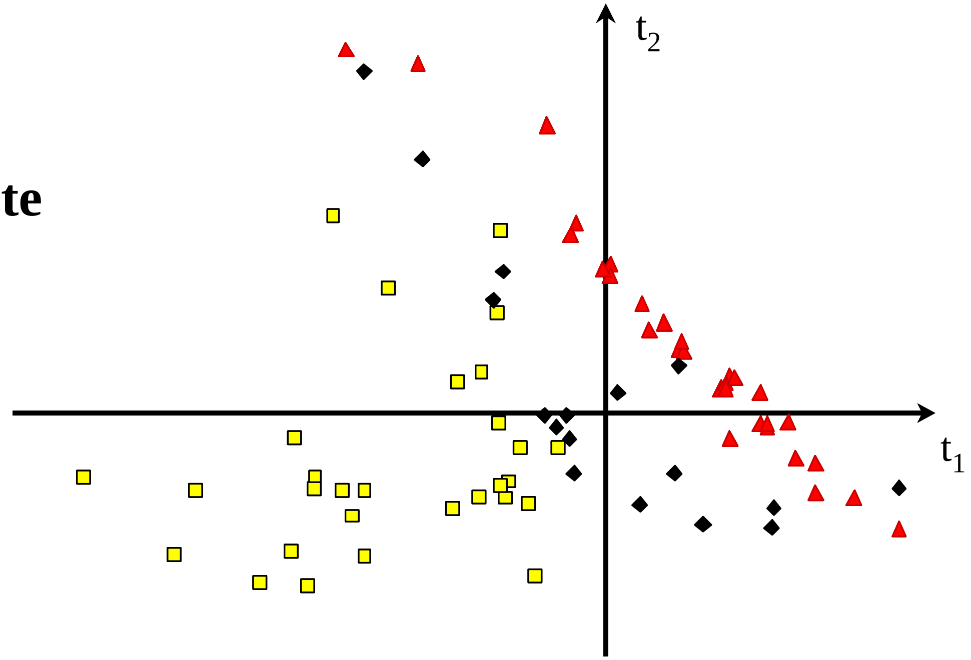
Multivariate data analysis (MVA) - Introduction

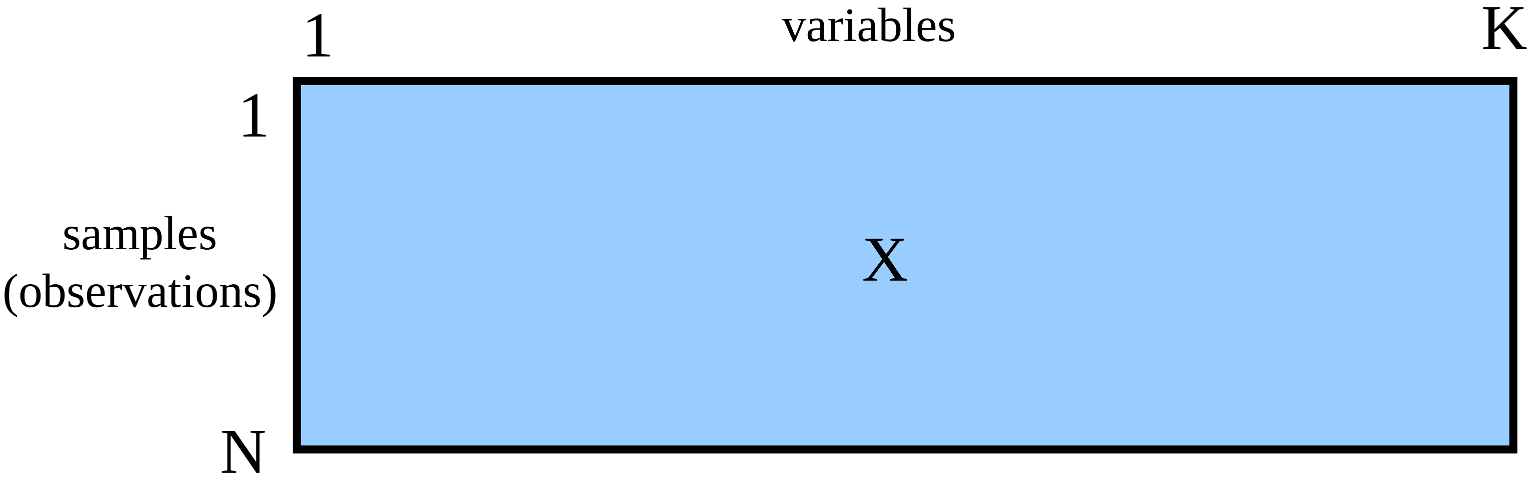
- Introduction
- Univariate/Multivariate
- Latent variables
- Projections
- PCA
- Examples



Chemical and Biological data are often of Multivariate character

Methods such as: GC, UV, IR, NIR, NMR, MS, E-fores, HPLC, TLC, Sequensing, Gene arrays ….

…. applied to complex samples in chemistry and biology creates large data tables!



Variables: Often many, co-linear (correlated), unknown relevance

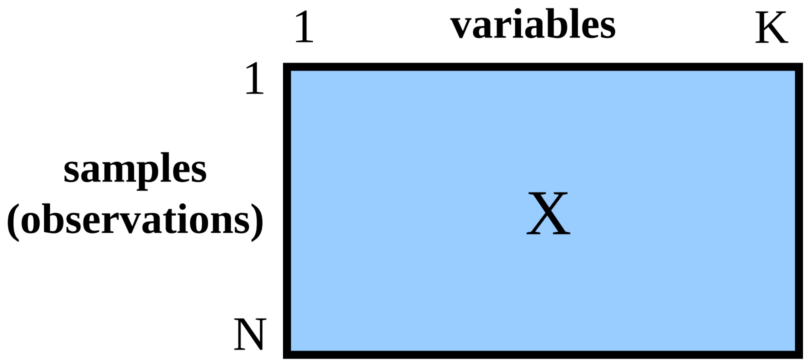
Measurements: Noisy, sometimes “missing values”

Different goals with Multivariate Analysis - **Overview** (understanding)

Relationships between observations (samples) - trends, groups, outliers

Relationships between variables - groupings, correlation

Explanation to trends, groups, outliers among observations
- which variables are important?

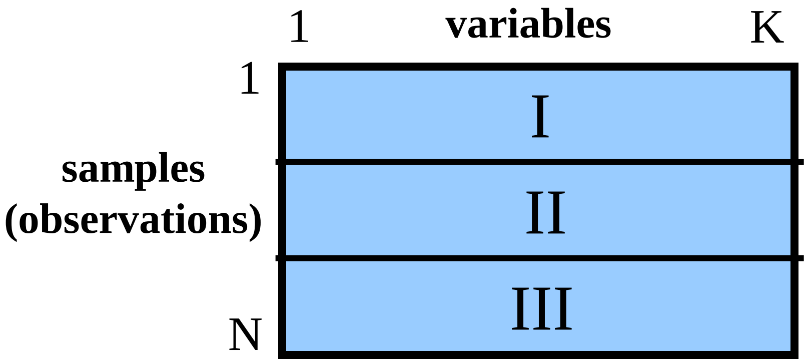


Different goals with Multivariate Analysis - **Classification**

Models for differences between known classes of observations

Explanation to differences between classes

Prediction of unknown samples with regards to class identity

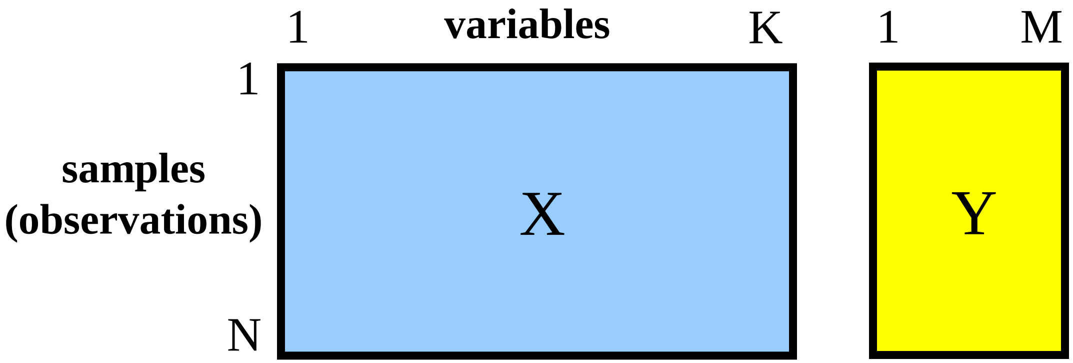


Different goals with Multivariate Analysis – **Correlation between blocks**

Relationships between two blocks of variables **(x and y)**.

Does a block of variables **(x)** contain information about the other block of variables **(y)?**

A Regression problem! (Multivariate regression)



Questions for Multivariate data tables

Questions about samples (observations)

Are there any outliers?
Are there groups and/or trends?
Are there similarities/dissimilarities between samples?
How do new samples behave?

?

Questions about variables

Which variables cause outliers?
Which variables are responsible for groupings and/or trends?
Which variables are responsible for class separations?
How do new variables behave?

Types of data

- What types of data for **Modelling** and **Analysis** are there?

- Univariate data $K = 1$
- Bivariate data $K = 2$
- Few-variate data $K \leq 5$
- Multivariate data $K \geq 6$
- Megavariate data $K \geq 1000$

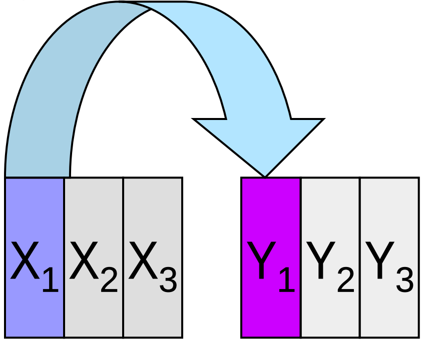
- Quantitative
- Qualitative

- Processes (Continuous/Batch)
- Time Series (Stationary/Dynamic)

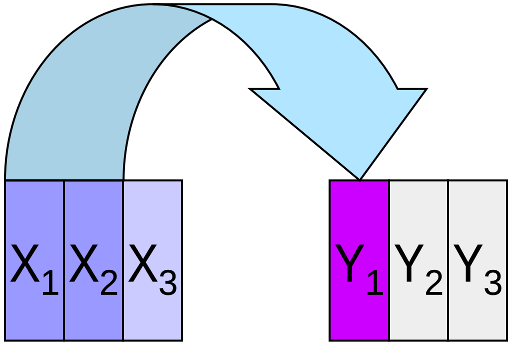
- Controlled/Uncontrolled

Methods of Analysis

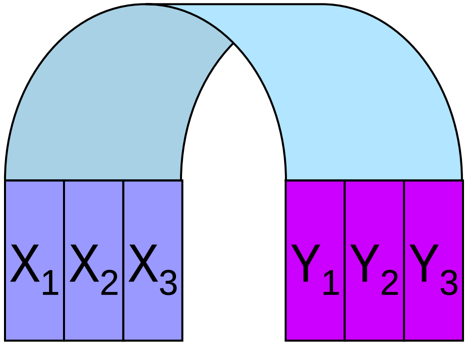
- **COST Approach**
  - Plot and evaluate one variable or a pair of variables at time
  - OK 50 years ago (few variables)



- **Classical Statistics**
  - Find a relationship between a few of the X's and one Y at a time
  - OK 50 years ago (few and essentially uncorrelated variables)



- **Multivariate Analysis**
  - Model all the variables together to find relationships between **all** the X's and all the Y's



Problems with univariate methods for Multivariate data

Univariate statistical analysis underestimates or overestimates the information in Multivariate data.

The solution to this problem is to use ***Multivariate Projection methods.***

By ***MultiVariate Analysis (MVA)*** all variables are analyzed simultaneously.

Multivariate tools

PCA	Principal Component Analysis (general overview of multivariate data)
PLS	Partial Least Squares Projection to Latent Structures (regression problem)
SIMCA	Soft Independent Modelling of Class Analogy (classification) (PCA + PLS)

Methods that can handle ***co-variation*** between ***variables***.

Why not univariate analysis of Multivariate data?

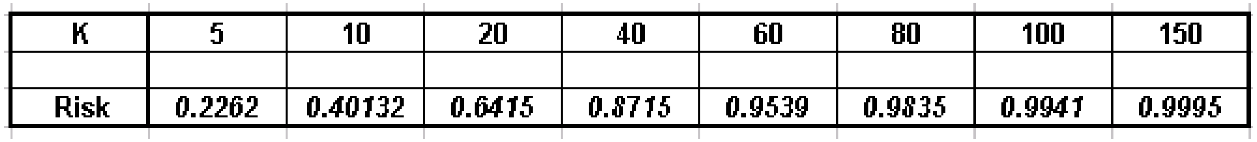
Two problems:

(1) Risk for random correlations (Type I error, ***false positives***)

(2) Risk for not seeing the information (Type II error, ***false negatives***)

Many variables increase the risk for random correlations between variables!

Risk for random correlation (Type I, false positives) = 1 - 0.95^K

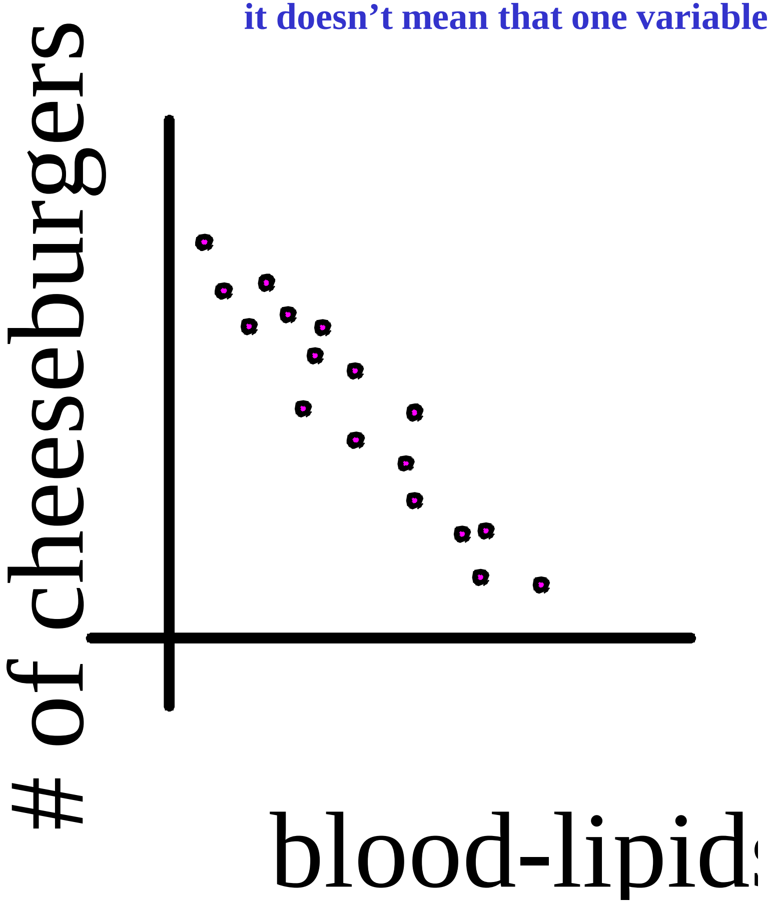


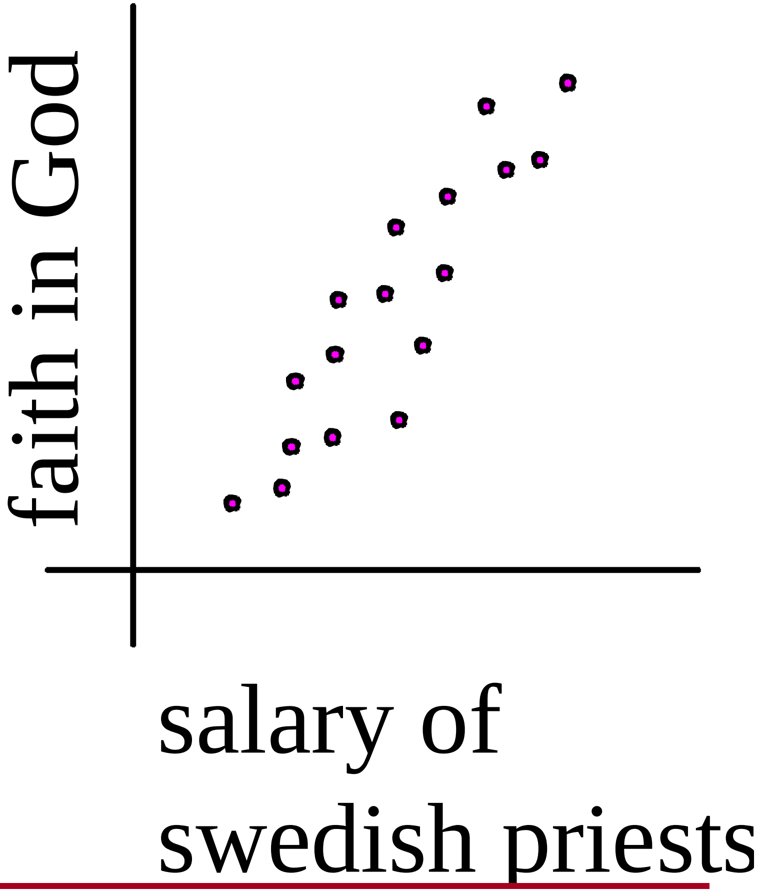
K	5	10	20	40	60	80	100	150
Risk	*0.2262*	*0.40132*	*0.6415*	*0.8715*	*0.9539*	*0.9835*	*0.9941*	*0.9995*

Why not univariate analysis of Multivariate data?

(1) Risk for random correlations (Type I error, ***false positives***)

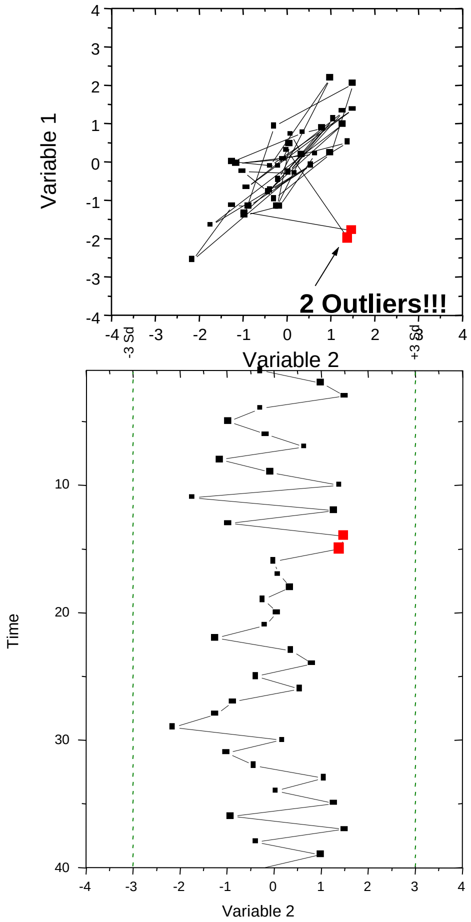
Even if two varaibles are correleated (correlation), it doesn’t mean that one variable causes the other (kausalitet)

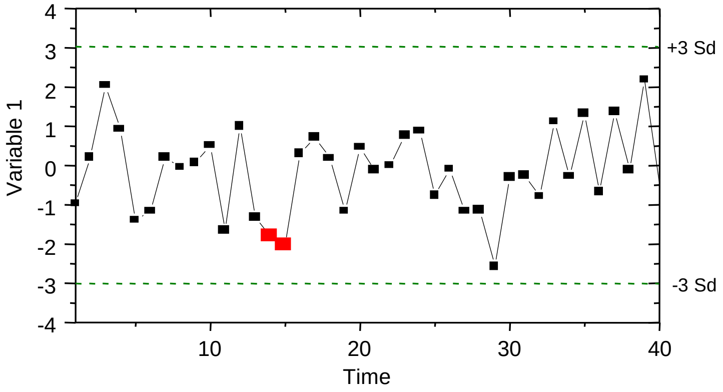




Why not univariate analysis of Multivariate data?

(2) Risk for not seeing information (Type II error, ***false negatives***)



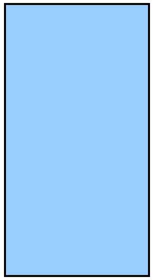


- The measured variables are often correlated
- Most deviating samples (outliers) aren’t found until all variables are analysed together (key to early fault detection)
- **The information is found in the variable correlations not in the individual signals!**

Univariate analysis/Multivariate analysis

Classical statistical methods

- Multiple Linear Regression (MLR)
- Canonical Correlation
- Linear Discriminant analysis (LDA)
- Analysis of variance (ANOVA)
- Maximum likelihood methods



Long and Thin

Assumptions

- Independent X-variables (orthogonal)
- X-variables are exact (no error in X)
- Residuals are normally distributed

Multivariate analysis

Projection methods

PCA, PLS, PCR, PLS-DA

Short and Fat

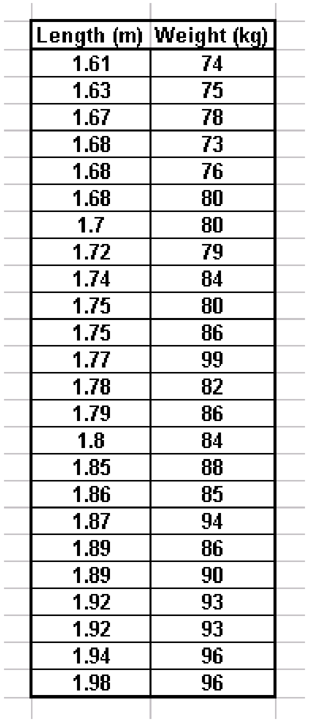
Assumptions

- X-variables not independent
- X-variables can contain errors
- Residuals can have structure

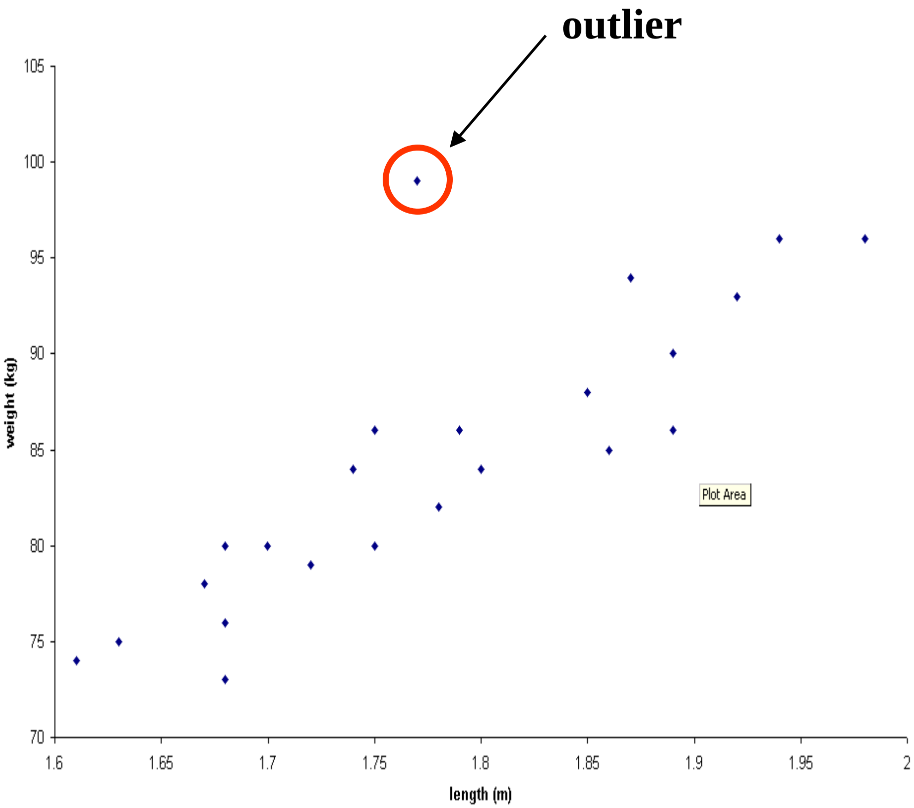
View data in plots

Two variablea - plot them against each other instead of analyzing them one at a time!

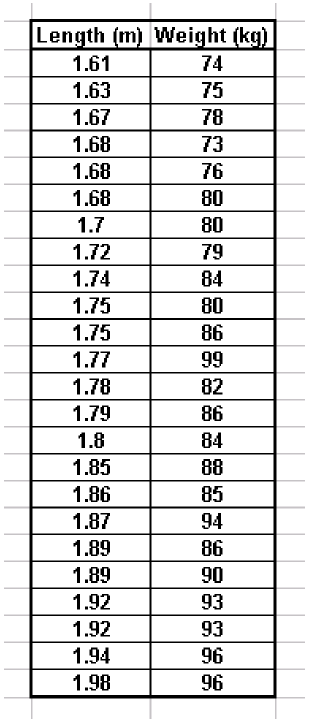
Plots of data gives information!



Length (m)	Weight (kg)
1.61	74
1.63	75
1.67	78
1.68	73
1.68	76
1.68	80
1.7	80
1.72	79
1.74	84
1.75	80
1.75	86
1.77	99
1.78	82
1.79	86
1.8	84
1.85	88
1.86	85
1.87	94
1.89	86
1.89	90
1.92	93
1.92	93
1.94	96
1.98	96



Construct appropriate plots!



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1.85	88
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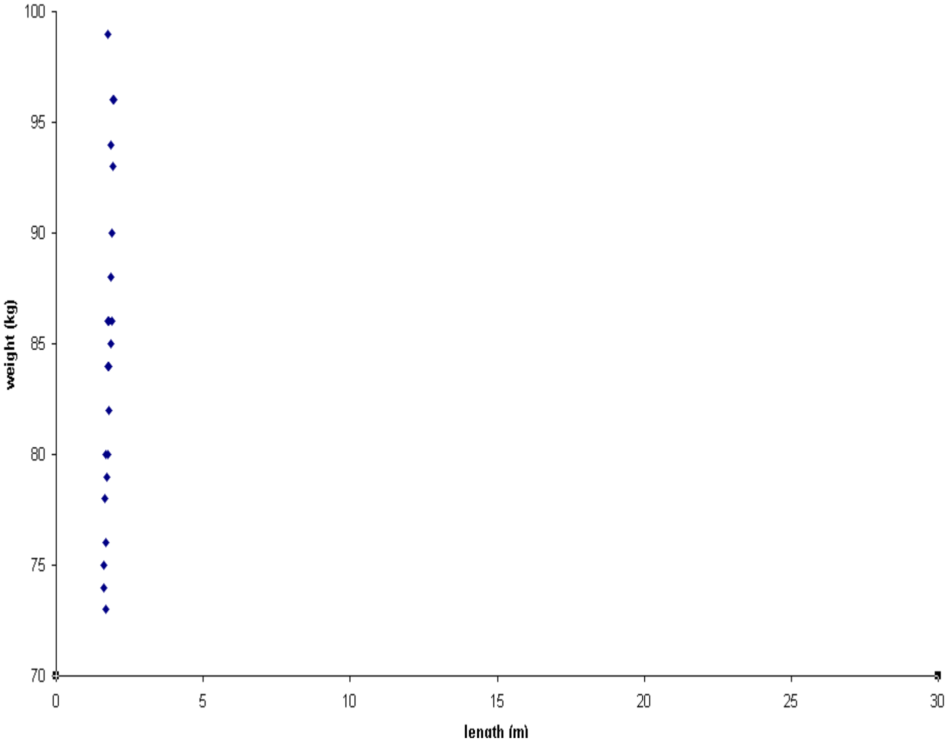
1.89	86
1.89	90
1.92	93
1.92	93
1.94	96
1.98	96



Latent variables

- **Latent variables describe the underlying (hidden) information (variation) in a studied system characterized by a number (K) of experimental variables.**

- **Many variables are correlated with each other, i.e. describe the same variation in the experimental space.**

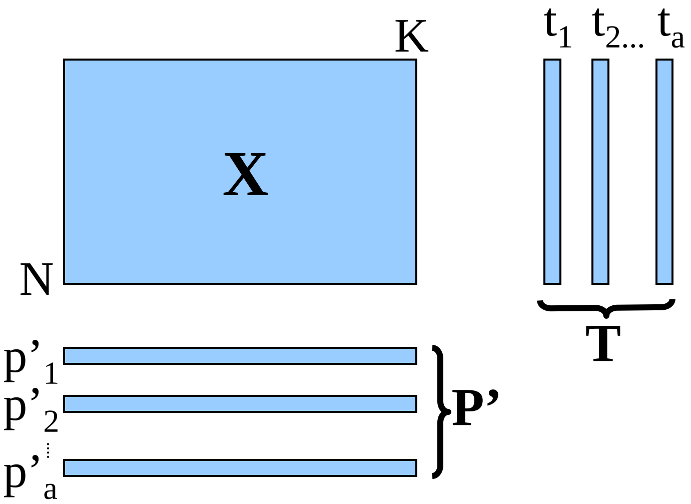
- **Latent variables – Principal components (describe the variation in the system)**

- ***PCA* - Models variation in one data block (X) in latent variables (Model: X = TP' + E)**

- ***PLS* – Models variation in two data blocks (X, Y) in latent variables and correlates these blocks by regression. (Model: X = TP' + E, Y = TC' + F)**

- **By using projection methods (PCA, PCR, PLS, …) the variation in a system can be describe by a few orthogonal latent variables (few compared to the (K) variables used to describe the system initially)**

Latent variables (PCA)



t_i: score vector
p_i: loading vector
T: matrix consisting of score vectors (N*A)
P: matrix consisting of loading vectors (K*A)

Residual

$$X = TP' + E = \sum_{a=1}^{A} t_a p_a' + E$$

Model

- **A principal component (latent variable) consists of two parts (score (t_i) + loading (p_i))**

- **Scores (t) describe the variation in the sample direction i.e. differences/similarities between samples**

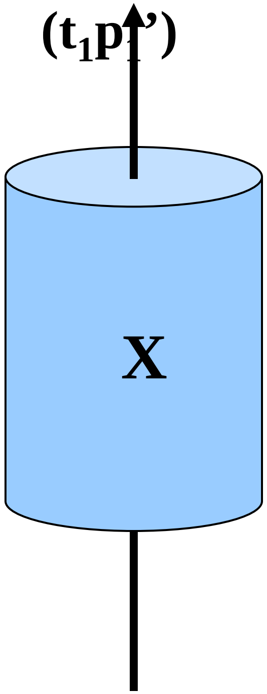
- **Loadings (p) describe the variation in the variable direction i.e. differences/similarities between variables and additionally give an explanation to the variation in scores.**

- **The principal components are orthogonal to each other and explain the variation in X that is based on a number (K) of often correlated variables.**

- **The number of principal components (A) is often a lot less than the number of variables (K) in X.**

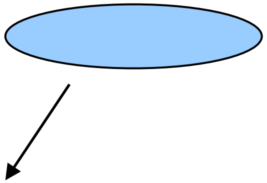
Latent variables (PCA)

PC_1
(t_1p_1')



X

residual (E_1)



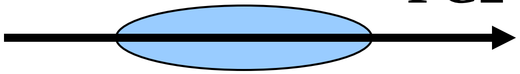
$$X = t_1p_1' + E_1$$

PC_1 describes the largest direction of variation in X.
The perpendicular distance to PC_1 defines the residual, E_1
The residual is the variation in X not described by the model.

After PC1, E_1 = X, for calculation of PC2 !

The direction described by PC1 is eliminated
and PC_2 is calculated from the remaining variation i.e. E_1

PC2 (t_2p_2')



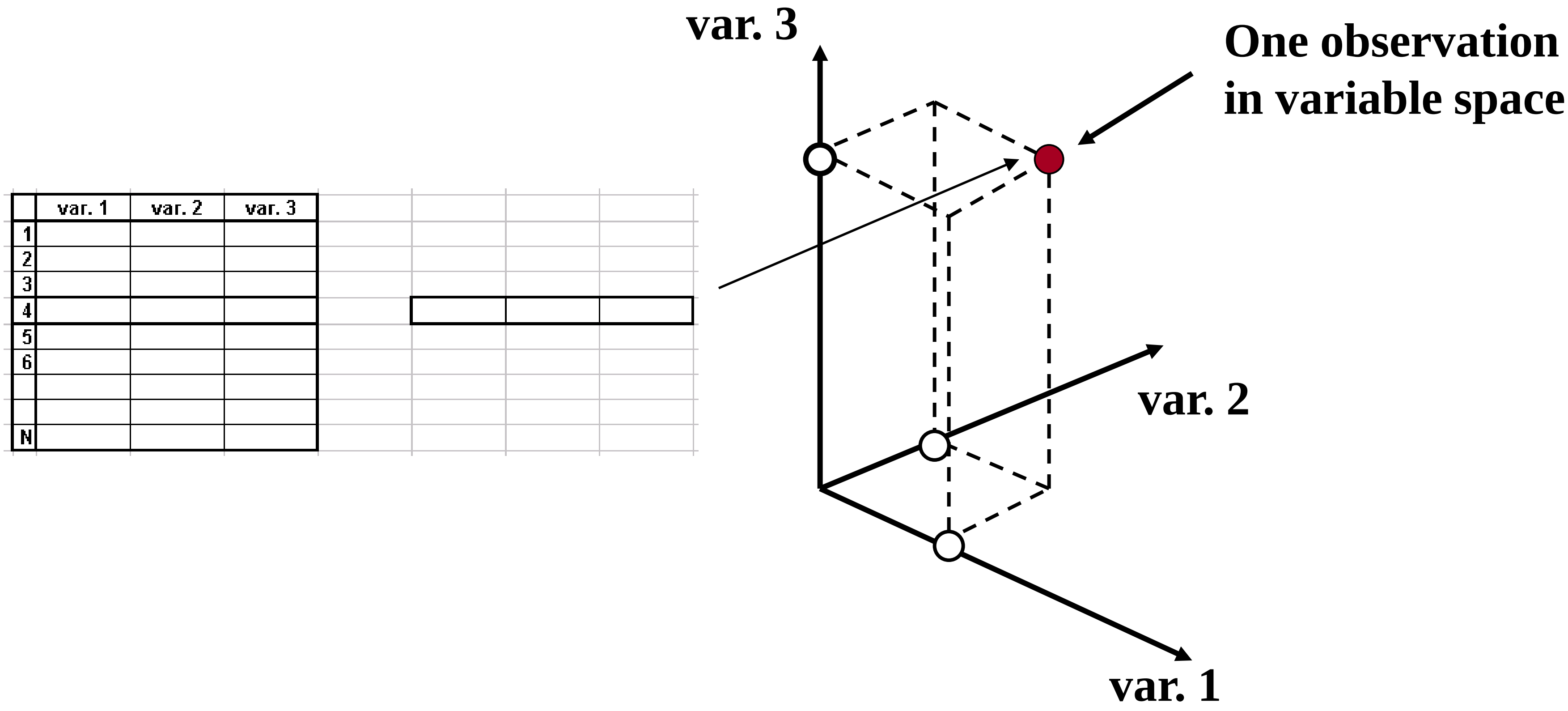
$X=E_1$

$$X = t_1p_1' + t_2p_2' + E_2$$

PC_2 describes the largest direction of variation in X = E_1

Projections

From data table to variable space



	var. 1	var. 2	var. 3
1			
2			
3			
4			
5			
6			
N			

var. 3

One observation in variable space

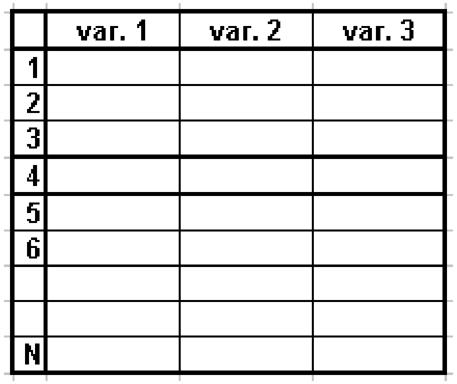
var. 2

var. 1

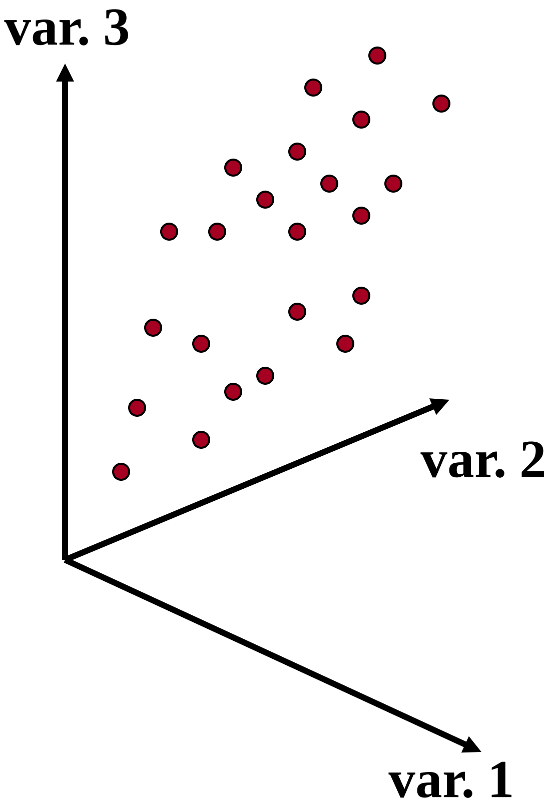
The whole table produces a swarm of points in variable space

Projections

The whole table produces a swarm of points in variable space

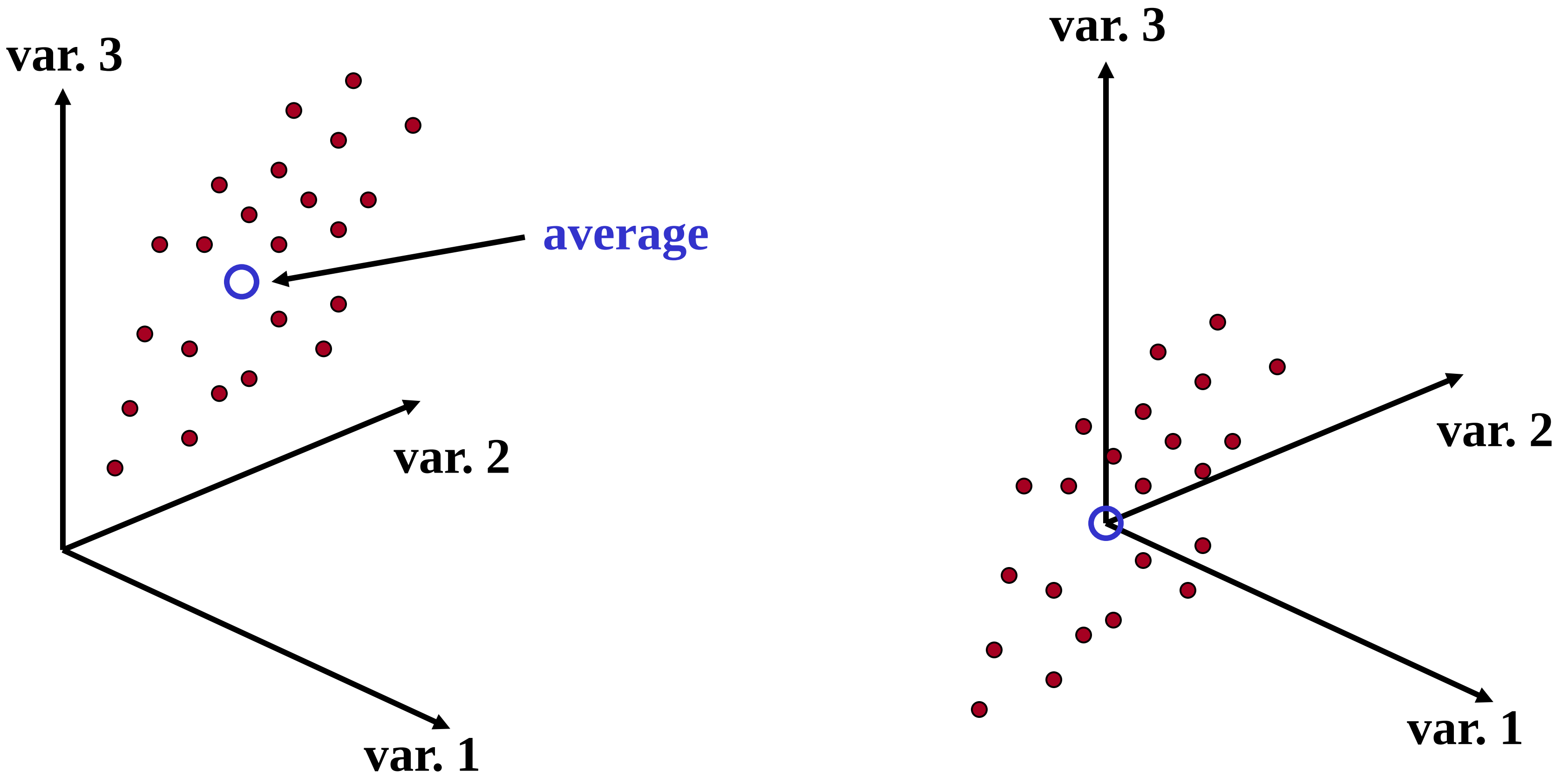


	var. 1	var. 2	var. 3
1			
2			
3			
4			
5			
6			
N			

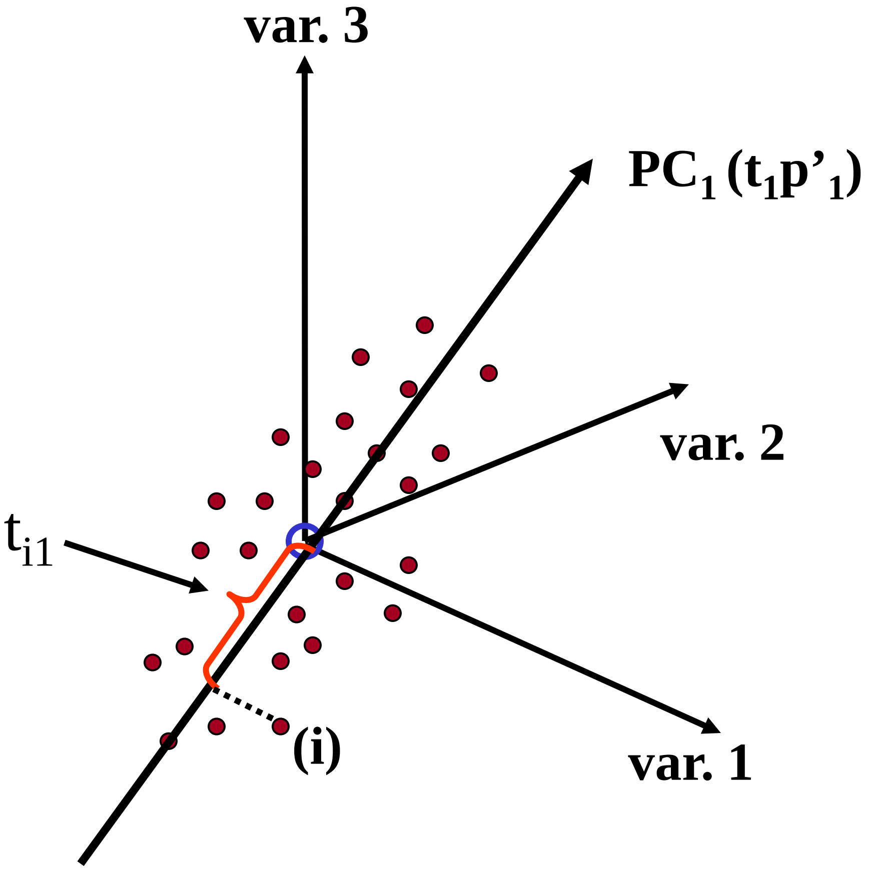


Projections

Mean Centering – move the centre of the points (average) to the origin of the variable space



Projections

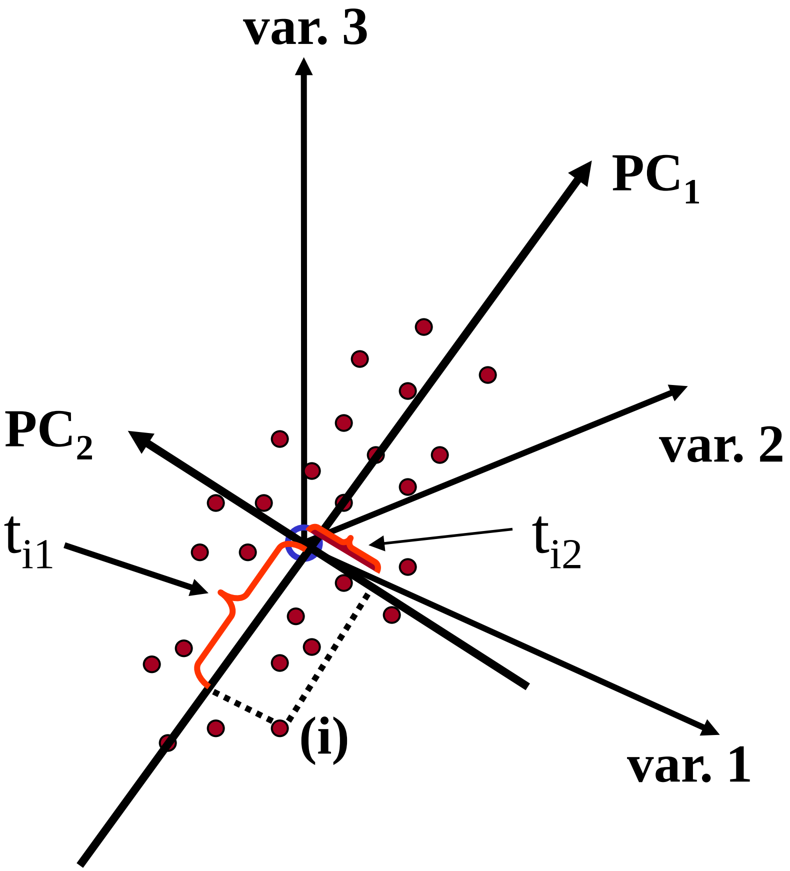


The first principal component (PC$_1$) is set to describe the largest variation in the data, which is the same as the direction in which the points spread most in the variable space

The Score value **(t$_{i1}$) for the point i is the distance from the projection of the point on the 1:st component to the origin.**

PC$_1$ hence is the first latent variable in a new coordinate system that describes the variation in the data.

Projections



The second principal component (PC_2)
is set to describe the largest variation in the data,
Perpendicular (orthogonal) to the 1:st component

The Score value (t_{i2}) for the point i is the distance from the projection of the point on the 2:nd component to the origin.

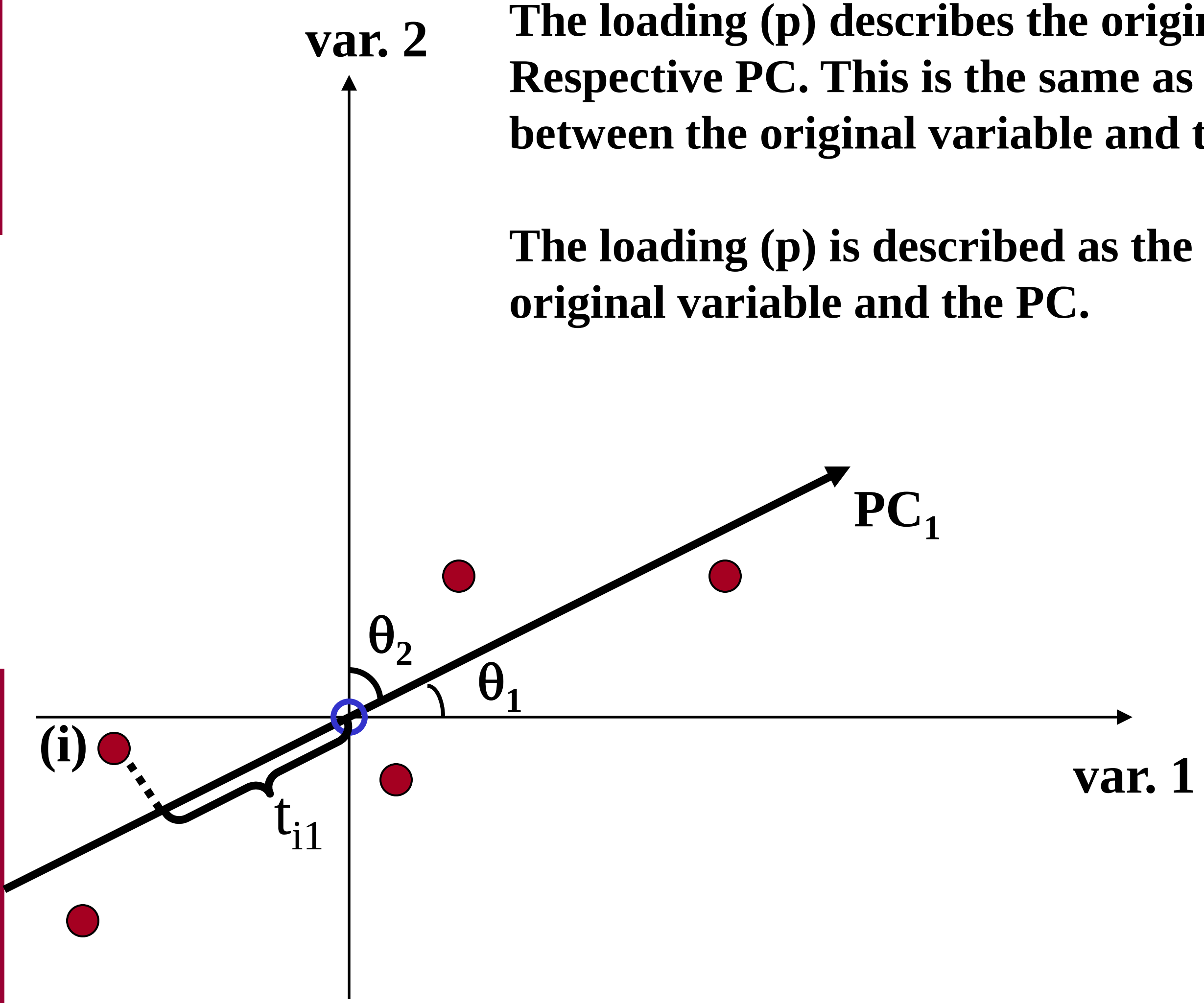
PC_2 hence is the second latent variable in a new coordinate system that describes the variation in the data.

Projections

The loading (p) describes the original variables importance for Respective PC. This is the same as the similarity in direction between the original variable and the PC.

The loading (p) is described as the cosine of the angle between the original variable and the PC.

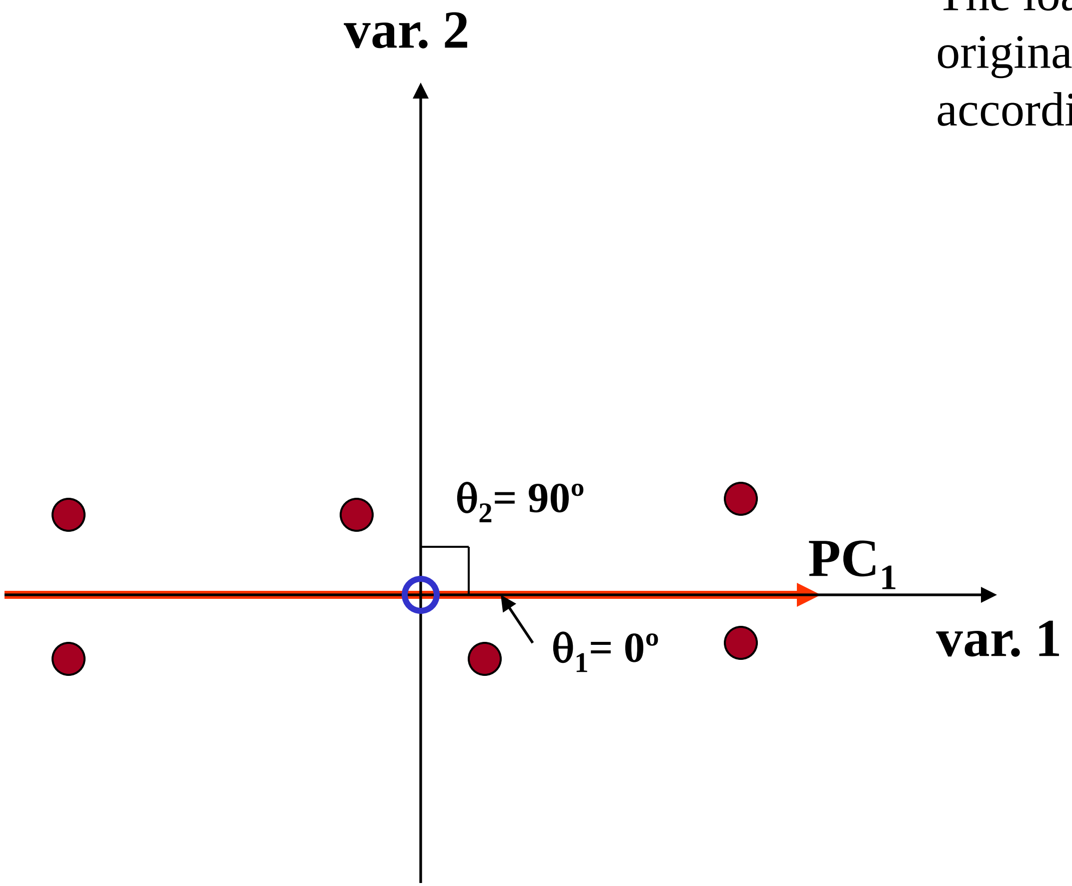
$$p = \cos\theta$$



Projections

Imagine a situation where the largest direction of variation in the data coincide with variable 1. This means that the direction for the 1:st principal component will coincide with the direction of variable no.1.

The loading **p** describes similarity between original variable and principal component according to direction!



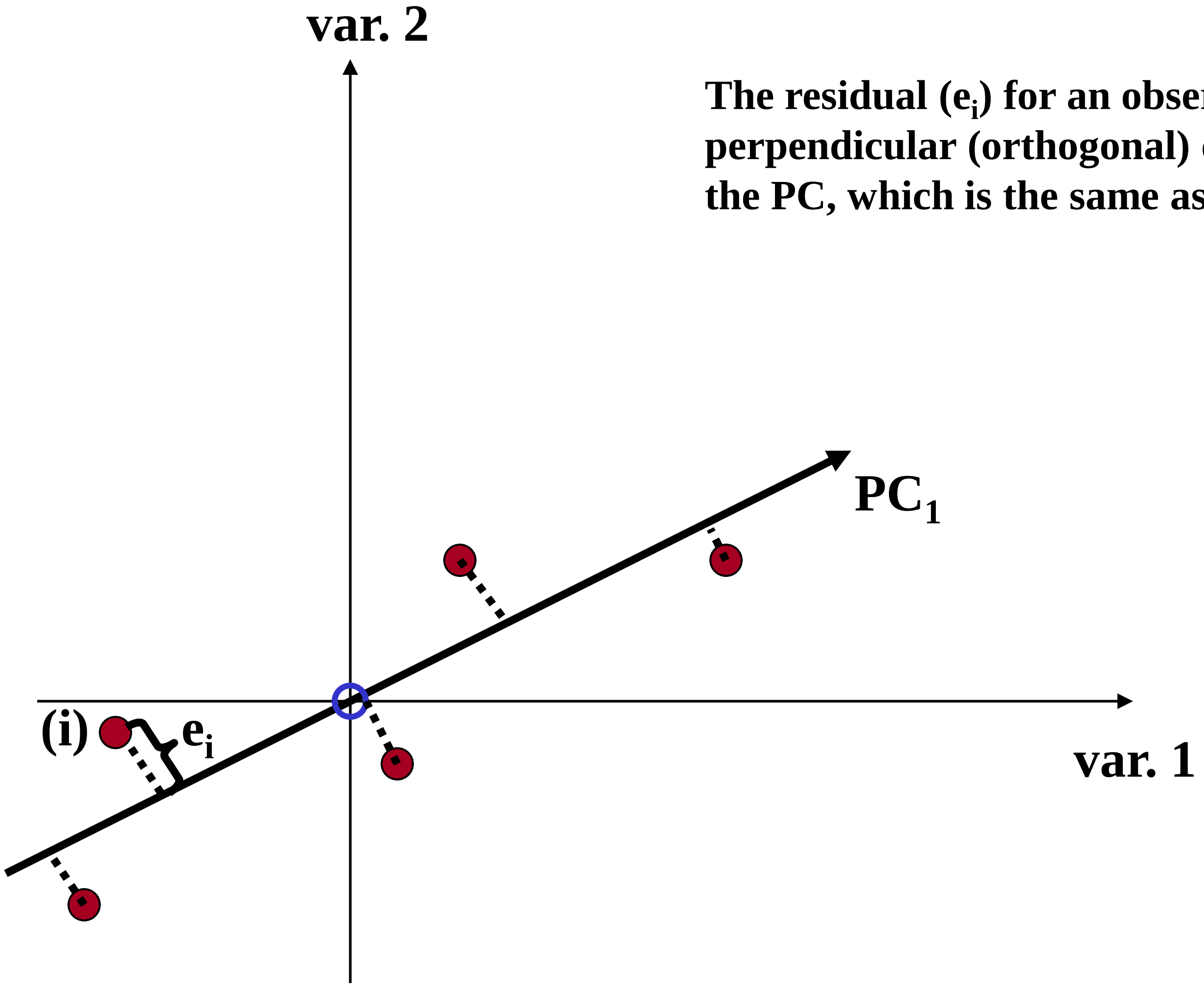
$$\boxed{\begin{array}{l} \mathbf{p = \cos\theta} \\ \\ \mathbf{p_1 = \cos 0 = 1} \\ \\ \mathbf{p_2 = \cos 90 = 0} \end{array}}$$

$\mathbf{p_1 = \cos 0 = 1}$ → **100% weight for PC1**

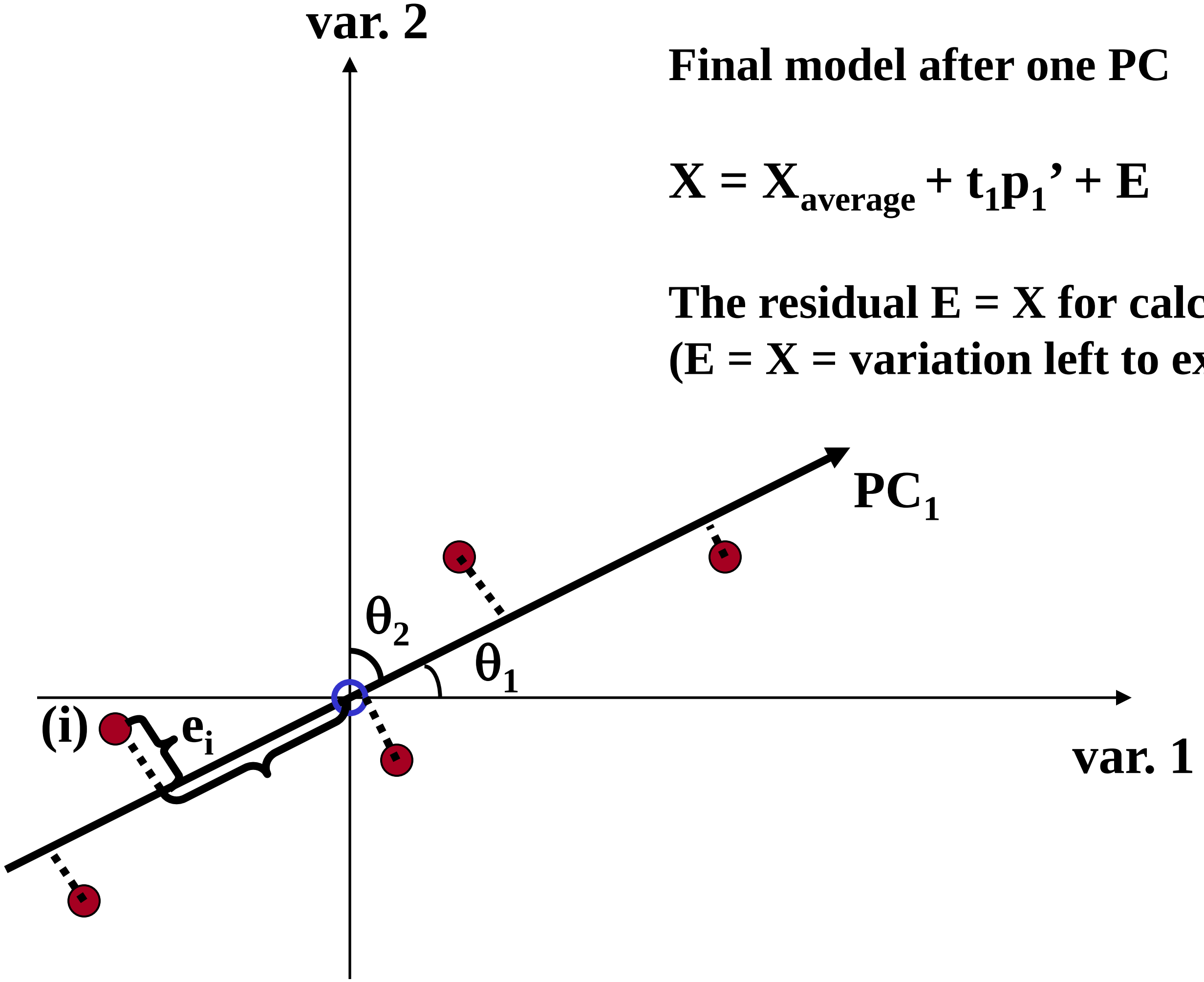
$\mathbf{p_2 = \cos 90 = 0}$ → **0% weight for PC1**

Projections

The residual (e_i) for an observation is described by the perpendicular (orthogonal) distance from the point to the PC, which is the same as the unexplained variation



Projections

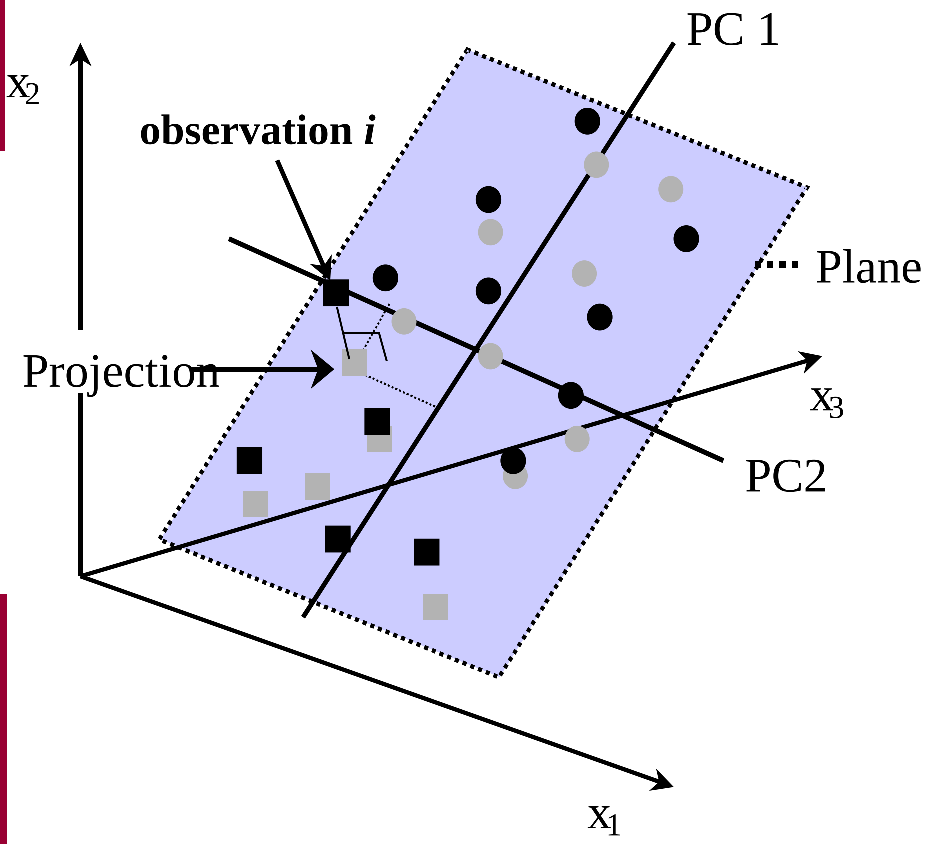


Final model after one PC

$\mathbf{X = X_{average} + t_1p_1' + E}$

The residual E = X for calculation of PC$_2$
(E = X = variation left to explain)

Projections



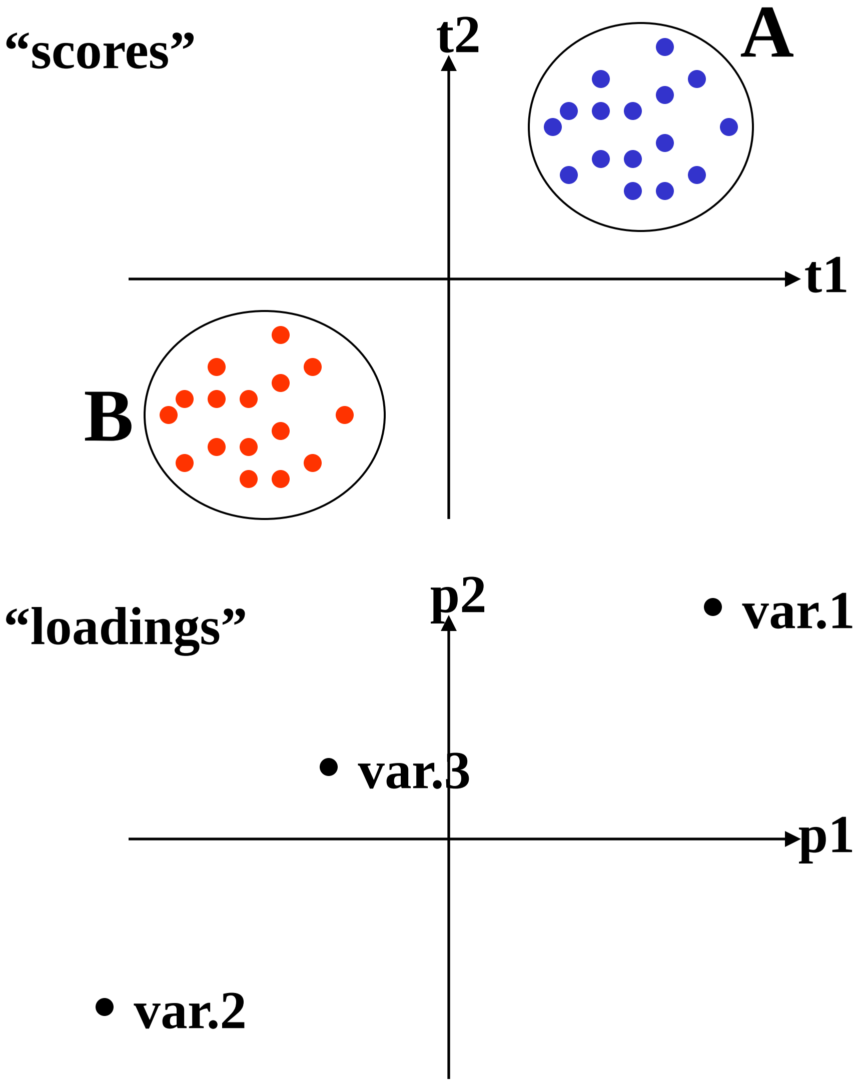
Two PC:s make up a plane (window) in the K-dimensional variable space.

If the points are projected down on the plane, it can be lifted out and be viewed as a two dimensional plot describing the objects relationships, a so called *score plot (t_1/t_2)*. In this plot similarities/dissimilarities between objects (samples) can be seen.

The corresponding *loading plot (p1/p2)* describes the variables relationships and is also a means for interpreting the score plot by telling which variables are responsible for similaritie/dissimilarities between objects.

Det perpendicular distance from the object to the Projection on the plane is the *residual (E)* or the variation not described by the two PC:s.

Projections



The Score plot t1/t2 shows two clearly separated classes of observations (A and B).

The Loading plot p1/p2 show the Three variables influence on the two principal components.

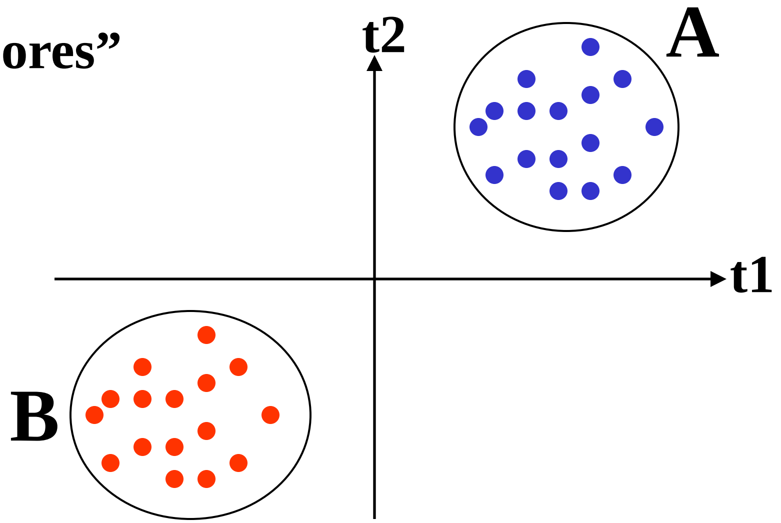
Questions!

1. What is causing the samples in class A to be similar to each other and the samples in class B to be similar to each other.

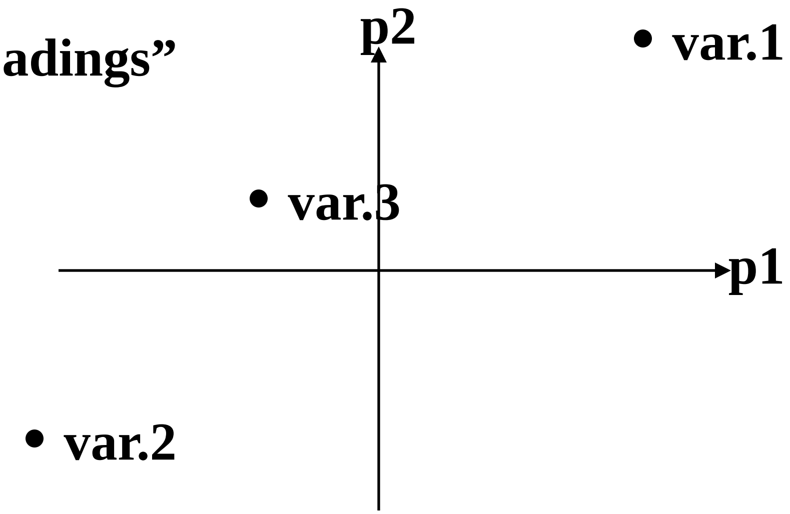
2. What is causing the samples in class A to be different from the samples in class B?

Projections

“scores”



“loadings”



<u>Answer Question 1</u>

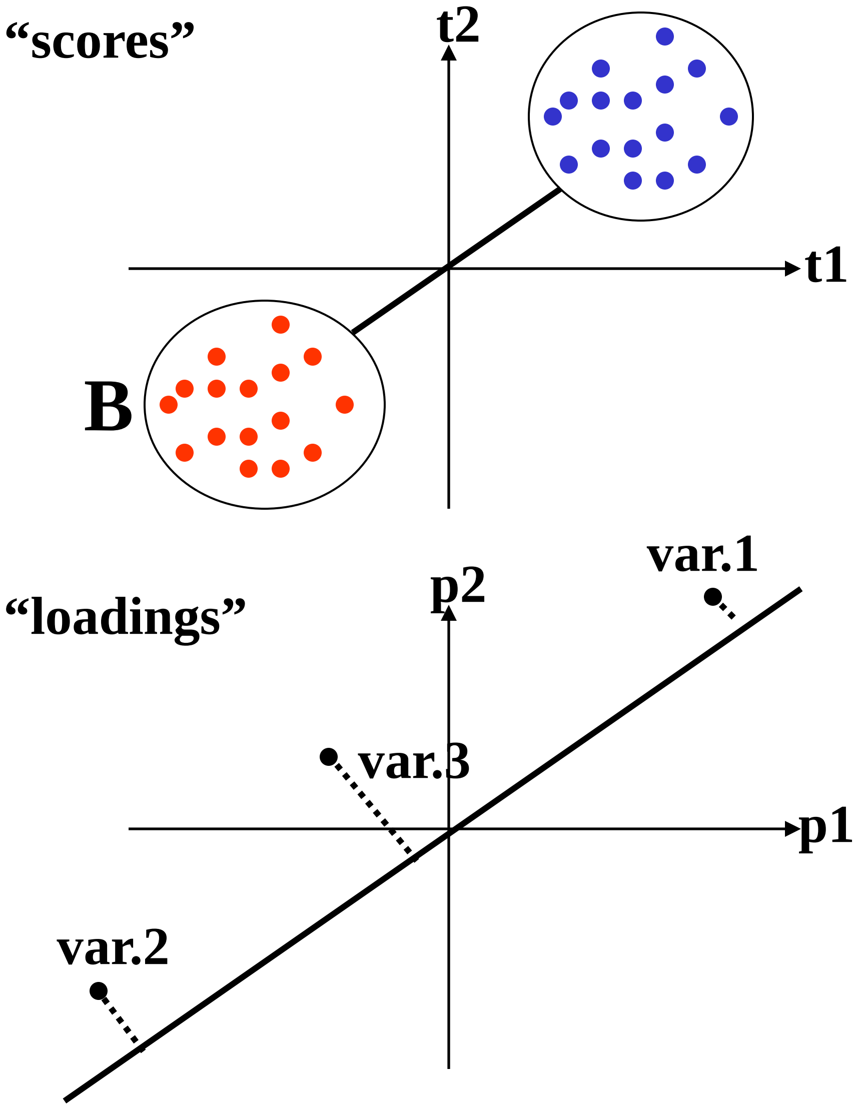
Overlay the plots!

- All samples in class A have got high values for var. 1 (positively correlated)

- All samples in class B have got high values for var. 2 (positively correlated)

- Var. 3 has got low loading values in both components (no influence)

Projections



Answer Question 2

Define the direction for the difference between A and B in both plots.

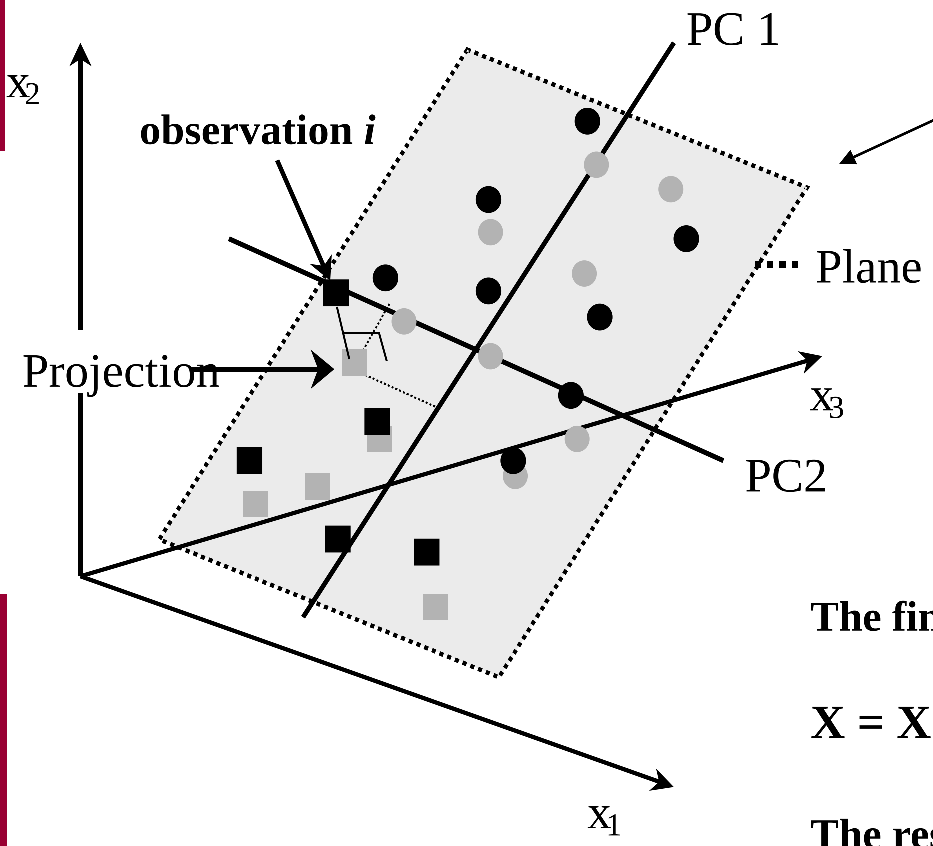
Project the variables onto the direction in the loading plot.

The distance from the projection on the line to the origin is equal to the individual variables weight for the variation in that direction i.e. for the difference between A and B.

-Var. 1 and Var. 2 are the variables that are most important for the separation between A and B. They are negatively correlated, which means that when one goes up the other one goes down. Class A has got high values for var. 1 in comparison with class B and vice versa.

- Var. 3 has got no significant influence on the separation in the identified direction.

Projections



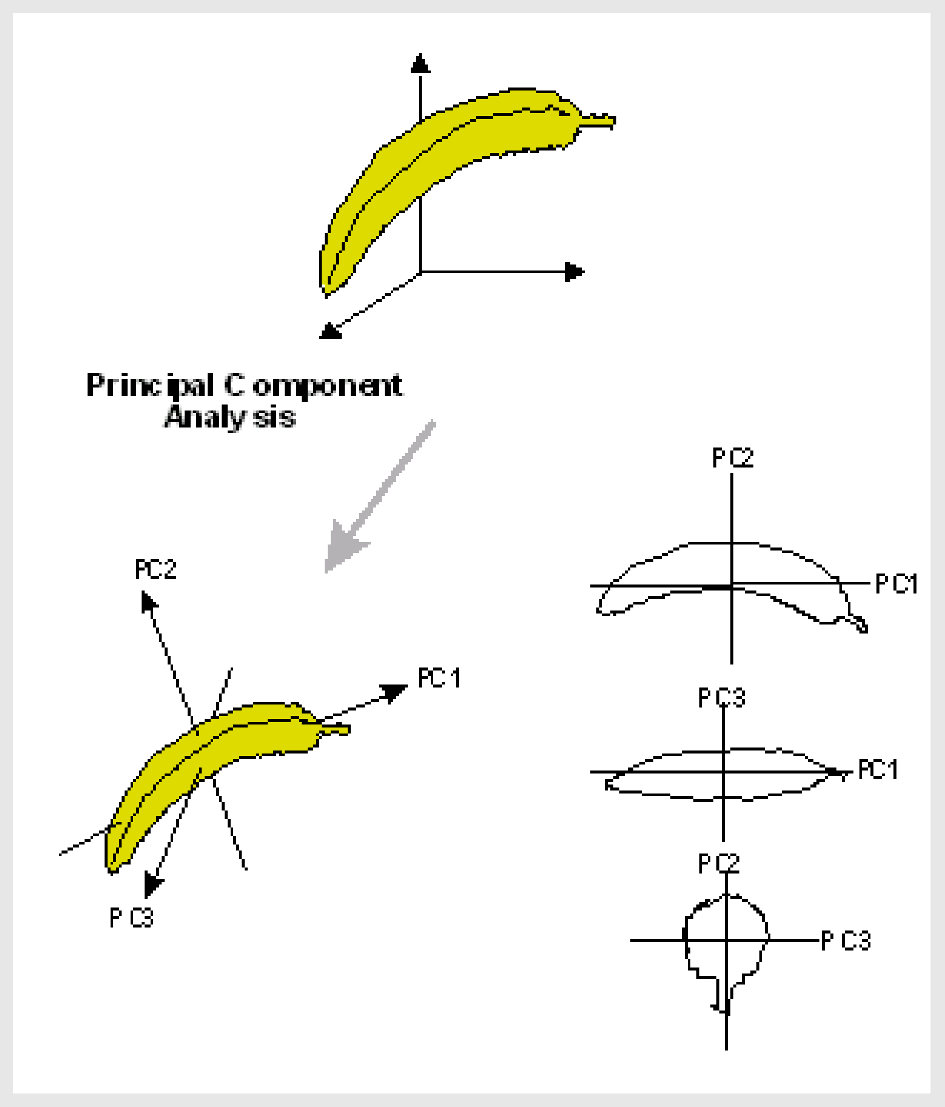
PC_1 mot PC_2 defines a plane in the 3-dimensional variable space.

The final model after two principal components

$$\mathbf{X = X_{average} + t_1p_1' + t_2p_2' + E}$$

The residual E = X for calculation of PC_3
(E = X = variation left to describe)

PCA (Principal Component Analysis)

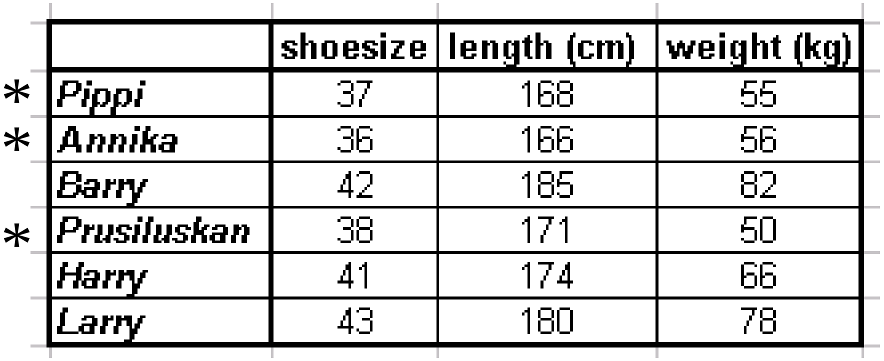


Example, PCA (3 variables)

Six people (three women and three men) described by three variables (shoe size, length, weight)

* **women**

X =

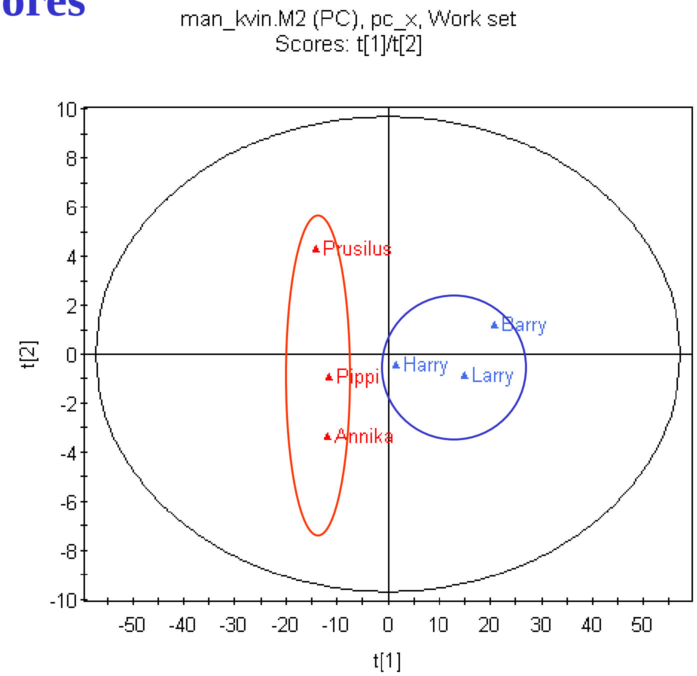


		shoesize	length (cm)	weight (kg)
*	*Pippi*	37	168	55
*	*Annika*	36	166	56
	Barry	42	185	82
*	*Prusiluskan*	38	171	50
	Harry	41	174	66
	Larry	43	180	78

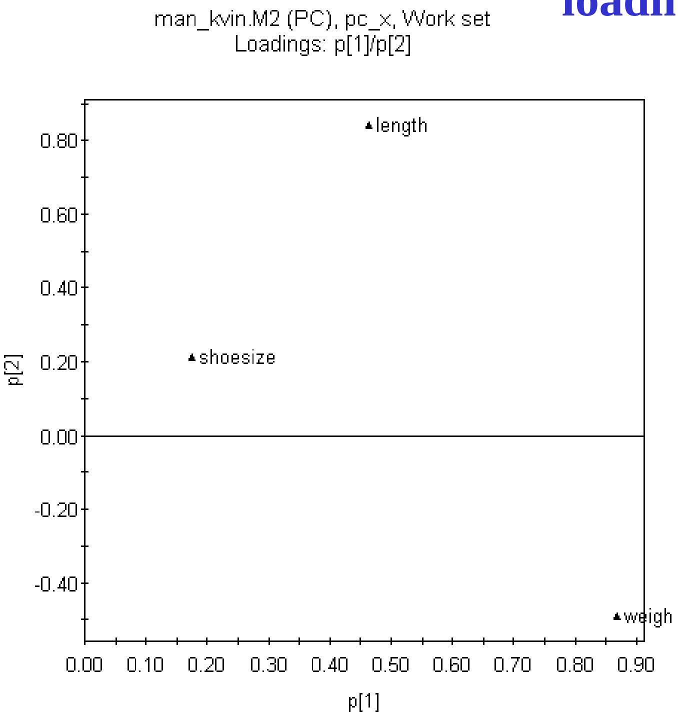
The values are presented in a data table X where each person defines an object and the three measures the variables.

Example, PCA (3 variables)

“scores”



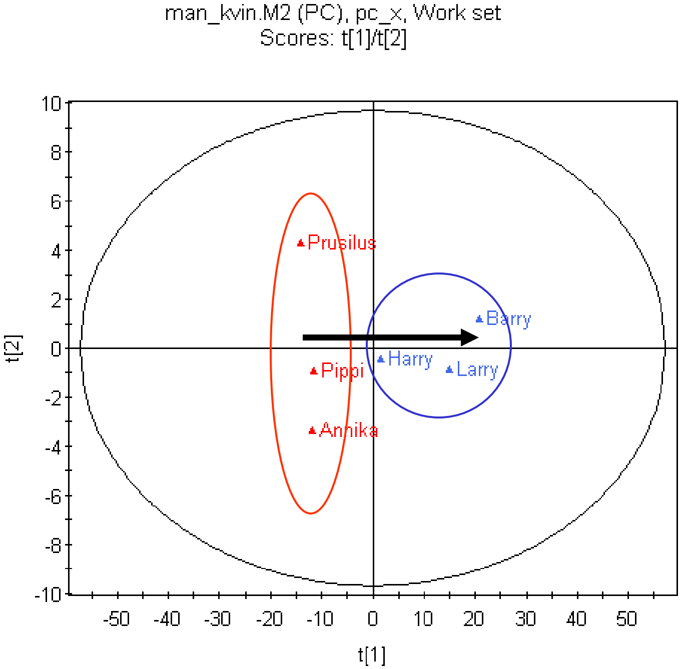
“loadings”

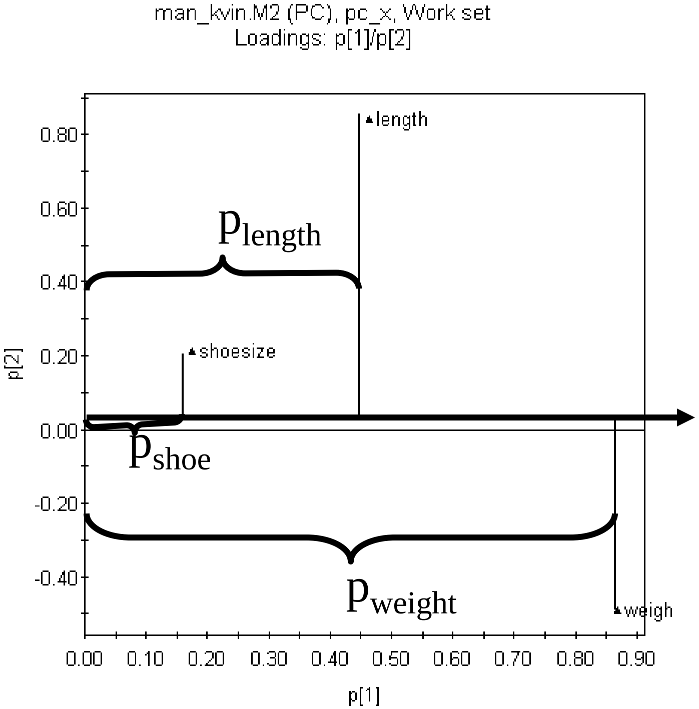


Scores (t1/t2) show that men and women are separated in the first PC

Loadings (p1/p2) shows the variable importance for the two PC:s

Example, PCA (3 variables)

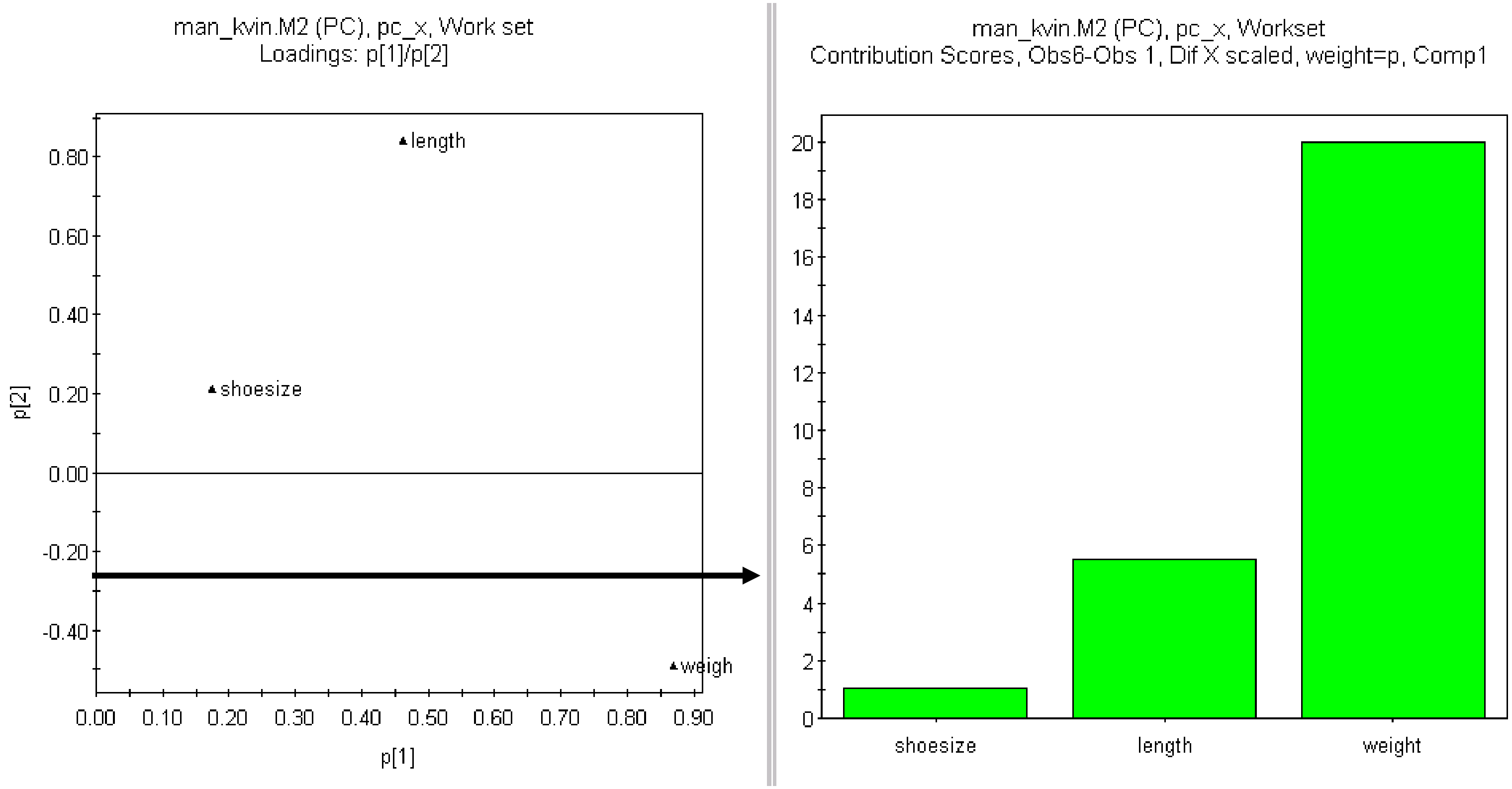




Interpretation of scores and loadings together tell us that the difference between men and women, in this case, is that the men are heavier, are longer and also have bigger feet.
The variable importance (weight) for the separation in PC 1 can be viewed in the loading plot.

Variable weights for the separation in PC 1: weight > length > shoe size

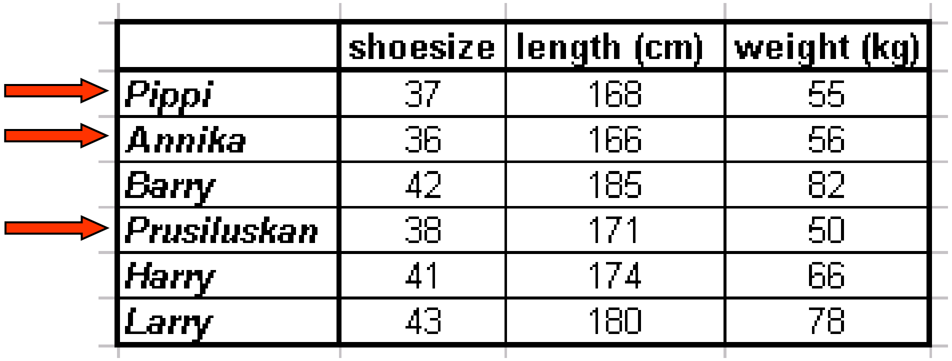
Example, PCA (3 variables)



A comparison of visual interpretation of scores and loadings to "Contribution plot" in SIMCA shows that the same result is yielded.

Example, PCA (3 variables)

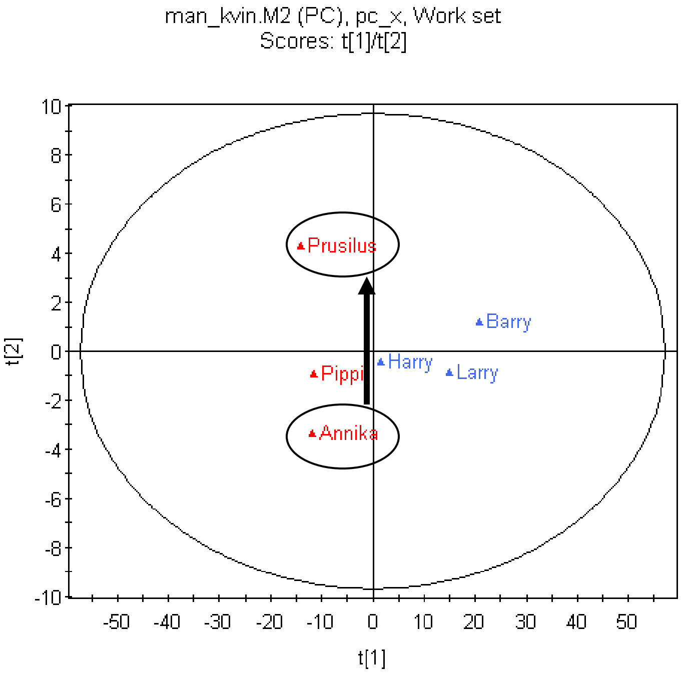
Interpretation of the data table show that the conclusions drawn based on the model seem to picture the reality quite well

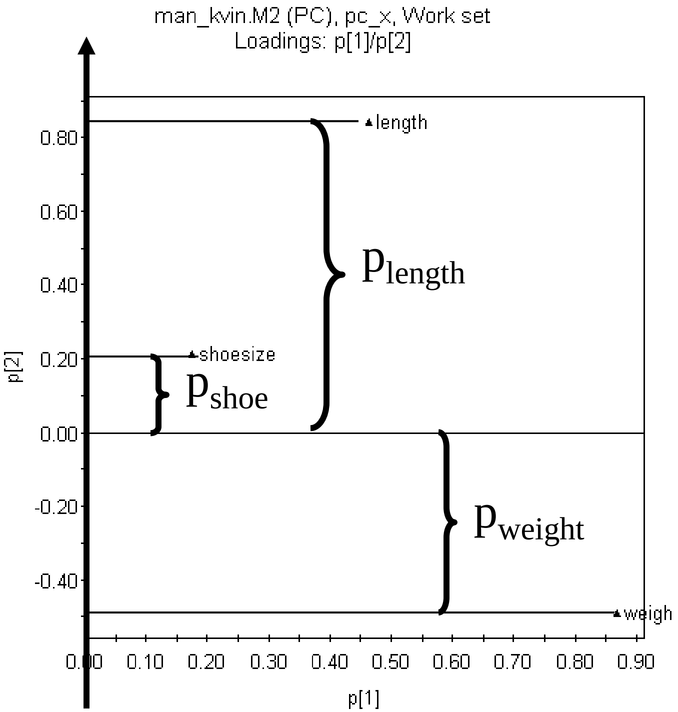


	shoesize	length (cm)	weight (kg)
Pippi	37	168	55
Annika	36	166	56
Barry	42	185	82
Prusiluskan	38	171	50
Harry	41	174	66
Larry	43	180	78

PCA has reduced the problem from three dimensions down to two dimensions without loosing any important information about the variation in the data.

Example, PCA (3 variables)

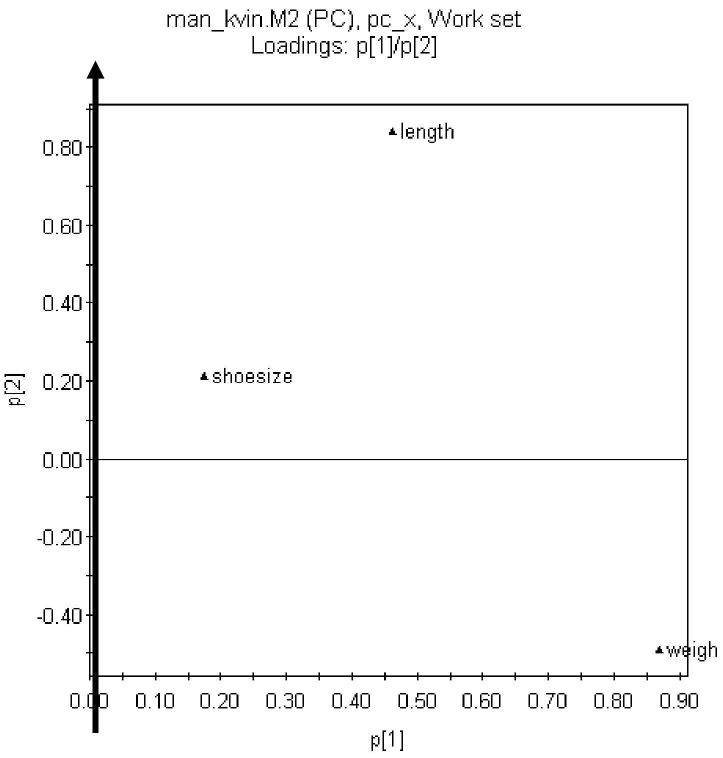


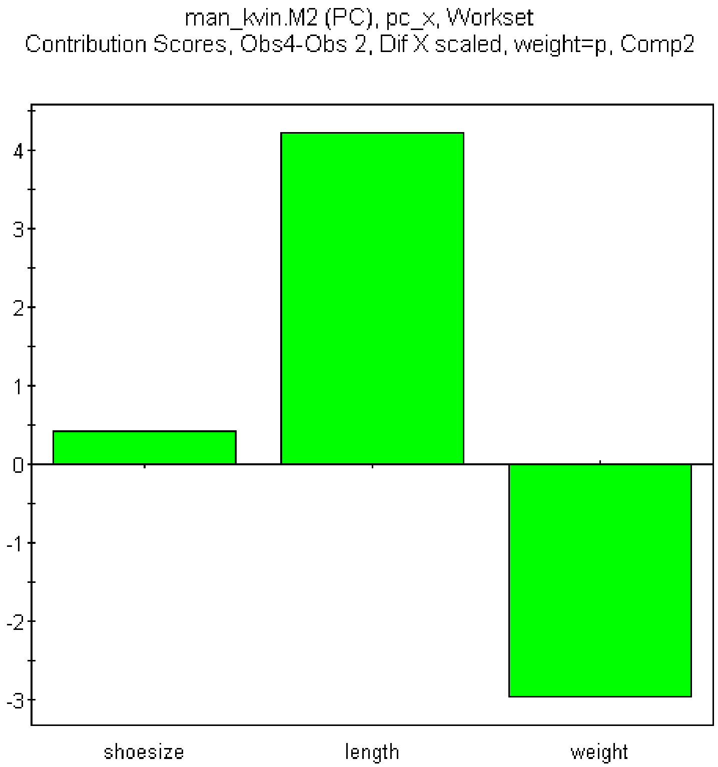


Now we are interested in the difference within the group of women since it seems like there is a fairly large difference between Prusiluskan and Annika described by PC 2.

Interpretation of scores and loadings show that the difference is due to that Prusiluskan is longer, weighs less and has got bigger feet than Annika.

Example, PCA (3 variables)

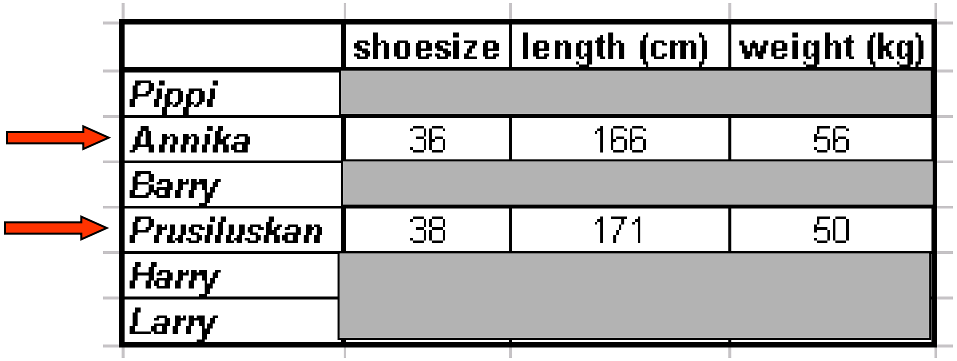




A comparison of visual interpretation of scores and loadings to "Contribution plot" in SIMCA shows that the same result is yielded.

Example, PCA (3 variables)

Interpretation of the data table show that the conclusions drawn based on the model seem to picture the reality quite well



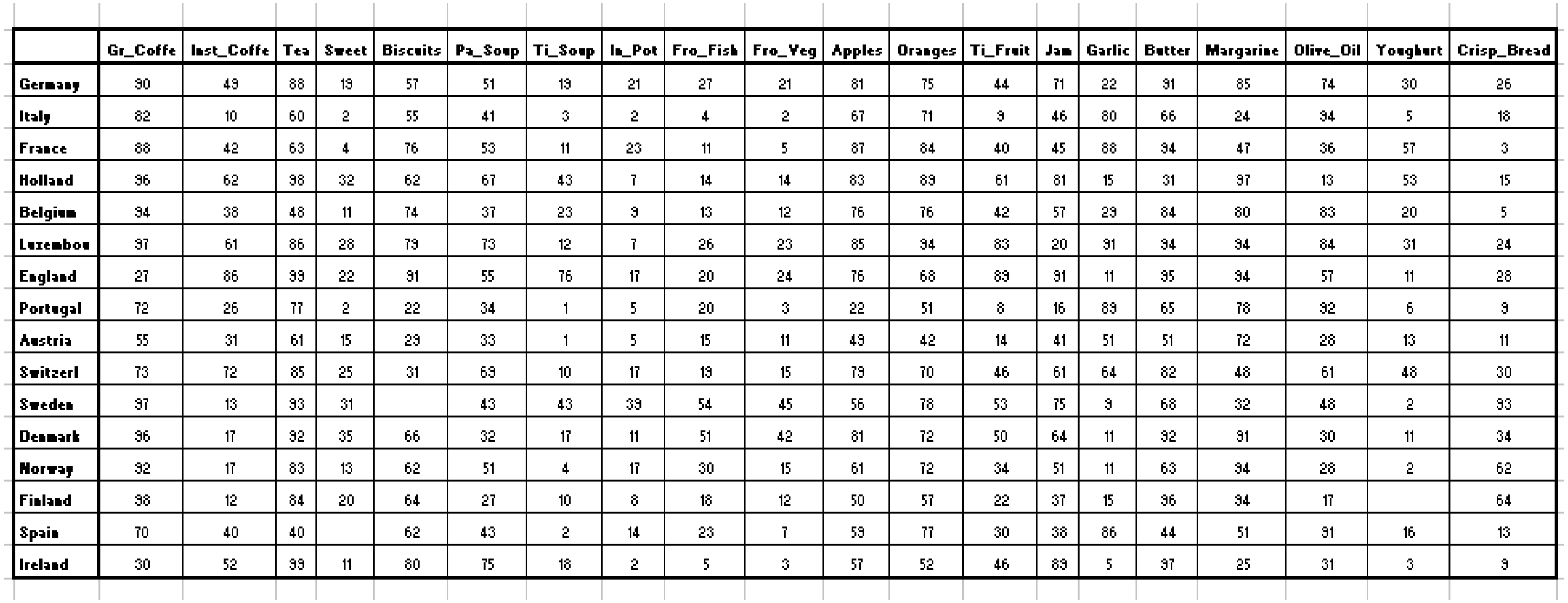
	shoesize	length (cm)	weight (kg)
Pippi			
Annika	36	166	56
Barry			
Prusiluskan	38	171	50
Harry			
Larry			

PCA has reduced the problem from three dimensions down to two dimensions without loosing any important information about the variation in the data.

Example, PCA (many variables)

The data table X is a summary of the consumption of 20 different food stuffs in 16 European countries

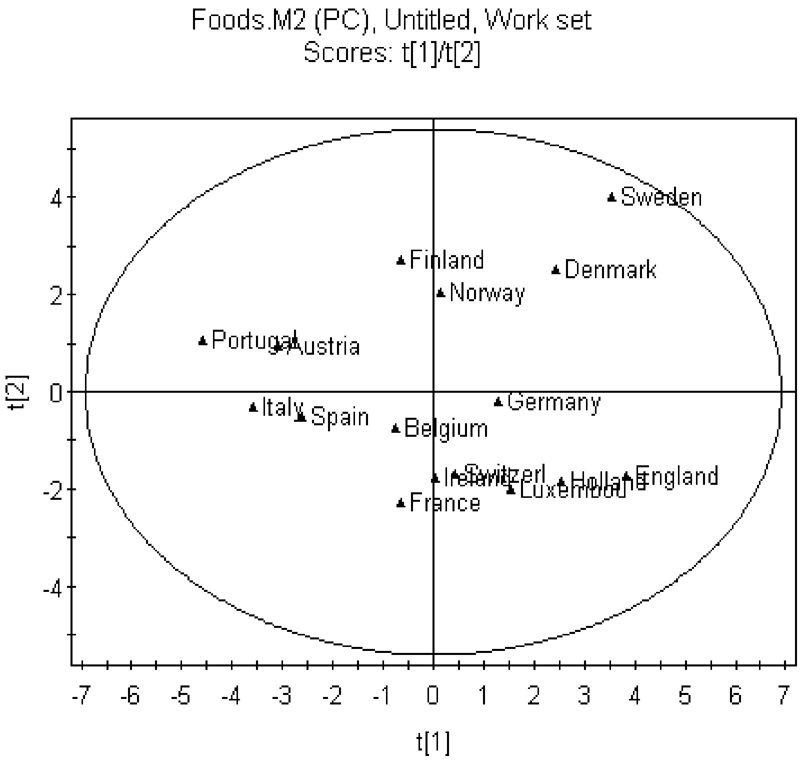
Difficult to see differences/similarities when variables become many!



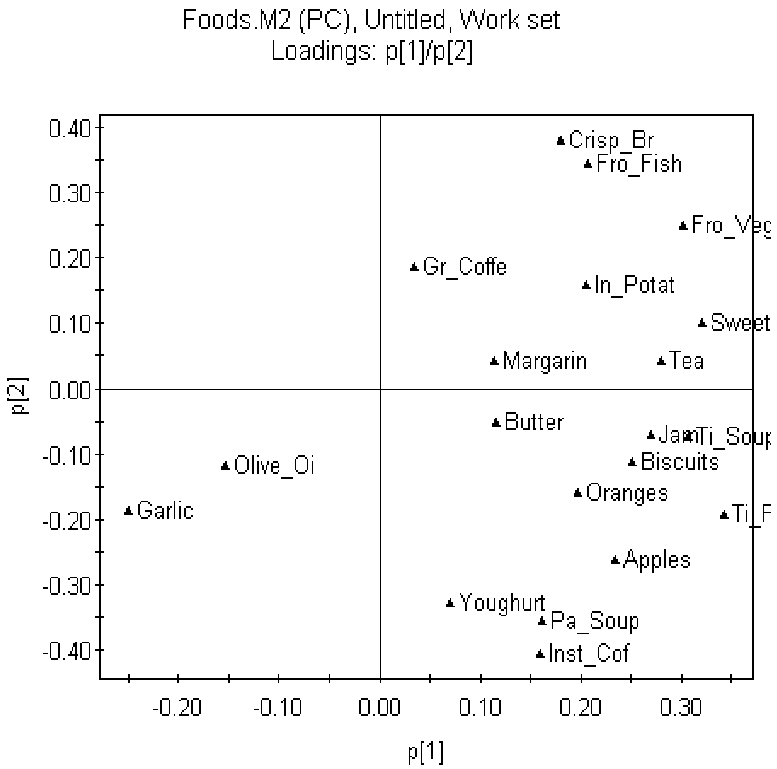
	Gr_Coffe	Inst_Coffe	Tea	Sweet	Biscuits	Pa_Soup	Ti_Soup	In_Pot	Fro_Fish	Fro_Veg	Apples	Oranges	Ti_Fruit	Jam	Garlic	Butter	Margarine	Olive_Oil	Youghurt	Crisp_Bread
Germany	90	49	88	19	57	51	19	21	27	21	81	75	44	71	22	91	85	74	30	26
Italy	82	10	60	2	55	41	3	2	4	2	67	71	9	46	80	66	24	94	5	18
France	88	42	63	4	76	53	11	23	11	5	87	84	40	45	88	94	47	36	57	3
Holland	96	62	98	32	62	67	43	7	14	14	83	89	61	81	15	31	97	13	53	15
Belgium	94	38	48	11	74	37	23	9	13	12	76	76	42	57	29	84	80	83	20	5
Luxembou	97	61	86	28	79	73	12	7	26	23	85	94	83	20	91	94	94	84	31	24
England	27	86	99	22	91	55	76	17	20	24	76	68	89	91	11	95	94	57	11	28
Portugal	72	26	77	2	22	34	1	5	20	3	22	51	8	16	89	65	78	92	6	9
Austria	55	31	61	15	29	33	1	5	15	11	49	42	14	41	51	51	72	28	13	11
Switzerl	73	72	85	25	31	69	10	17	19	15	79	70	46	61	64	82	48	61	48	30
Sweden	97	13	93	31		43	43	39	54	45	56	78	53	75	9	68	32	48	2	93
Denmark	96	17	92	35	66	32	17	11	51	42	81	72	50	64	11	92	91	30	11	34
Norway	92	17	83	13	62	51	4	17	30	15	61	72	34	51	11	63	94	28	2	62
Finland	98	12	84	20	64	27	10	8	18	12	50	57	22	37	15	96	94	17		64
Spain	70	40	40		62	43	2	14	23	7	59	77	30	38	86	44	51	91	16	13
Ireland	30	52	99	11	80	75	18	2	5	3	57	52	46	89	5	97	25	31	3	9

Example, PCA (many variables)

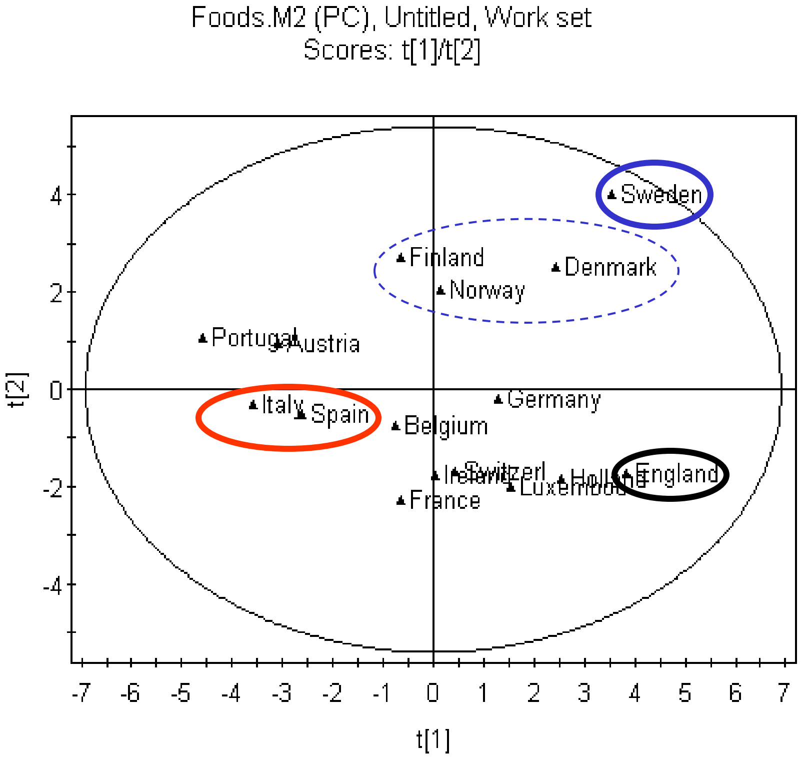
“scores”

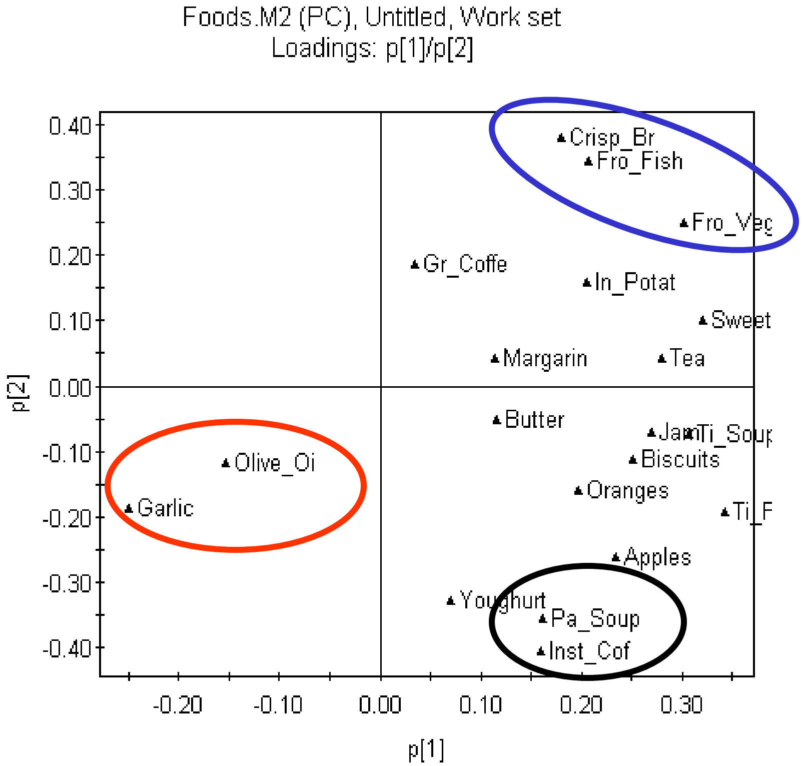


“loadings”



Example, PCA (many variables)

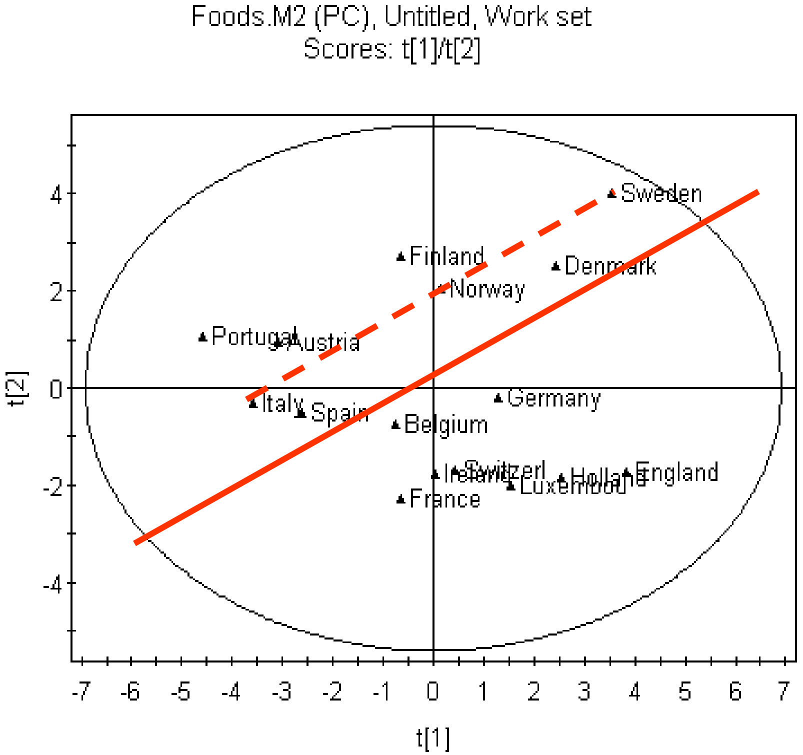


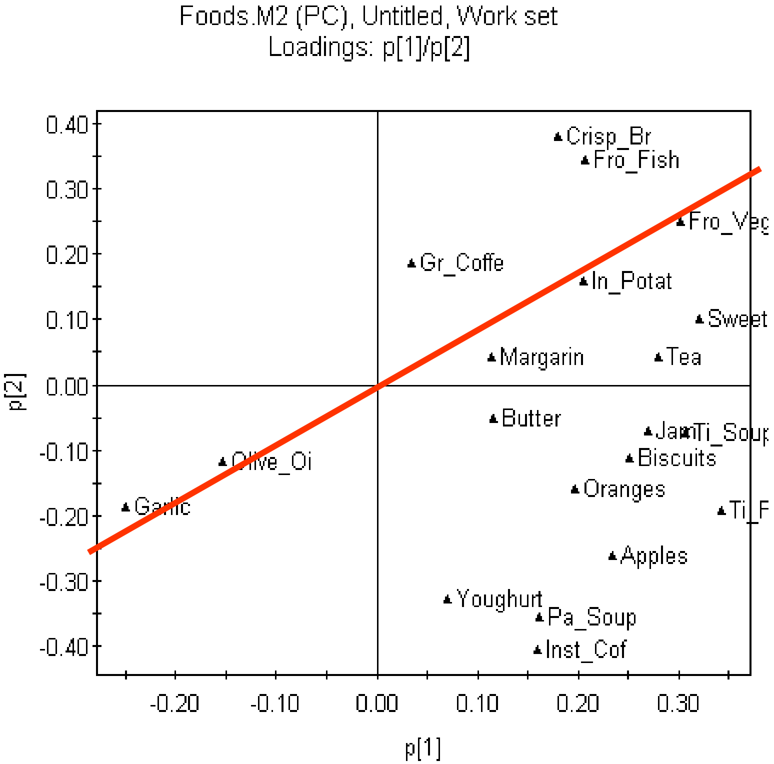


Characteristic food stuffs for different regions in Europe can be identified by interpreting scores and loadings together. ***E.g. The nordic countries including Sweden consume high amounts of crisp bread (knäckebröd), frozen fish (fiskpinnar) and frozen vegetables.***

Example, PCA (many variables)

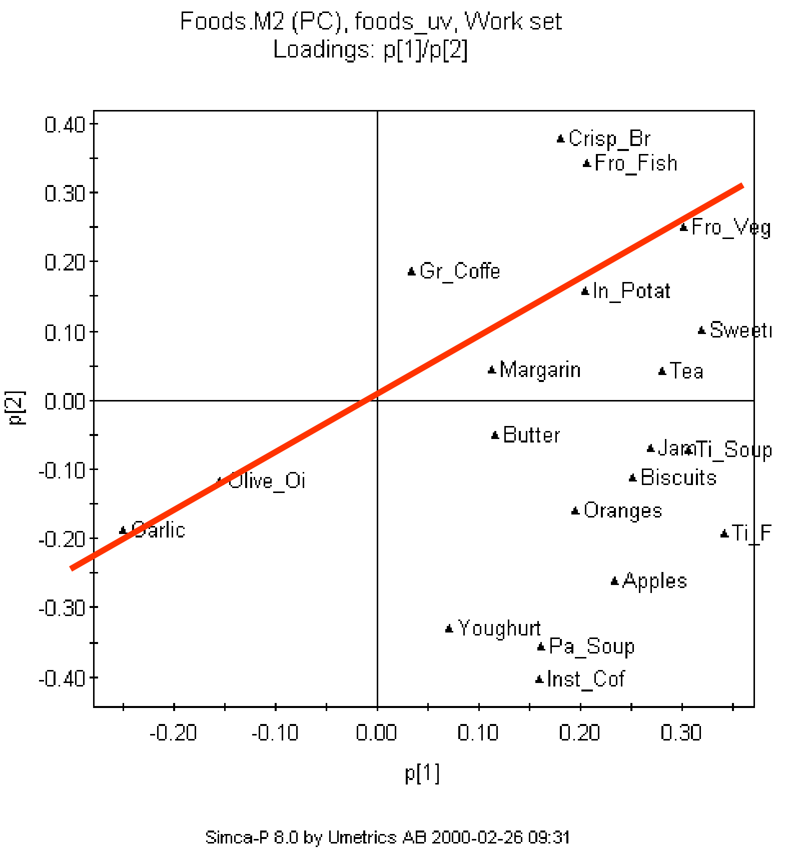
Difference between Sweden and Italy?

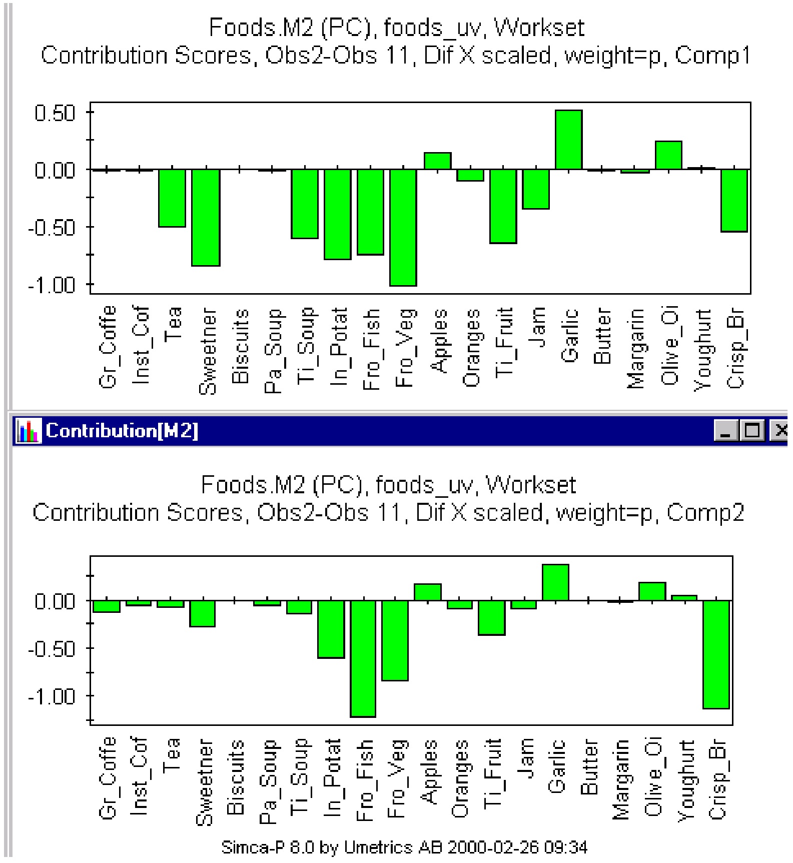

Foods.M2 (PC), Untitled, Work set
Scores: t[1]/t[2]


Foods.M2 (PC), Untitled, Work set
Loadings: p[1]/p[2]

Define the direction for the separation between Sweden and Italy in scores and transfer it to the loadings. Interpretation can now be carried out by projecting the variables onto the line and measure the distance to the origin, which is equal to the variables weight for the explaining the variation along that direction .

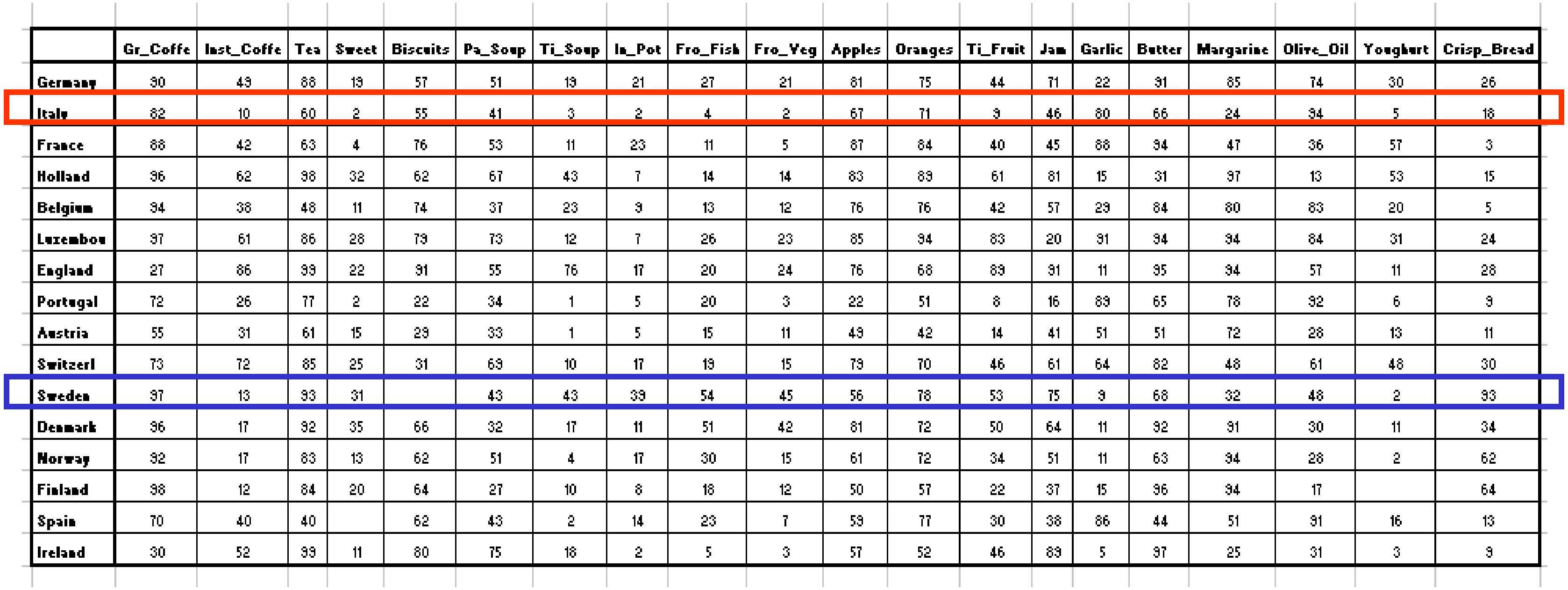
Example, PCA (many variables)





Example, PCA (many variables)

Viewing the data table reveals that the interpretations based on the model seem to match the true results in the data!



	Gr_Coffe	Inst_Coffe	Tea	Sweet	Biscuits	Pa_Soup	Ti_Soup	In_Pot	Fro_Fish	Fro_Veg	Apples	Oranges	Ti_Fruit	Jam	Garlic	Butter	Margarine	Olive_Oil	Youghurt	Crisp_Bread
Germany	90	49	88	19	57	51	19	21	27	21	81	75	44	71	22	91	85	74	30	26
Italy	82	10	60	2	55	41	3	2	4	2	67	71	9	46	80	66	24	94	5	18
France	88	42	63	4	76	53	11	23	11	5	87	84	40	45	88	94	47	36	57	3
Holland	96	62	98	32	62	67	43	7	14	14	83	89	61	81	15	31	97	13	53	15
Belgium	94	38	48	11	74	37	23	9	13	12	76	76	42	57	29	84	80	83	20	5
Luxembou	97	61	86	28	79	73	12	7	26	23	85	94	83	20	91	94	94	84	31	24
England	27	86	99	22	91	55	76	17	20	24	76	68	89	91	11	95	94	57	11	28
Portugal	72	26	77	2	22	34	1	5	20	3	22	51	8	16	89	65	78	92	6	9
Austria	55	31	61	15	29	33	1	5	15	11	49	42	14	41	51	51	72	28	13	11
Switzerl	73	72	85	25	31	69	10	17	19	15	79	70	46	61	64	82	48	61	48	30
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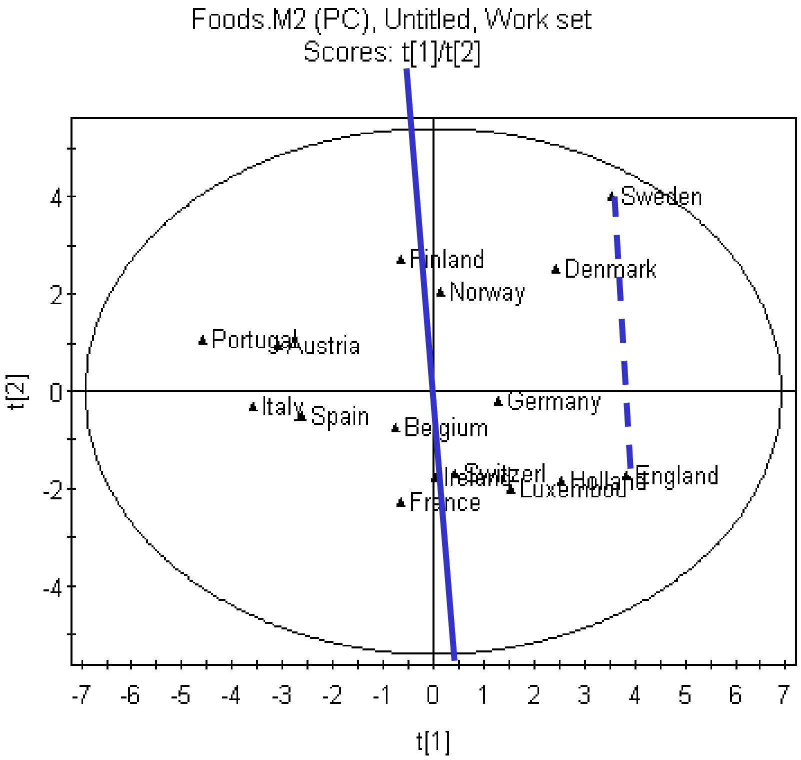
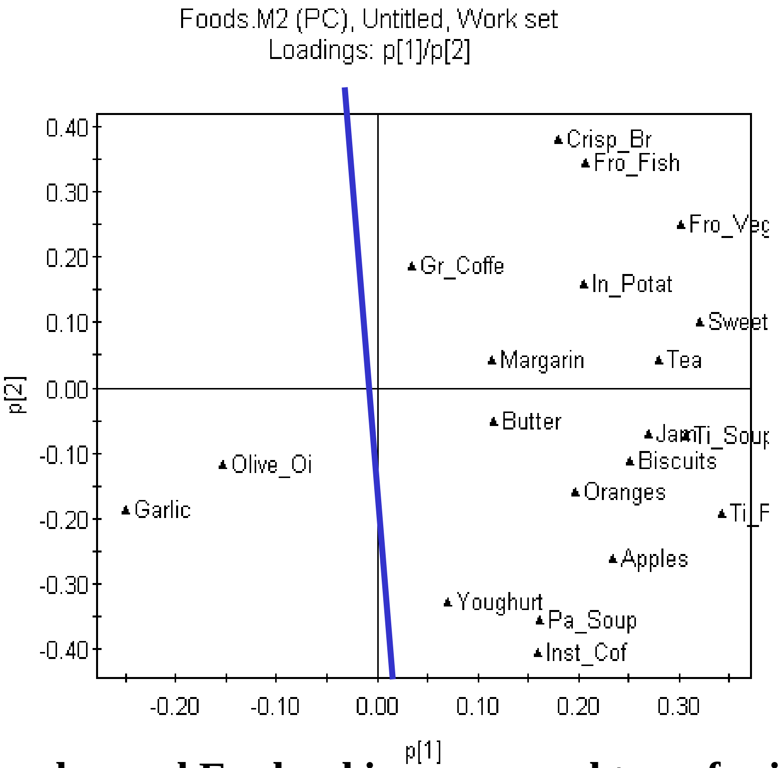
Finland	98	12	84	20	64	27	10	8	18	12	50	57	22	37	15	96	94	17		64
Spain	70	40	40		62	43	2	14	23	7	59	77	30	38	86	44	51	91	16	13
Ireland	30	52	99	11	80	75	18	2	5	3	57	52	46	89	5	97	25	31	3	9

Projection (PCA) has reduced the problem from 20 dimensions to 2 dimensions without loosing information about the important variation in the data. By using adequate plots and diagrams we can instead clarify the interpretation of the multivariate data table .

Example, PCA (many variables)

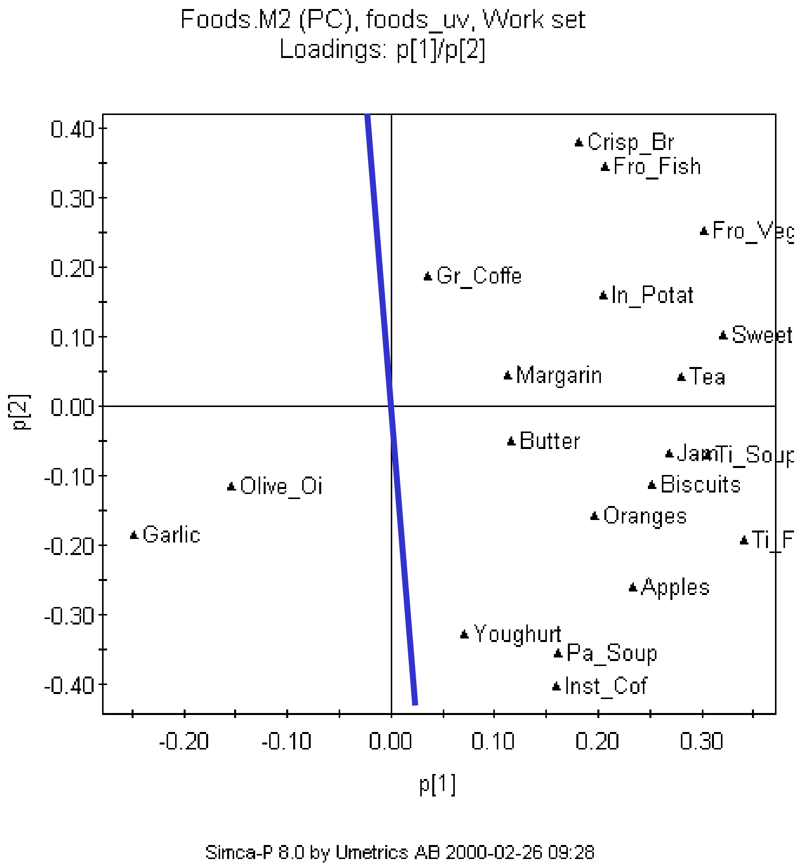
Difference between Sweden and England?





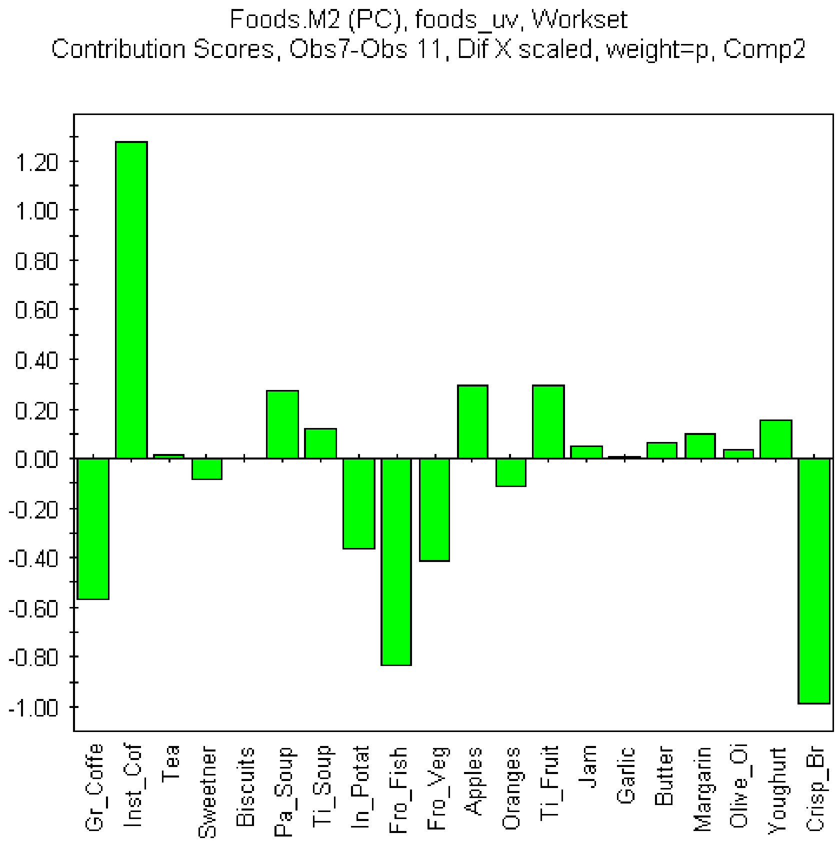
Define the direction for the separation between Sweden and England in scores and transfer it to the loadings. Interpretation can now be carried out by projecting the variables onto the line and measure the distance to the origin, which is equal to the variables weight for the explaining the variation along that direction .

Example, PCA (many variables)



Foods.M2 (PC), foods_uv, Work set
Loadings: p[1]/p[2]

Simca-P 8.0 by Umetrics AB 2000-02-26 09:28



Foods.M2 (PC), foods_uv, Workset
Contribution Scores, Obs7-Obs 11, Dif X scaled, weight=p, Comp2

Example, PCA (many variables)

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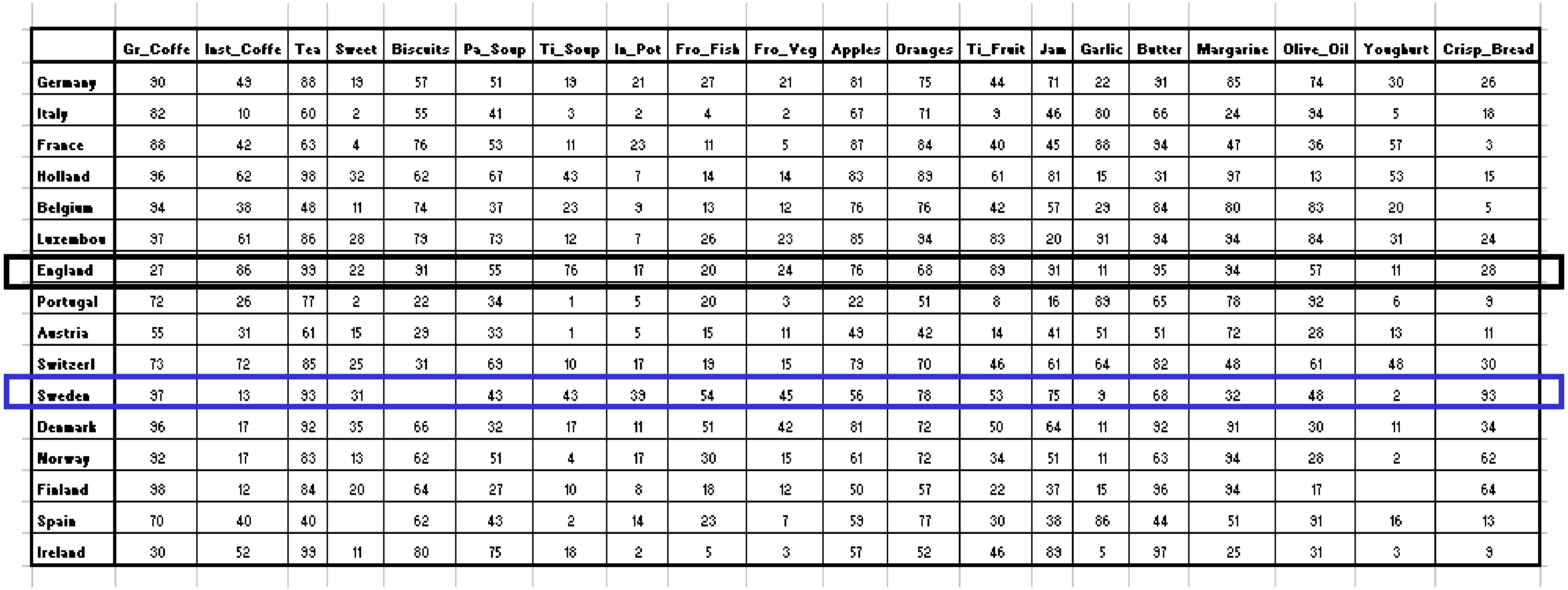

	Gr_Coffe	Inst_Coffe	Tea	Sweet	Biscuits	Pa_Soup	Ti_Soup	In_Pot	Fro_Fish	Fro_Veg	Apples	Oranges	Ti_Fruit	Jam	Garlic	Butter	Margarine	Olive_Oil	Youghurt	Crisp_Bread
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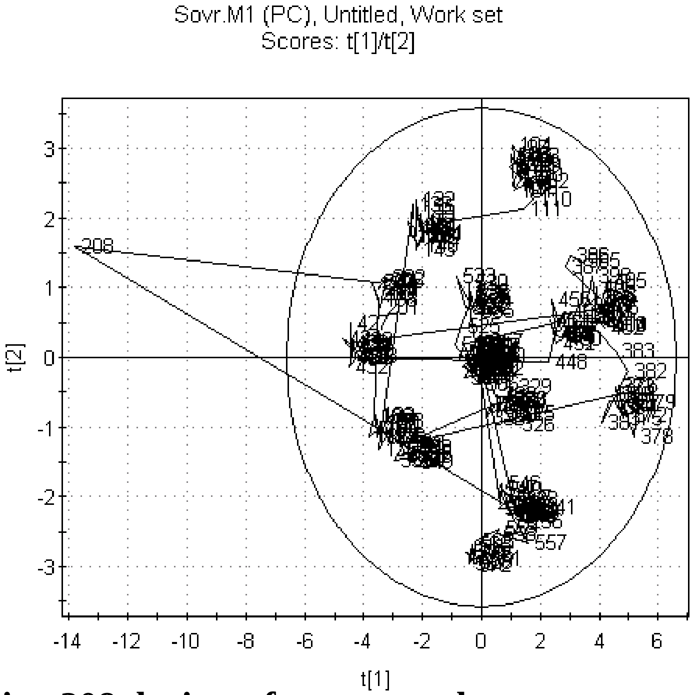
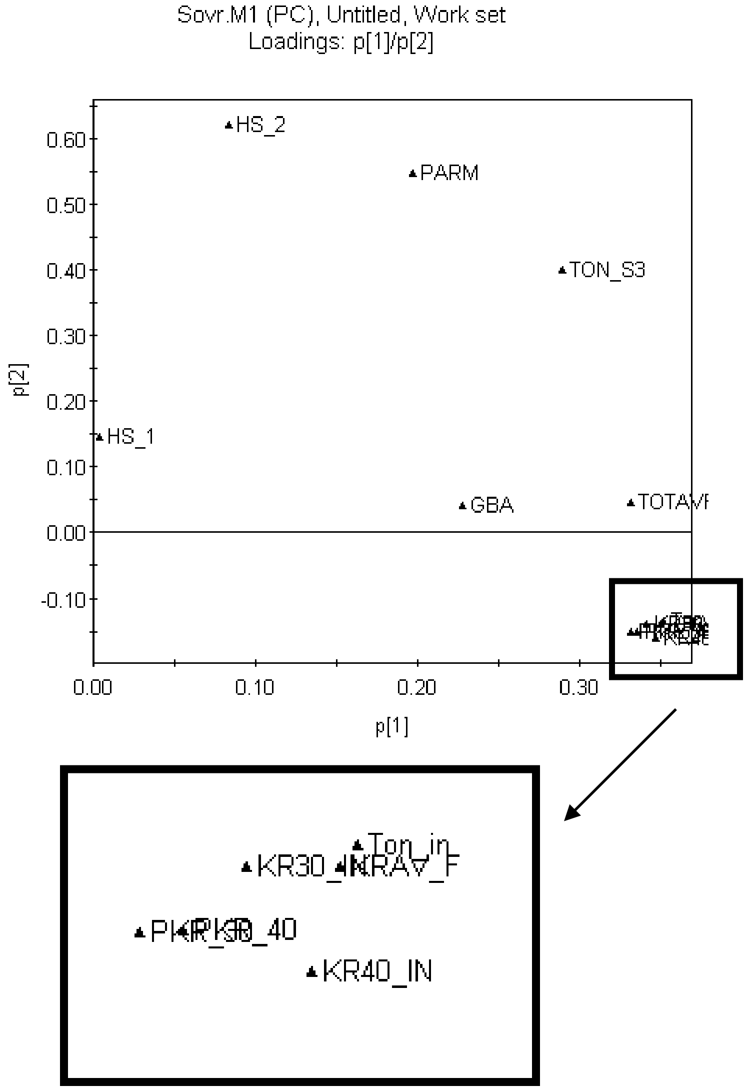
Holland	96	62	98	32	62	67	43	7	14	14	83	89	61	81	15	31	97	13	53	15
Belgium	94	38	48	11	74	37	23	9	13	12	76	76	42	57	29	84	80	83	20	5
Luxembou	97	61	86	28	79	73	12	7	26	23	85	94	83	20	91	94	94	84	31	24
England	27	86	99	22	91	55	76	17	20	24	76	68	89	91	11	95	94	57	11	28
Portugal	72	26	77	2	22	34	1	5	20	3	22	51	8	16	89	65	78	92	6	9
Austria	55	31	61	15	29	33	1	5	15	11	49	42	14	41	51	51	72	28	13	11
Switzerl	73	72	85	25	31	69	10	17	19	15	79	70	46	61	64	82	48	61	48	30
Sweden	97	13	93	31		43	43	39	54	45	56	78	53	75	9	68	32	48	2	93
Denmark	96	17	92	35	66	32	17	11	51	42	81	72	50	64	11	92	91	30	11	34
Norway	92	17	83	13	62	51	4	17	30	15	61	72	34	51	11	63	94	28	2	62
Finland	98	12	84	20	64	27	10	8	18	12	50	57	22	37	15	96	94	17		64
Spain	70	40	40		62	43	2	14	23	7	59	77	30	38	86	44	51	91	16	13
Ireland	30	52	99	11	80	75	18	2	5	3	57	52	46	89	5	97	25	31	3	9

Projection (PCA) has reduced the problem from 20 dimensions to 2 dimensions without loosing information about the important variation in the data. By using adequate plots and diagrams we can instead clarify the interpretation of the multivariate data table .

Example, PCA (process)



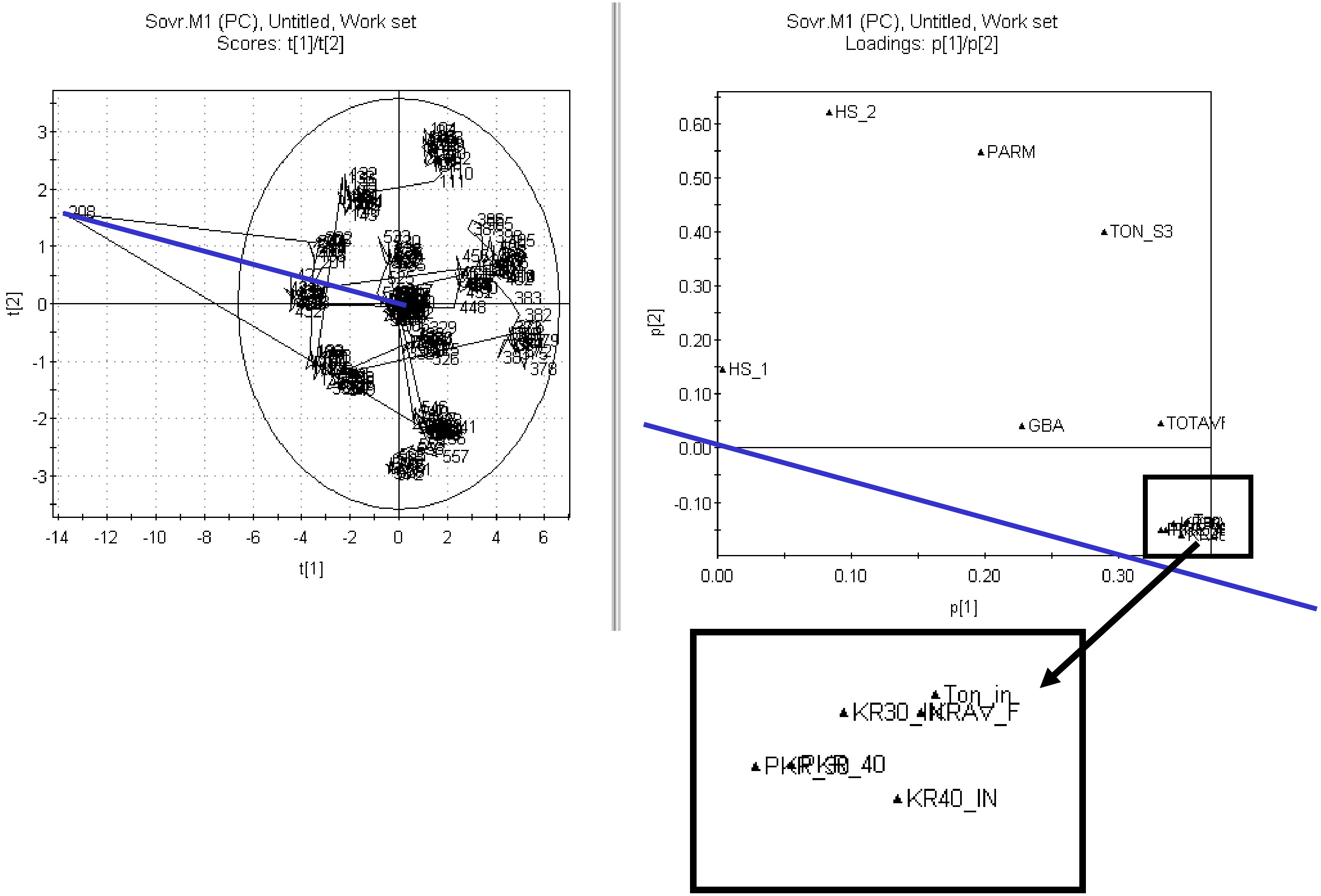


Observation 208 deviates from normal process behaviour.

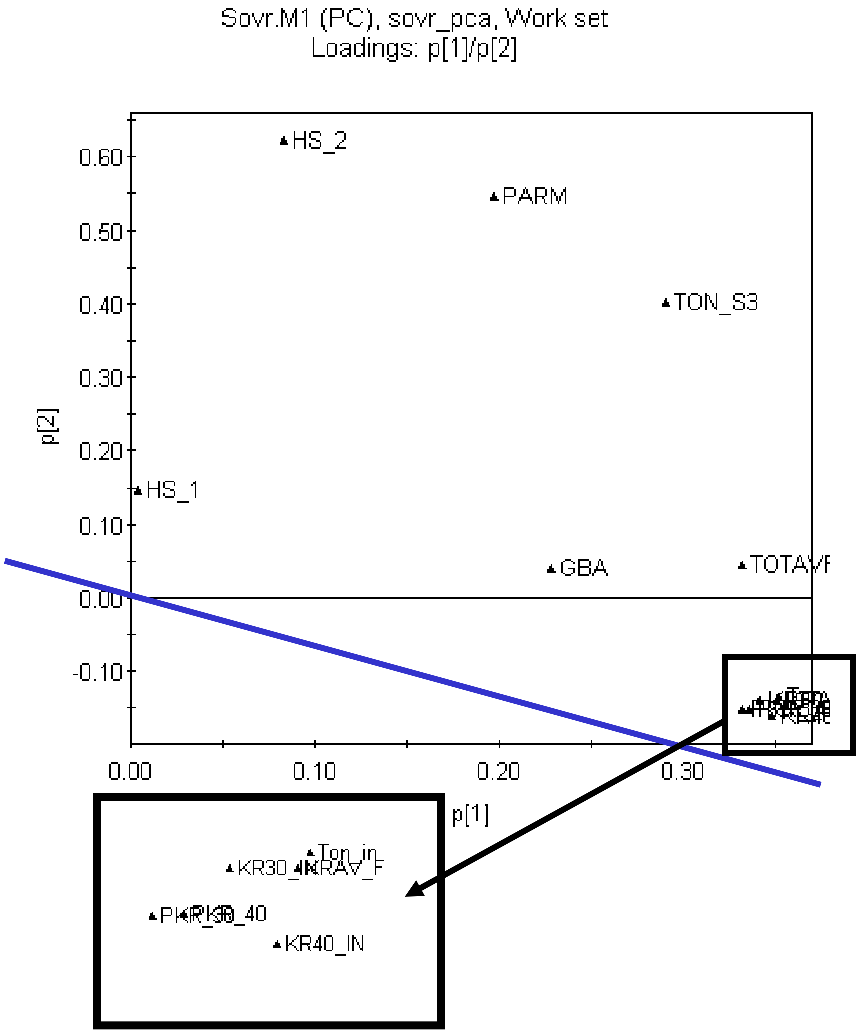
Scores give an indication that something is wrong. Scores as a multivariate control chart of the process provides the possibility for early fault detection.

By interpreting scores and loadings together an explanation can be found on which corrections can be based!

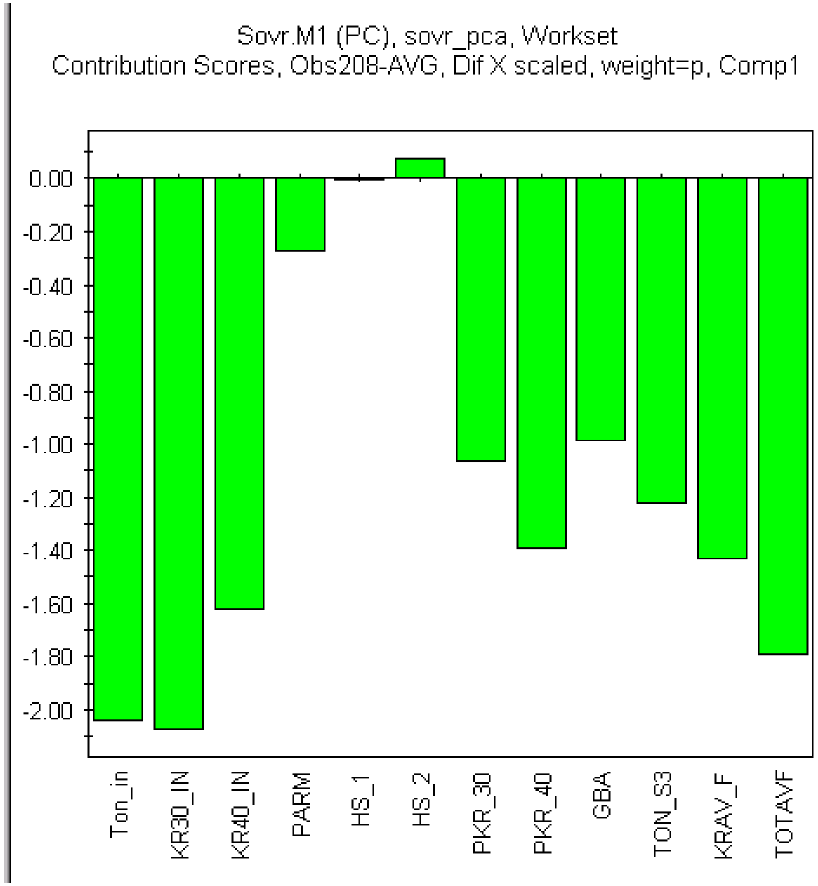
Example, PCA (process)



Example, PCA (process)

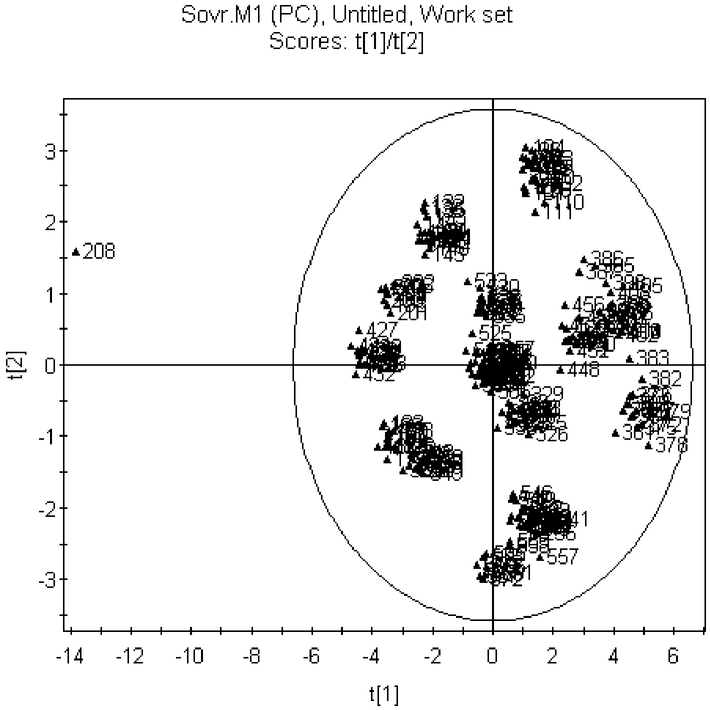


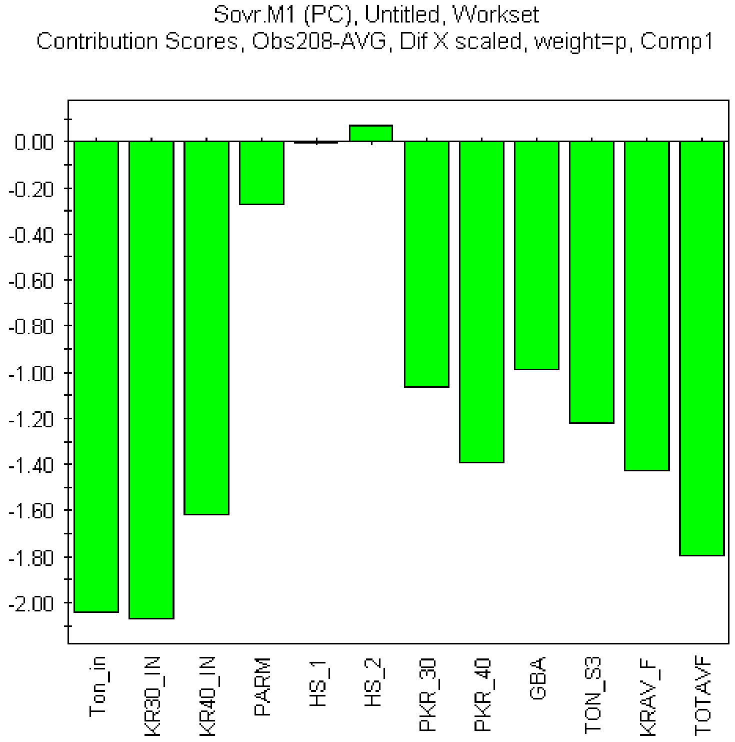
Sovr.M1 (PC), sovr_pca, Work set
Loadings: p[1]/p[2]



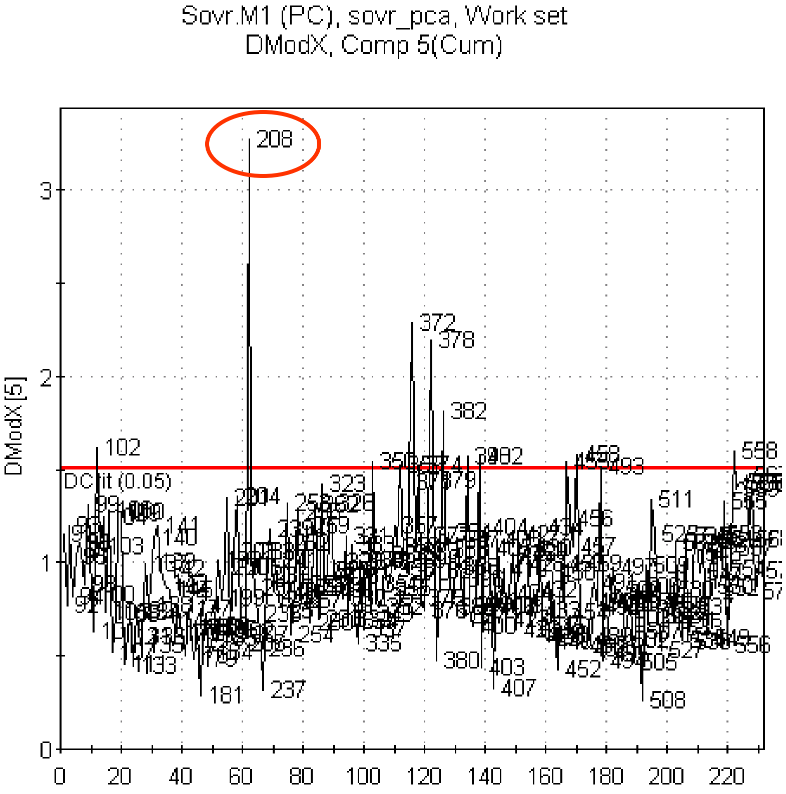
Sovr.M1 (PC), sovr_pca, Workset
Contribution Scores, Obs208-AVG, Dif X scaled, weight=p, Comp1

Example, PCA (process)





Example, PCA (process), DModX

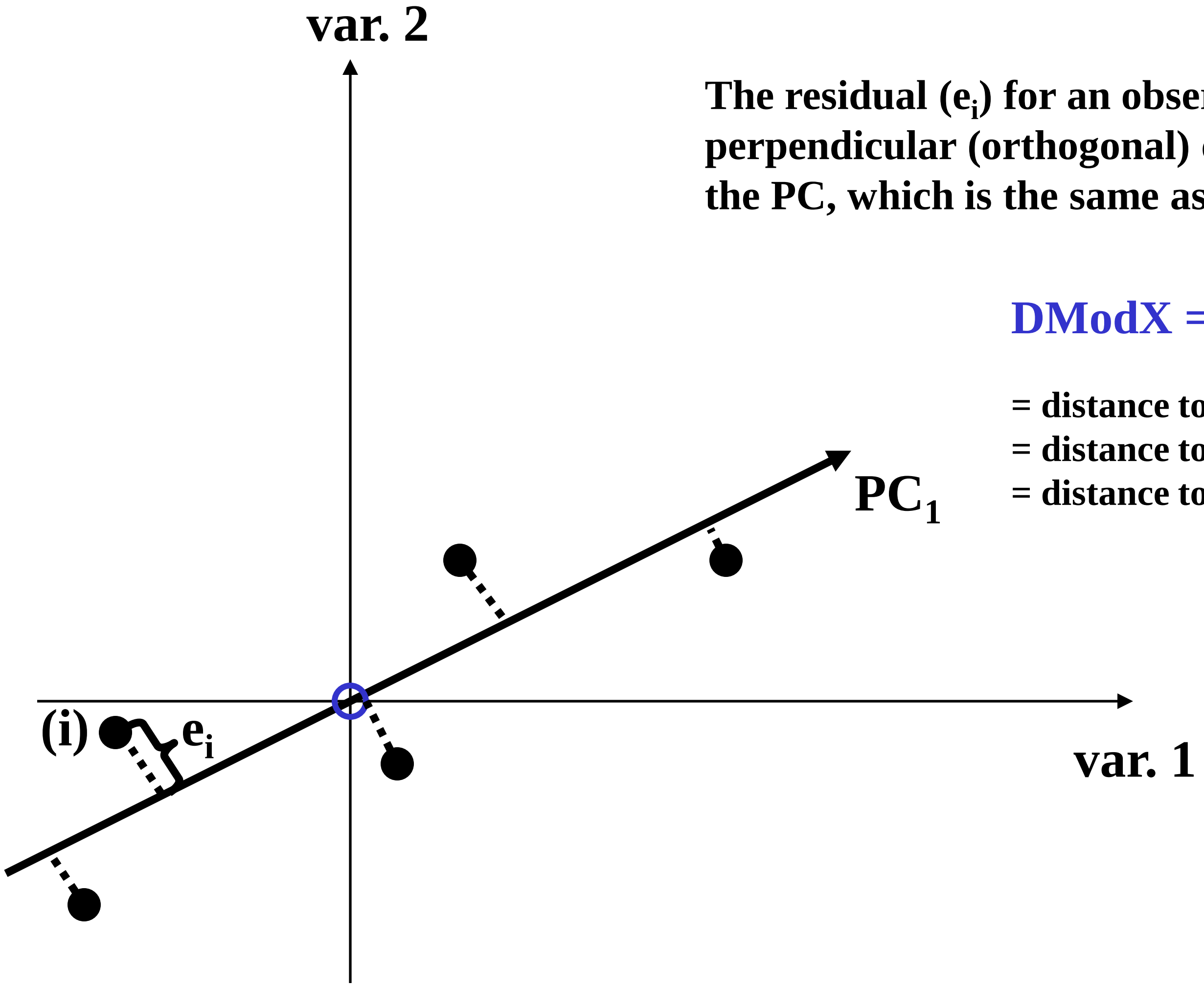


Outliers can also be found in DModX

DModX = Distance to Model in X (residual)

If the distance to the model for one observation is to large i.e. the residual for the observation is abnormally large, then the observation is considered to be an "outlier"
(belongs to another class of observations).

DModX (Distance to Model in X)



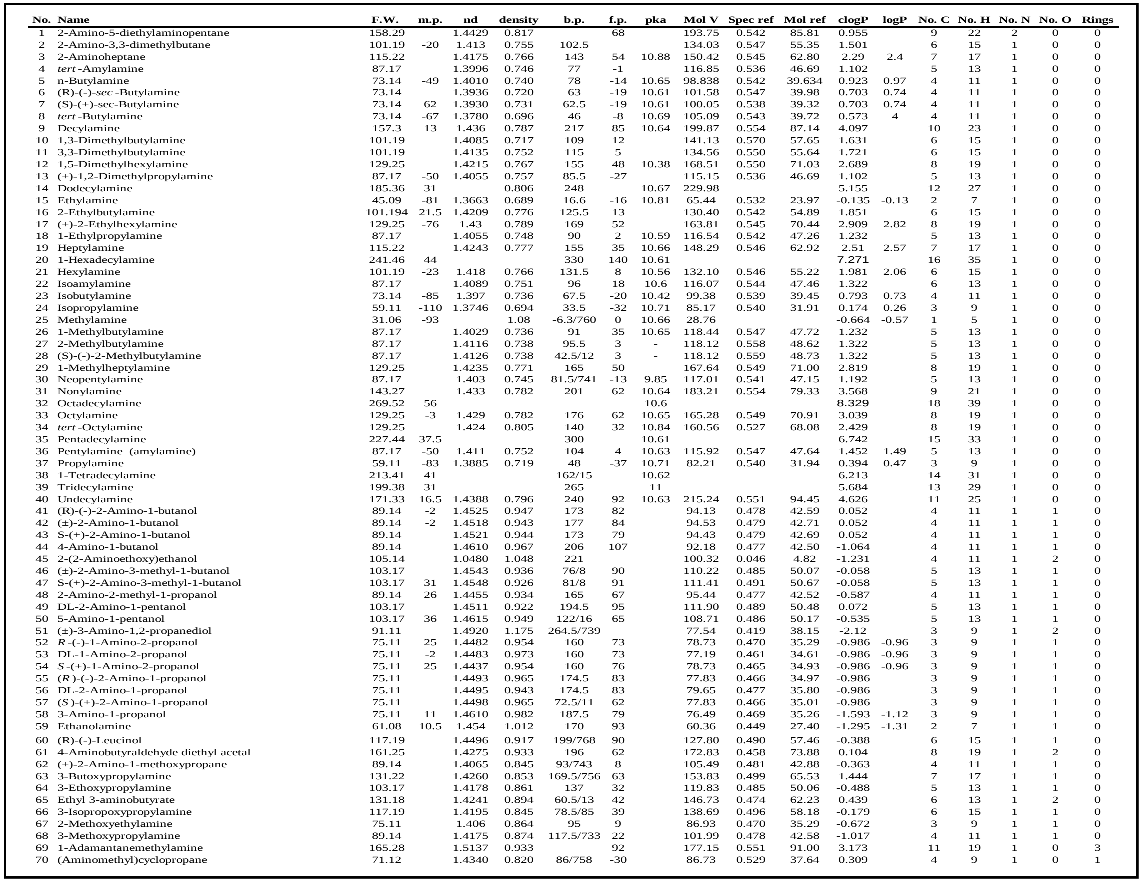
The residual (e_i) for an observation is described by the perpendicular (orthogonal) distance from the point to the PC, which is the same as the unexplained variation

$$\text{DModX} = \sum \sqrt{e_i^2}$$

= distance to the line (1 PC)
= distance to the plane (2 PCs)
= distance to the hyper plane (3 or more PCs)

Example, PCA (known classes)

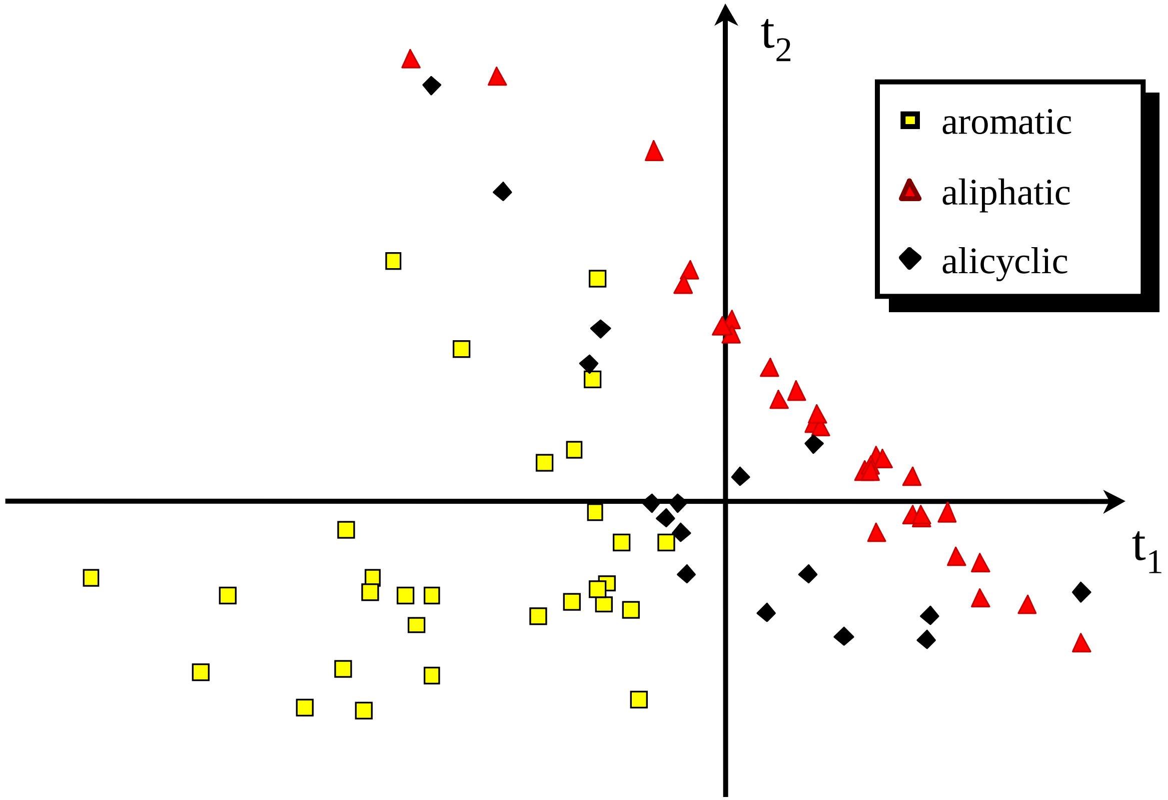
70 aliphatic, alicyclic and aromatic amines for synthesis of pharmaceutical drugs were characterized by 17 property variables from the literature.



No.	Name	F.W.	m.p.	nd	density	b.p.	f.p.	pka	Mol V	Spec ref	Mol ref	clogP	logP	No. C	No. H	No. N	No. O	Rings
1	2-Amino-5-diethylaminopentane	158.29		1.4429	0.817		68		193.75	0.542	85.81	0.955		9	22	2	0	0
2	2-Amino-3,3-dimethylbutane	101.19	-20	1.413	0.755	102.5			134.03	0.547	55.35	1.501		6	15	1	0	0
3	2-Aminoheptane	115.22		1.4175	0.766	143	54	10.88	150.42	0.545	62.80	2.29	2.4	7	17	1	0	0
4	*tert* -Amylamine	87.17		1.3996	0.746	77	-1		116.85	0.536	46.69	1.102		5	13	1	0	0
5	n-Butylamine	73.14	-49	1.4010	0.740	78	-14	10.65	98.838	0.542	39.634	0.923	0.97	4	11	1	0	0
6	(R)-(-)-*sec* -Butylamine	73.14		1.3936	0.720	63	-19	10.61	101.58	0.547	39.98	0.703	0.74	4	11	1	0	0
7	(S)-(+)-sec-Butylamine	73.14	62	1.3930	0.731	62.5	-19	10.61	100.05	0.538	39.32	0.703	0.74	4	11	1	0	0
8	*tert* -Butylamine	73.14	-67	1.3780	0.696	46	-8	10.69	105.09	0.543	39.72	0.573	4	4	11	1	0	0
9	Decylamine	157.3	13	1.436	0.787	217	85	10.64	199.87	0.554	87.14	4.097		10	23	1	0	0
10	1,3-Dimethylbutylamine	101.19		1.4085	0.717	109	12		141.13	0.570	57.65	1.631		6	15	1	0	0
11	3,3-Dimethylbutylamine	101.19		1.4135	0.752	115	5		134.56	0.550	55.64	1.721		6	15	1	0	0
12	1,5-Dimethylhexylamine	129.25		1.4215	0.767	155	48	10.38	168.51	0.550	71.03	2.689		8	19	1	0	0
13	(±)-1,2-Dimethylpropylamine	87.17	-50	1.4055	0.757	85.5	-27		115.15	0.536	46.69	1.102		5	13	1	0	0
14	Dodecylamine	185.36	31		0.806	248		10.67	229.98			5.155		12	27	1	0	0
15	Ethylamine	45.09	-81	1.3663	0.689	16.6	-16	10.81	65.44	0.532	23.97	-0.135	-0.13	2	7	1	0	0
16	2-Ethylbutylamine	101.194	21.5	1.4209	0.776	125.5	13		130.40	0.542	54.89	1.851		6	15	1	0	0
17	(±)-2-Ethylhexylamine	129.25	-76	1.43	0.789	169	52		163.81	0.545	70.44	2.909	2.82	8	19	1	0	0
18	1-Ethylpropylamine	87.17		1.4055	0.748	90	2	10.59	116.54	0.542	47.26	1.232		5	13	1	0	0
19	Heptylamine	115.22		1.4243	0.777	155	35	10.66	148.29	0.546	62.92	2.51	2.57	7	17	1	0	0
20	1-Hexadecylamine	241.46	44			330	140	10.61				7.271		16	35	1	0	0
21	Hexylamine	101.19	-23	1.418	0.766	131.5	8	10.56	132.10	0.546	55.22	1.981	2.06	6	15	1	0	0
22	Isoamylamine	87.17		1.4089	0.751	96	18	10.6	116.07	0.544	47.46	1.322		6	13	1	0	0
23	Isobutylamine	73.14	-85	1.397	0.736	67.5	-20	10.42	99.38	0.539	39.45	0.793	0.73	4	11	1	0	0
24	Isopropylamine	59.11	-110	1.3746	0.694	33.5	-32	10.71	85.17	0.540	31.91	0.174	0.26	3	9	1	0	0
25	Methylamine	31.06	-93		1.08	-6.3/760	0	10.66	28.76			-0.664	-0.57	1	5	1	0	0
26	1-Methylbutylamine	87.17		1.4029	0.736	91	35	10.65	118.44	0.547	47.72	1.232		5	13	1	0	0
27	2-Methylbutylamine	87.17		1.4116	0.738	95.5	3	-	118.12	0.558	48.62	1.322		5	13	1	0	0
28	(S)-(-)-2-Methylbutylamine	87.17		1.4126	0.738	42.5/12	3	-	118.12	0.559	48.73	1.322		5	13	1	0	0
29	1-Methylheptylamine	129.25		1.4235	0.771	165	50		167.64	0.549	71.00	2.819		8	19	1	0	0
30	Neopentylamine	87.17		1.403	0.745	81.5/741	-13	9.85	117.01	0.541	47.15	1.192		5	13	1	0	0
31	Nonylamine	143.27		1.433	0.782	201	62	10.64	183.21	0.554	79.33	3.568		9	21	1	0	0
32	Octadecylamine	269.52	56					10.6				8.329		18	39	1	0	0
33	Octylamine	129.25	-3	1.429	0.782	176	62	10.65	165.28	0.549	70.91	3.039		8	19	1	0	0
34	*tert* -Octylamine	129.25		1.424	0.805	140	32	10.84	160.56	0.527	68.08	2.429		8	19	1	0	0
35	Pentadecylamine	227.44	37.5			300		10.61				6.742		15	33	1	0	0
36	Pentylamine (amylamine)	87.17	-50	1.411	0.752	104	4	10.63	115.92	0.547	47.64	1.452	1.49	5	13	1	0	0
37	Propylamine	59.11	-83	1.3885	0.719	48	-37	10.71	82.21	0.540	31.94	0.394	0.47	3	9	1	0	0
38	1-Tetradecylamine	213.41	41			162/15		10.62				6.213		14	31	1	0	0
39	Tridecylamine	199.38	31			265		11				5.684		13	29	1	0	0
40	Undecylamine	171.33	16.5	1.4388	0.796	240	92	10.63	215.24	0.551	94.45	4.626		11	25	1	0	0
41	(R)-(-)-2-Amino-1-butanol	89.14	-2	1.4525	0.947	173	82		94.13	0.478	42.59	0.052		4	11	1	1	0
42	(±)-2-Amino-1-butanol	89.14	-2	1.4518	0.943	177	84		94.53	0.479	42.71	0.052		4	11	1	1	0
43	S-(+)-2-Amino-1-butanol	89.14		1.4521	0.944	173	79		94.43	0.479	42.69	0.052		4	11	1	1	0
44	4-Amino-1-butanol	89.14		1.4610	0.967	206	107		92.18	0.477	42.50	-1.064		4	11	1	1	0
45	2-(2-Aminoethoxy)ethanol	105.14		1.0480	1.048	221			100.32	0.046	4.82	-1.231		4	11	1	2	0
46	(±)-2-Amino-3-methyl-1-butanol	103.17		1.4543	0.936	76/8	90		110.22	0.485	50.07	-0.058		5	13	1	1	0
47	S-(+)-2-Amino-3-methyl-1-butanol	103.17	31	1.4548	0.926	81/8	91		111.41	0.491	50.67	-0.058		5	13	1	1	0
48	2-Amino-2-methyl-1-propanol	89.14	26	1.4455	0.934	165	67		95.44	0.477	42.52	-0.587		4	11	1	1	0
49	DL-2-Amino-1-pentanol	103.17		1.4511	0.922	194.5	95		111.90	0.489	50.48	0.072		5	13	1	1	0
50	5-Amino-1-pentanol	103.17	36	1.4615	0.949	122/16	65		108.71	0.486	50.17	-0.535		5	13	1	1	0
51	(±)-3-Amino-1,2-propanediol	91.11		1.4920	1.175	264.5/739			77.54	0.419	38.15	-2.12		3	9	1	2	0
52	*R* -(-)-1-Amino-2-propanol	75.11	25	1.4482	0.954	160	73		78.73	0.470	35.29	-0.986	-0.96	3	9	1	1	0
53	DL-1-Amino-2-propanol	75.11	-2	1.4483	0.973	160	73		77.19	0.461	34.61	-0.986	-0.96	3	9	1	1	0
54	*S* -(+)-1-Amino-2-propanol	75.11	25	1.4437	0.954	160	76		78.73	0.465	34.93	-0.986	-0.96	3	9	1	1	0
55	(*R*)-(-)-2-Amino-1-propanol	75.11		1.4493	0.965	174.5	83		77.83	0.466	34.97	-0.986		3	9	1	1	0
56	DL-2-Amino-1-propanol	75.11		1.4495	0.943	174.5	83		79.65	0.477	35.80	-0.986		3	9	1	1	0
57	(*S*)-(+)-2-Amino-1-propanol	75.11		1.4498	0.965	72.5/11	62		77.83	0.466	35.01	-0.986		3	9	1	1	0
58	3-Amino-1-propanol	75.11	11	1.4610	0.982	187.5	79		76.49	0.469	35.26	-1.593	-1.12	3	9	1	1	0
59	Ethanolamine	61.08	10.5	1.454	1.012	170	93		60.36	0.449	27.40	-1.295	-1.31	2	7	1	1	0
60	(R)-(-)-Leucinol	117.19		1.4496	0.917	199/768	90		127.80	0.490	57.46	-0.388		6	15	1	1	0
61	4-Aminobutyraldehyde diethyl acetal	161.25		1.4275	0.933	196	62		172.83	0.458	73.88	0.104		8	19	1	2	0
62	(±)-2-Amino-1-methoxypropane	89.14		1.4065	0.845	93/743	8		105.49	0.481	42.88	-0.363		4	11	1	1	0
63	3-Butoxypropylamine	131.22		1.4260	0.853	169.5/756	63		153.83	0.499	65.53	1.444		7	17	1	1	0
64	3-Ethoxypropylamine	103.17		1.4178	0.861	137	32		119.83	0.485	50.06	-0.488		5	13	1	1	0
65	Ethyl 3-aminobutyrate	131.18		1.4241	0.894	60.5/13	42		146.73	0.474	62.23	0.439		6	13	1	2	0
66	3-Isopropoxypropylamine	117.19		1.4195	0.845	78.5/85	39		138.69	0.496	58.18	-0.179		6	15	1	1	0
67	2-Methoxyethylamine	75.11		1.406	0.864	95	9		86.93	0.470	35.29	-0.672		3	9	1	1	0
68	3-Methoxypropylamine	89.14		1.4175	0.874	117.5/733	22		101.99	0.478	42.58	-1.017		4	11	1	1	0
69	1-Adamantanemethylamine	165.28		1.5137	0.933		92		177.15	0.551	91.00	3.173		11	19	1	0	3
70	(Aminomethyl)cyclopropane	71.12		1.4340	0.820	86/758	-30		86.73	0.529	37.64	0.309		4	9	1	0	1

Example, PCA (known classes)

Scores summarizes the variation between molecules in the data table based on the included variables. From scores we can now chose molecules suitable for synthesis and analysis. (D-optimal choice, Multivariate design)

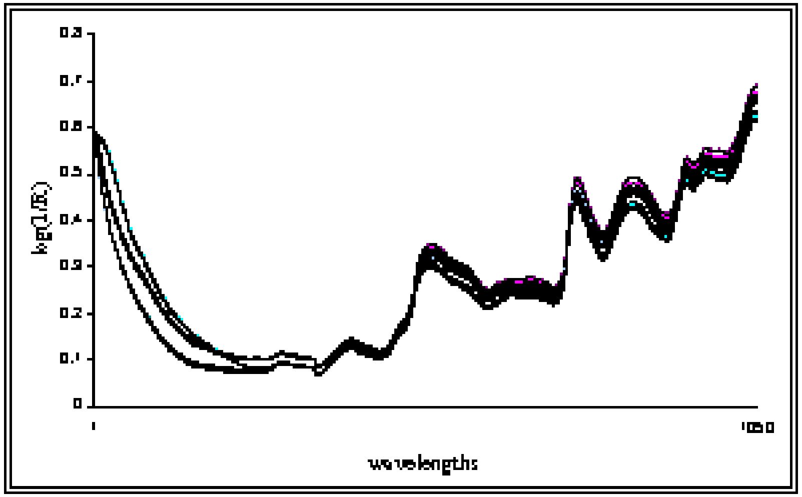


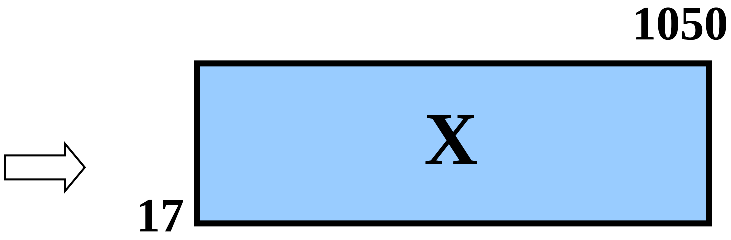
Example, PCA (spectroscopic data)

NIR spectra for 17 wood samples from three different species (spruce, pine, birch).

Each wavelength in the spectrum becomes a variable (1050 variables)

Strong correlation between variables (wavelengths)

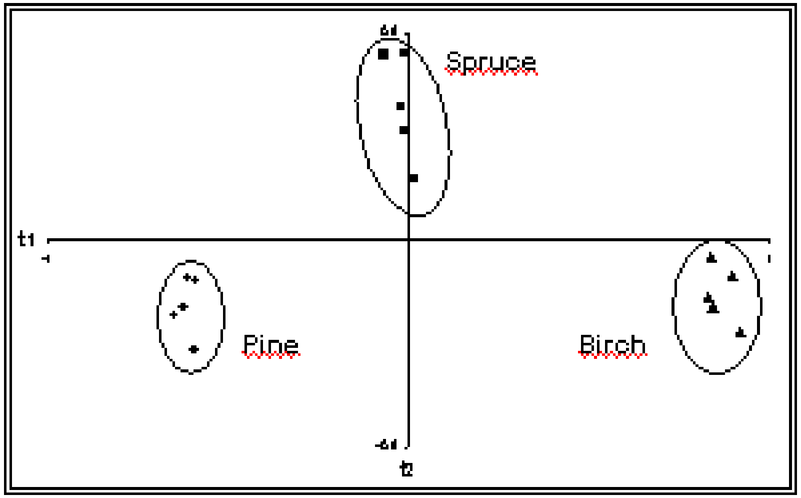


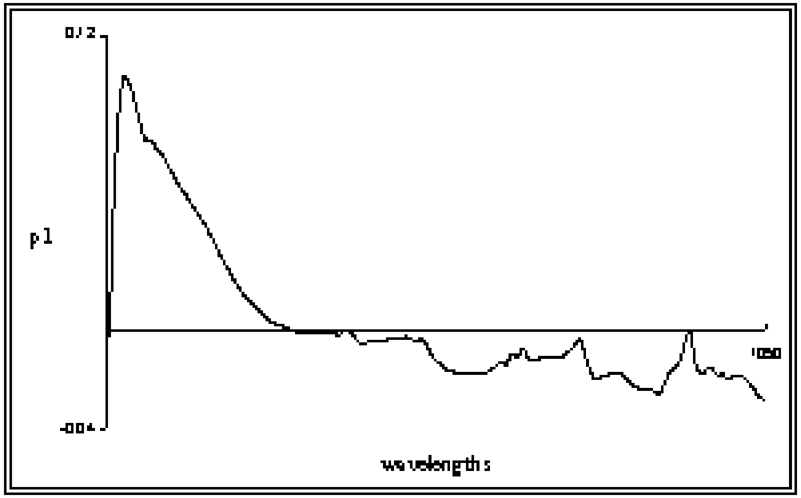


Example, PCA (spectroscopic data)

“scores”

“loadings”





Scores show that NIR spectra contain information that can be used to distinguish between the three species. Three evident classes!

<u>PCA of NIR spectra</u>

From 1050 to 2 dimensions (clear class information)

Loading (p_1) plotted against variable number. gives a loading spectrum that can be compared to the original spectra.

Separation in 1st PC is due to differences in absorption for early wavelengths.

Conclusion

- Multivariate data
  - How are they generated
  - Properties
  - Definition of problems (Overview, Classification, Regression)

- Methods
  - -Univariate
  - -Multivariate (PCA, PCR, PLS, PLS-DA)

- Latent variables

- Projections

- PCA
  - Basic theory
  - Model (scores, loadings, residuals)
  - Interpretation (scores, loadings)
  - Examples