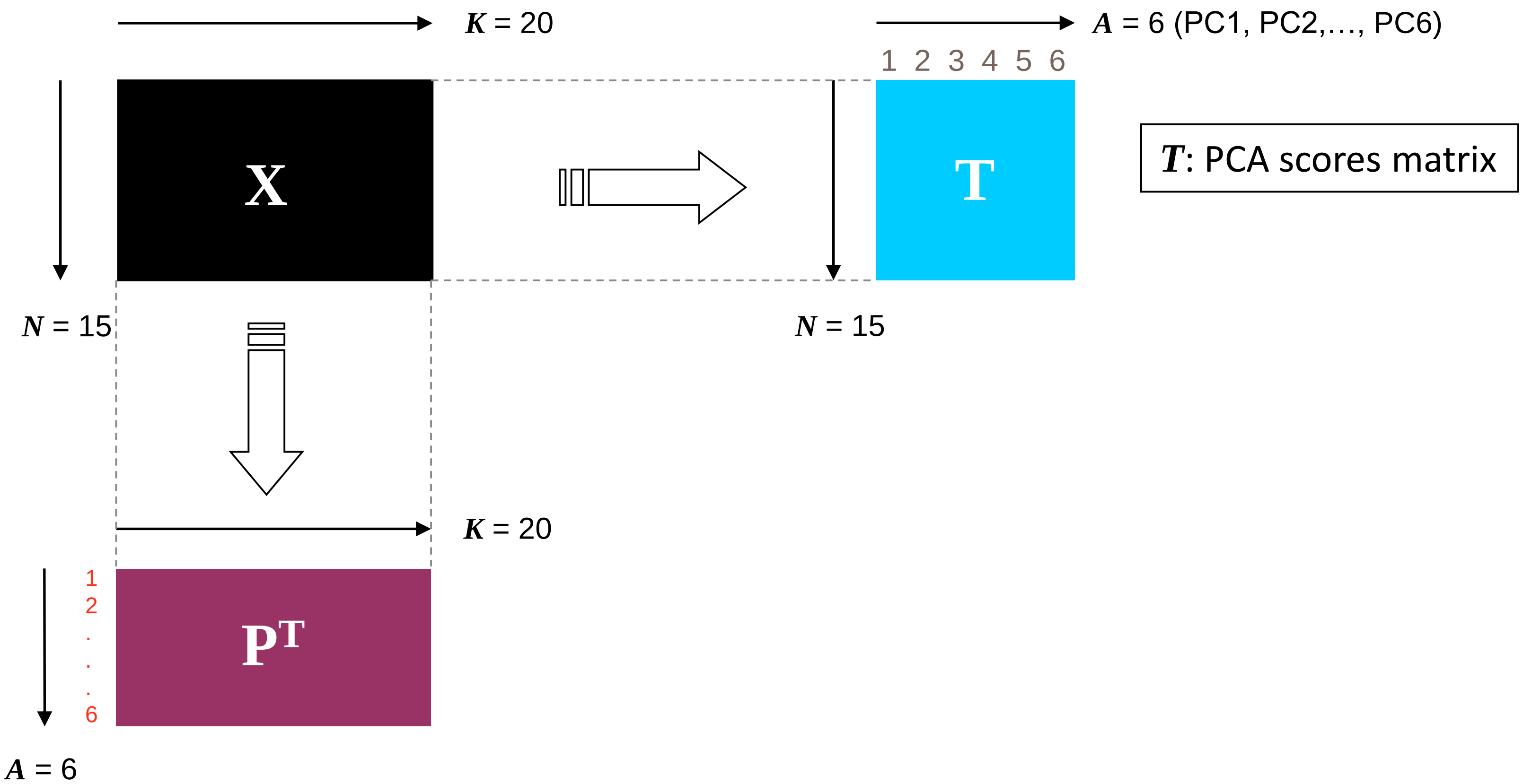
Centered data

Person	Height (cm)	Weight (kg)	Shoe size
Person A	-0.4321317	-1.3572123	0.1291
Person B	0.4321317	0.4469861	-0.2582
Person C	-1.4198613	-0.8695911	-1.42009
Person D	1.2963951	1.3247043	1.29099
Person E	-0.617331	0.6420346	-0.6455
Person F	0.7407972	-0.1869215	0.9037
Mean	0.00	0.00	0.00
STD	1	1	1

Standardised data

PCA – more on concept

PCA basics – more on concept



P: PCA loadings matrix
A: number of components computed

PCA basics

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{P}^T$$

(15×20)

T

(15×6)

$\mathbf{P}^{\mathbf{T}}$

(6×20)

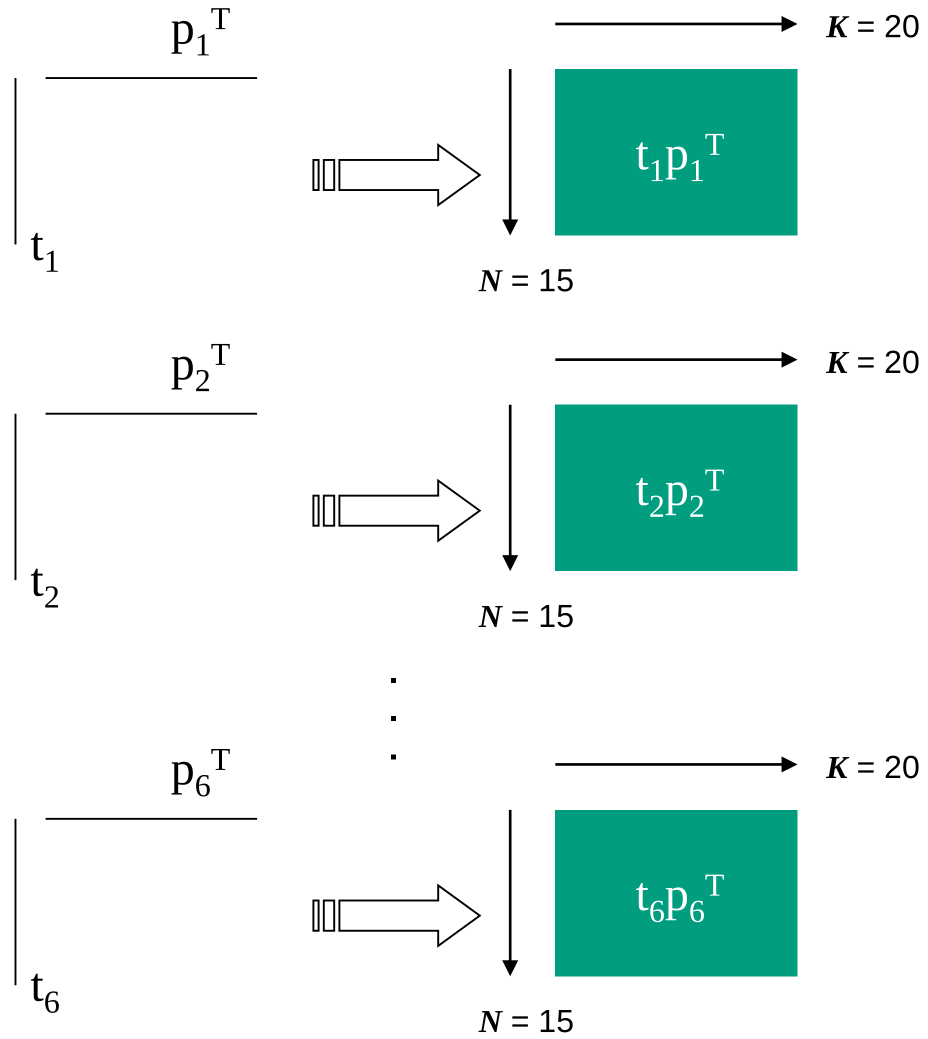
Example

$A = 6$

$$\boldsymbol{X} = \sum_{a=1}^{A} \boldsymbol{t}_a \boldsymbol{p}_a^T = \boldsymbol{t}_1 \boldsymbol{p}_1^T + \boldsymbol{t}_2 \boldsymbol{p}_2^T + \cdots + \boldsymbol{t}_A \boldsymbol{p}_A^T$$

PCA basics – more on concept

$$X = t_1 p_1^T + t_2 p_2^T + \ldots + t_6 p_6^T$$



Holds 69.9% of variance in X

Holds 19.2% of variance in X

.
.
.

Holds 0.7% of variance in X

PCA basics – more on concept

$$X = t_1p_1^T + t_2p_2^T + \ldots + t_6p_6^T$$

$$X = t_1p_1^T + t_2p_2^T + t_3p_3^T + t_4p_4^T + t_5p_5^T + t_6p_6^T$$

Explained variance in each component

PC1: 69.9%
PC2: 19.2%
PC3: 6.1%
PC4: 3.1%
PC5: 1.0%
PC6: 0.7%

Total: 100%

Systematic variation ?

Residuals ?

PCA basics

$$X = t_1p_1^T + t_2p_2^T + \ldots + t_6p_6^T$$

$$X = t_1p_1^T + t_2p_2^T + t_3p_3^T + t_4p_4^T + t_5p_5^T + t_6p_6^T$$

Explained variance in each component

PC1: 69.9%
PC2: 19.2%

PC3: 6.1%
PC4: 3.1%
PC5: 1.0%
PC6: 0.7%

Systematic variation ?

Noise ?

Total: 100%

How many components are appropriate for the PCA model? **Validation!**

PCA basics

$$X = t_1p_1' + t_2p_2' + E$$

$$X = t_1p_1' + t_2p_2' + E$$

$$\hat{X} = t_1p_1' + t_2p_2'$$

$$\hat{X} = t_1p_1' + t_2p_2'$$

➔ $\hat{\boldsymbol{X}}$ is a filtered, ”noise free” version of $\boldsymbol{X}$ (approximation of $\boldsymbol{X}$)

PCA – validation

PCA basics – validation

- Validation is necessary to gain knowledge on **how many** components are **appropriate** for the model, i.e. how many components can be used for …
  - Interpretation
  - Further analysis

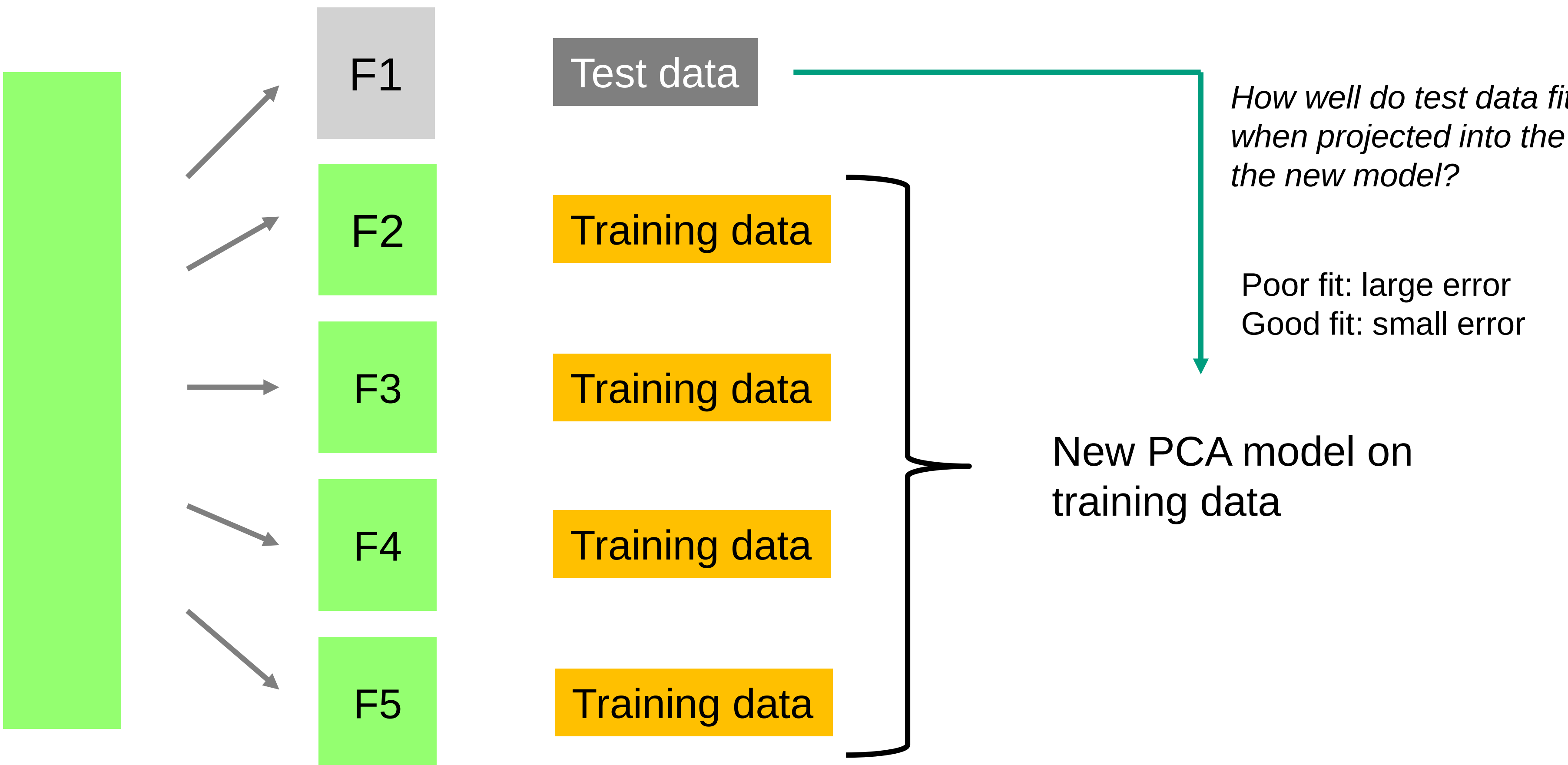
- Use of *internal cross validation* in PCA
  - **K-fold** cross validation (number of folds / splits used)
  - **LOO** cross validation ("Leave-one-out")
    - LOO computationally more expensive compared to K-Fold
    - LOO is special case of K-Fold

PCA basics – validation

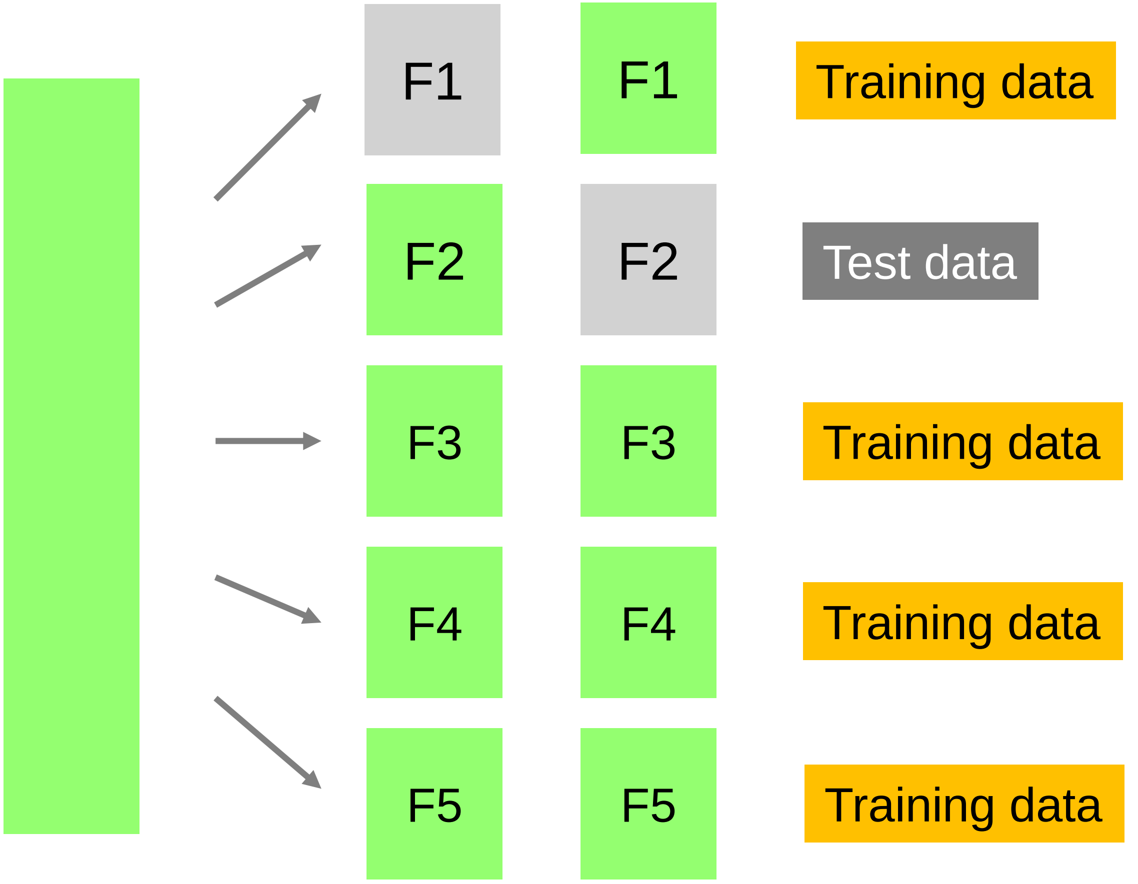
- More details on cross validation will be discussed in Ch. 6 – Learning Best Practices for Model Evaluation and Hyperparameter Tuning

- Use explained **validation** variance for choice of number of components
  - Point where curve of explained validated variance clearly flattens out ➔ point where one should stop interpreting components

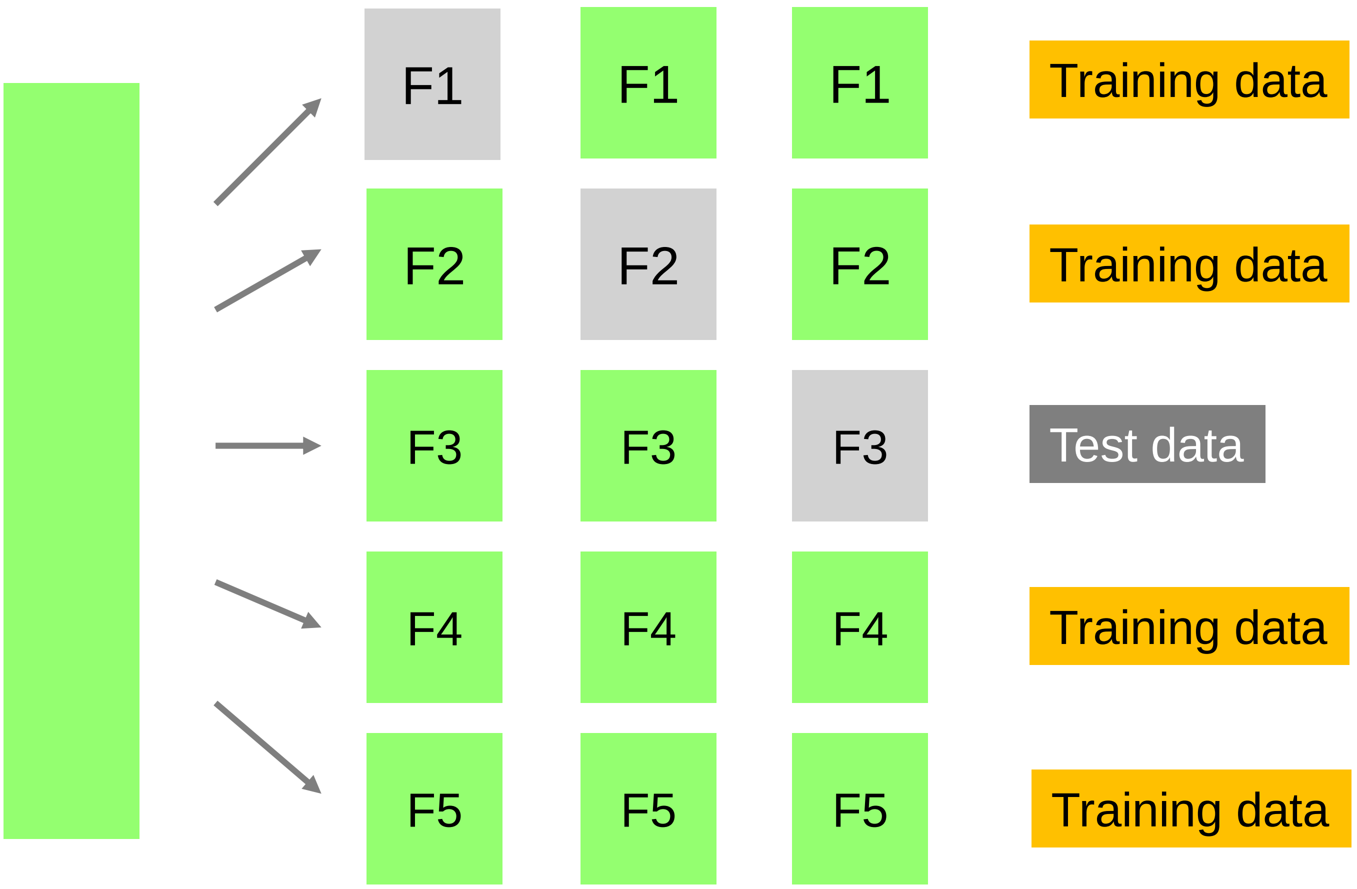
PCA basics - K-fold cross-validation process



PCA basics - K-fold cross-validation process



PCA basics - K-fold cross-validation process



PCA basics - K-fold cross-validation process

PCA basics - K-fold cross-validation process

K-fold cross-validation process

Error of **F1**

Error of **F2**

Error of **F3**

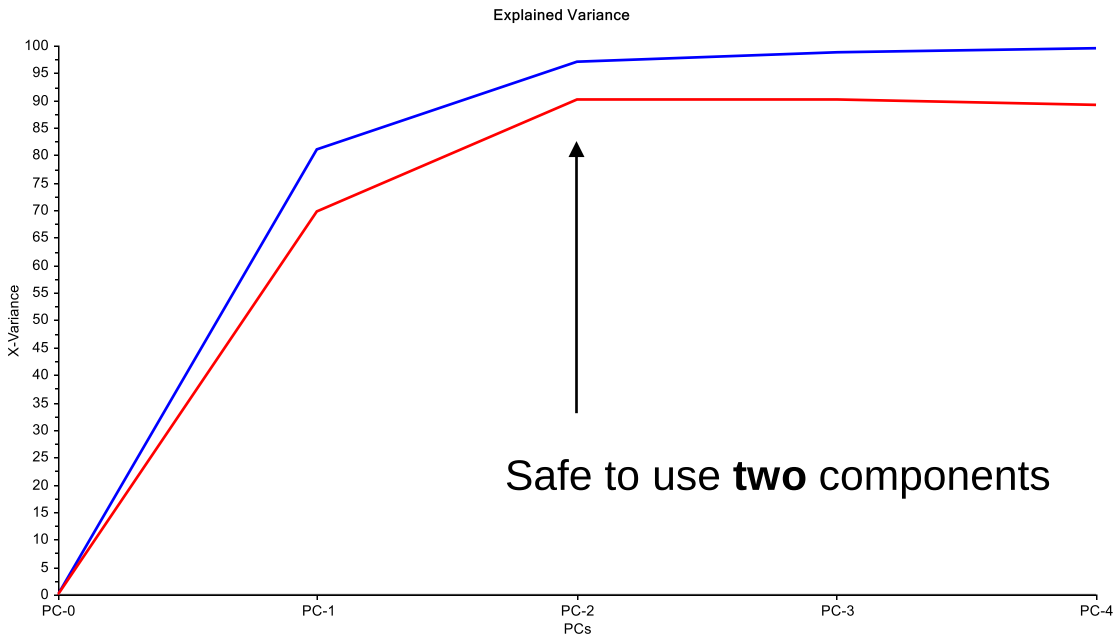
Error of **F4**

Error of **F5**

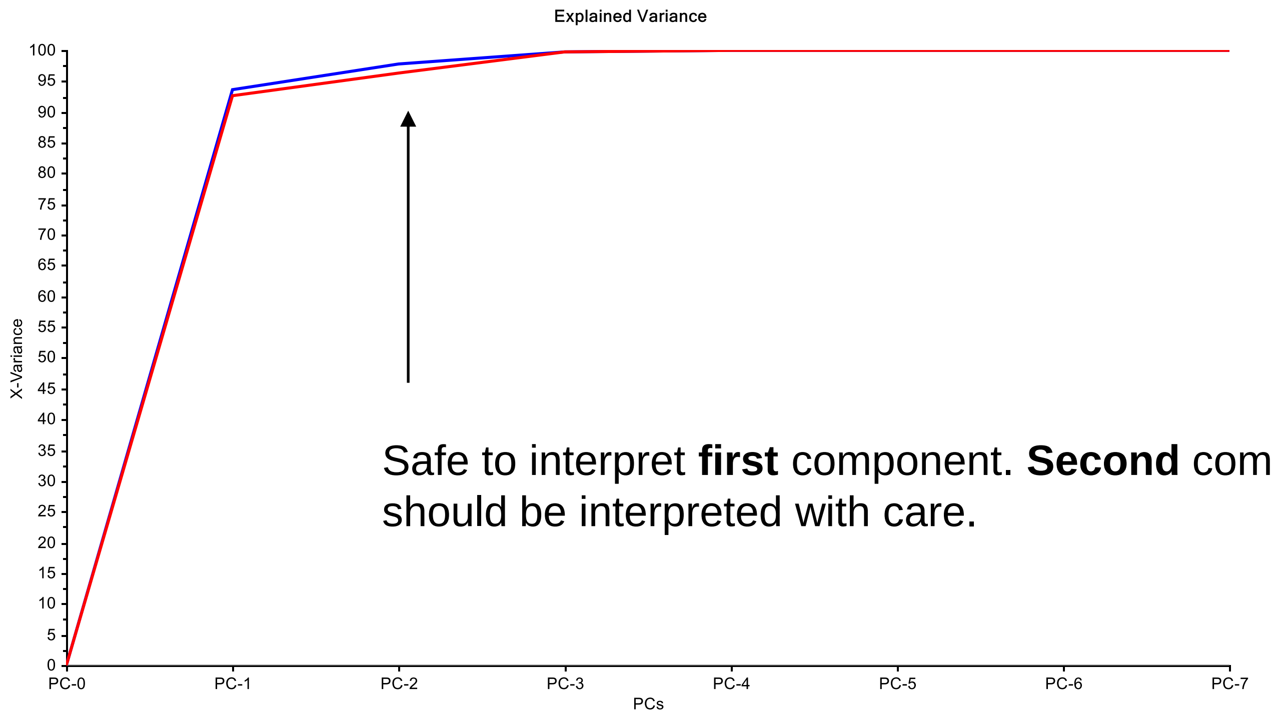
Compute average error across all folds

- Provides information on how many components are “safe” to use (explained validated variance plot)
- Provides information on the variance in the data

PCA basics – validation

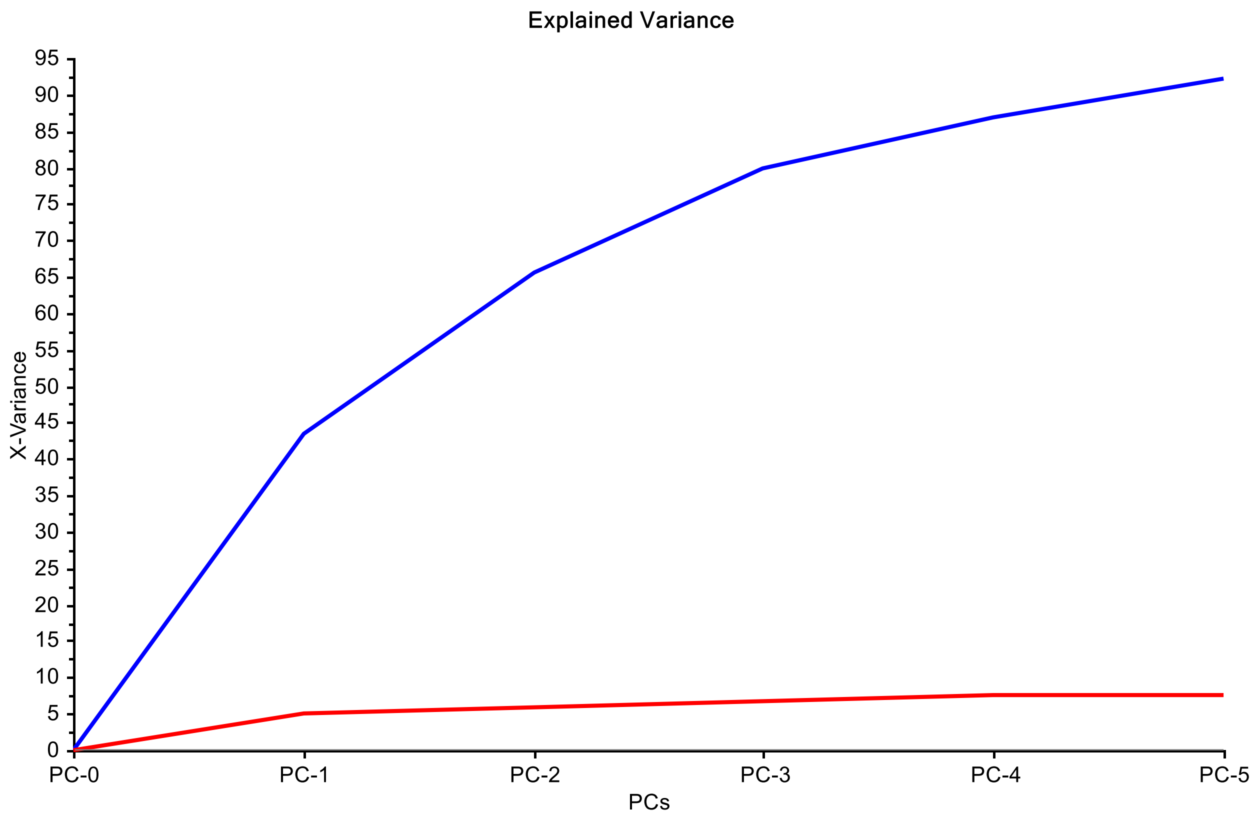


PCA basics – validation



Safe to interpret **first** component. **Second** component should be interpreted with care.

PCA basics – validation



Poor model – may be a result of few objects that are very different from each other

PCA with **Hoggorm** and **HoggormPlot**

Hoggorm, HoggormPlot and examples

- **Hoggorm** package for multivariate statistics
  - GitHub: https://github.com/olivertomic/hoggorm
  - Read the Docs: http://hoggorm.readthedocs.io/en/latest/

- **HoggormPlot** package for convenient plotting of Hoggorm results
  - GitHub: https://github.com/olivertomic/hoggormPlot
  - Read the Docs: http://hoggormplot.readthedocs.io/en/latest/

- **Examples** of how to use Hoggorm illustrated in Jupyter notebooks
  - GitHub: https://github.com/khliland/hoggormExamples

Resources

- PCA:
  - Python Machine Learning SE, Chapter 5, pages 141 – 154
- PLSR:
  - Video lectures: https://www.youtube.com/playlist?list=PL4C8FE6F00CBBF34A
  - Introduction and examples in R: «The pls Package (Mevik & Wehrens)»