# EPSC 552: Data analysis and Geostatistics:

## Lecture XI: Eigenvector methods: PCA and FA

# A few words of caution….

Eigenvector and clustering methods are extremely powerful aids in understanding your data, and the underlying processes that control the variability in your study

However;

“Principal component analysis belongs to that category of techniques, including cluster analysis, in which appropriateness is judged more by performance and utility than by theoretical considerations”
*Davis, 3rd ed., 2002*

And;

Eigenvector methods require there to be multidimensional correlations in the data set with meaningful causation —> if these are absent, they are not going to magically appear, and eigenvector methods are useless.

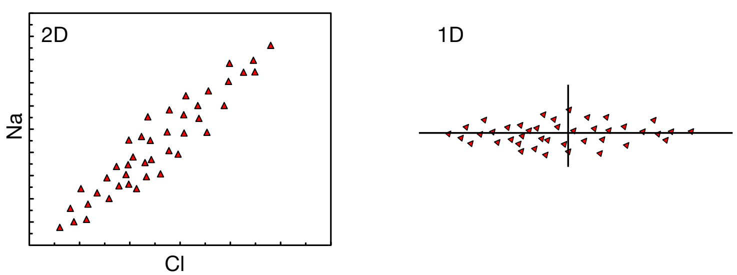
Also, if they are present in 2-D, there is no added value in multi-D —> you look for hidden directions in your data in eigenvector methods

# Eigenvector methods

## Two main techniques: principle component and factor analysis

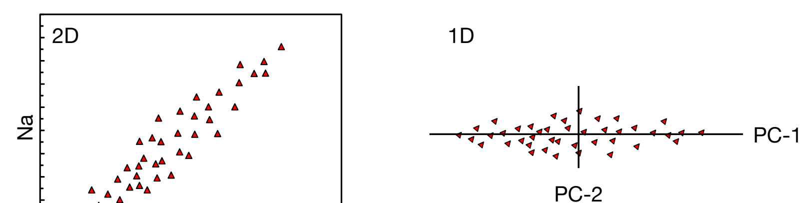
both techniques perform a transformation of the data to allow for easier interpretation through:

- reduction of variables
- suggestion of underlying processes




# Eigenvector methods

## System can be transformed to its principle components




The data have been re-cast into a new coordinate system where the axes are the principal processes operating on your data + noise

majority of the variance in this system resides in PC-1 and PC-2 can be interpreted as just the scatter/noise in the data:

dimensionality of the system reduced from 2-D to 1-D without losing any information !

# Eigenvector methods - PCA and FA

## General notes on Principle Component Analysis and Factor Analysis

- Principle components are the principle non-correlated directions in your data set (maximized variation along, minimized variation perpendicular to PC)
- Nowadays datasets with 50 to 100 variables are not uncommon. A reduction to a much smaller number of unrelated variables (the Factors) makes it much easier to mine such a dataset
- In PCA all variance is redistributed to new PCs, resulting in the same number of PCs as original variables.
- In FA, only those PCs that are informative are retained and the remainder is discarded as noise. The PCs can also be rotated to simplify interpretation.
- Strictly speaking PCA is a mathematical transformation of your data that retains all information, whereas FA is an interpretive model of your data.
- In reality, most software package call both PCA

# Principle component analysis - PCA

## Especially useful in multi-D space

have already seen an example of this approach when looking at DFA:

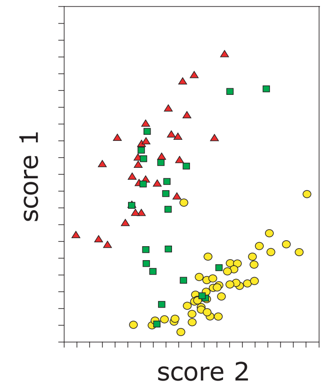
5-D replaced by 2 vectors that allow you to recognize clustering in the data:

this was not obvious in original data

However;

in this case the data are correlated in this 2-D vector space, whereas PCs are not allowed to be correlated

Principle components are the principle non-correlated directions in your data set




# Principle component analysis - PCA

## So what do we do in principle component analysis ?

look in the data for vectors that have maximum variance along them (i.e. a strong correlation/covariance)

as all variables that display the same correlation/covariance are grouped together, the trend they describe cannot be shared with any other PC

PC-1 = vector that explains most of the variance
the strongest direction in your data

PC-2 = vector that next explains most of the residual variance

PC-3 = vector that next explains most of the residual variance

etc

so PC-1 explains more variance than any single original variable and therefore, PC-n explains less variance than a single variable (noise)

# Principle component analysis - PCA

## So what do these principle components look like ?

PC:

$$PC_1 = a_{11}X_1 + a_{12}X_2 + a_{13}X_3 + a_{14}X_4 + a_{15}X_5 + \ldots.$$
$$PC_2 = a_{21}X_1 + a_{22}X_2 + a_{23}X_3 + a_{24}X_4 + a_{25}X_5 + \ldots.$$
$$PC_3 = a_{31}X_1 + a_{32}X_2 + a_{33}X_3 + a_{34}X_4 + a_{35}X_5 + \ldots.$$
$$PC_4 = a_{41}X_1 + a_{42}X_2 + a_{43}X_3 + a_{44}X_4 + a_{45}X_5 + \ldots.$$
.....

$X_i$ = original vars
$a_{ij}$ = coefficients that relate the original vars to the PCs

Note that to satisfy multi-non-colinearity some of the a-coefficients have to be 0

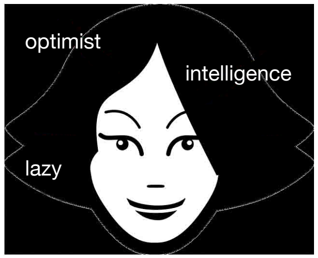
in matrix notation:

**PC = A X**

$$\begin{vmatrix} PC_1 \\ PC_2 \\ PC_3 \\ PC_4 \end{vmatrix} = \begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \end{vmatrix} \cdot \begin{vmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{vmatrix}$$

# Principle component analysis - PCA

## Another way to explain PCA: psychological questionnaires




A psychologist want to know your intelligence, whether you are extroverted, a pessimist, etc.

Have to work this out from indirect questions that correlate with the variable that you are interested in (e.g. intelligence, optimism, etc)

Many questions lead to a small number of ultimate variables

$$\begin{vmatrix} PC_1 \\ PC_2 \\ PC_3 \\ PC_4 \end{vmatrix} = \begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \end{vmatrix} \cdot \begin{vmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{vmatrix}$$

matrix A tells you how to score the answers

# Principle component analysis - PCA

## The transformation matrix A is what you want to obtain

the matrix that translates the original variables to line up with the principle directions in the data: the PCs

so, it redistributes the variance of the original variables over the PCs, maximizing it for $PC_1$: $Var(PC_1) = max$

it ensures that the PCs are uncorrelated: $Cov(PC_i - PC_{i+1}) = 0$

Note that we are only translating the data to a new coordination system: no info loss !

The matrix A is obtained from the covariance or the correlation matrix

when all variables are equivalent (e.g. all wt%, all ppm, etc)

when mixing variables (e.g. ppm + wt% + pH)

# Principle component analysis - PCA

## Link with correlation makes sense (I hope):

all variables that are correlated define one trend in the data so they should be combined in one PC, and this PC and its component variables should have an insignificant correlation with all remaining variables and PCs

e.g. 5 variables with the following correlation matrix:

| | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 1 | - | 0.85 | 0.14 | 0.23 | 0.78 |
| 2 | - | - | 0.21 | 0.19 | 0.95 |
| 3 | - | - | - | 0.9 | 0.25 |
| 4 | - | - | - | - | 0.13 |
| 5 | - | - | - | - | - |

strong correlations:

1 & 2
1 & 5
2 & 5

3 & 4

weak correlations:

1 & 3
1 & 4
2 & 3
2 & 4
5 & 3
5 & 4

so, this dat set has two PCs, with low correlation between them

# Principle component analysis - PCA

## Strong reduction in dimensionality: 5D to 2D

this allows for much easier data visualization and (hopefully) interpretation

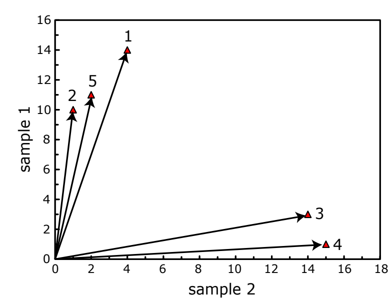
+

it may point to two underlying processes, affecting a different set of vars

a good way to represent this is to plot it in variable space

Now you get two clusters of variables and these are your PCs

So in a way, PCA is cluster analysis on your variables



# Principle component analysis - PCA

## So how do we obtain the transformation matrix from cor/cov ?

have to determine the eigenvectors in the correlation or covariance matrix

these are the weights that relate the original variables to the PC vectors

and scale these so that the variance of a PC equals 1

$$\mathbf{PC} = \mathbf{U}\,\mathbf{L}^{-0.5}\,\mathbf{X}$$ in matrix notation

pure mathematical transformation

this is the PC vector i.e. the new variables

the eigenvector matrix of the cor/cov matrix

the diagonal eigen-value matrix of the cor/cov matrix, i.e. the scale factor

these are the original variables, i.e. the input

input: original vars

operator: eigenvector matrix scaled by eigenvalues

output: PC vector

# Principle component analysis - PCA

## An example for thermal spring data from the Rockies:

| | Si | Al | Cu | Zn | pH | T |
|---|---|---|---|---|---|---|
| PC-1 | 0.6 | -0.2 | 0.1 | 0.3 | -0.4 | 0.9 |
| PC-2 | 0.3 | 0.7 | -0.2 | -0.1 | 0.6 | -0.1 |
| PC-3 | 0.1 | -0.1 | 0.9 | 0.8 | -0.7 | 0.4 |
| PC-4 | -0.2 | 0.2 | -0.3 | 0.1 | -0.4 | -0.2 |
| .... | | | | | | |

the coefficients are the factor loading:

the correlation between the original variables and the PCs

they display a clear grouping of variables

PC-1: Si and T - as T increases the solubility increases
PC-2: Al and pH - unclear, clay effect? speciation?
PC-3: Ca, Zn, -pH and ±T - low pH + high conc. base metals: sulfides
PC-4: no clear associations - residual noise ?

You get as many PCs as there are original variables, but not all will be meaningful.

# Principle component analysis - PCA

## The variance in the original variables is redistributed;

PC-1 will have a variance greater than a single original variable (it explains more variance in the data set than a single original variable)

so, subsequent PCs will eventually explain less variance than a single original var

such PCs can generally be ignored thereby reducing the dimensionality

but where should we put the boundary?

the eigenvalues show you how much variance a PC explains compared to the original variables and this value can therefore be used to define a cut-off:

- all eigenvalues less than 1 are insignificant (generally too restrictive)
- use a scree plot (PC-number versus eigenvalue) - where there is a kink in this plot: boundary - use all PCs up to this point and one beyond
- maximum likelihood method - the goodness-of-fit of the factor model is iteratively tested using the $X^2$ test and additional factors are calculated from the residual covariance/correlation matrix only if it fails the $X^2$ test

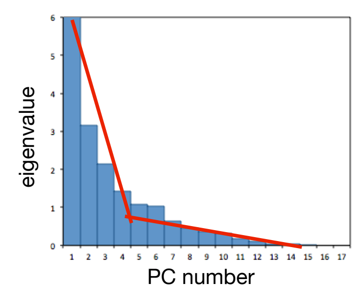
# Restricting the number of PCs: FA

## The variance in the original variables is redistributed;

PC-1 will have a variance greater than a single original variable (it explains more variance in the data set than a single original variable)

so, subsequent PCs will eventually explain less variance than a single original var

such PCs can generally be ignored thereby reducing the dimensionality




The cut-off can be determined in a scree-plot

# Principle component analysis - PCA

## To facilitate interpretation the resulting PCs are commonly rotated in multi-dimensional space

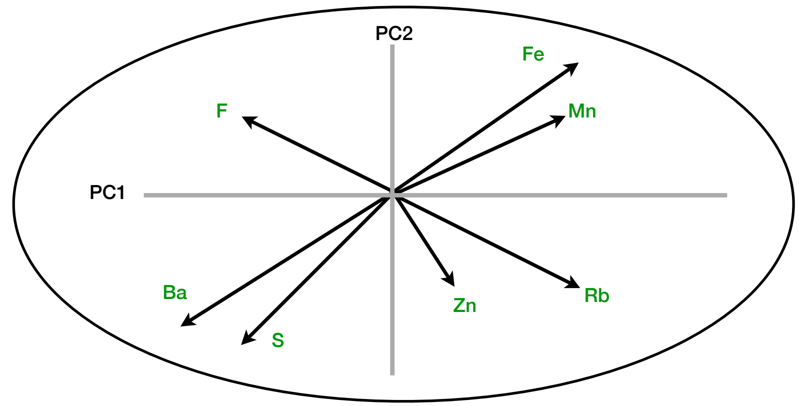
The most popular technique is Varimax rotation:

“rotation to maximize the variance of the squared loadings within each column of the loadings matrix”

this rotation results in the correlations with the original variables to be either large or small, so it enhances the contrast, producing PCs that are highly correlated with a few original variables and weakly with the rest:

much easier to interpret, because it is immediately clear which variables are important and that in turn can directly point to the underlying process

# Varimax rotation




# A Factor Analysis example using PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

6 km$^2$
55 samples

After cleaning
15 elements

All elements log-transformed

# A Factor Analysis example

## The Sn-W mineralized granite of Regoufe (Portugal)

| NR | XCO | YCO | F | ZR | SR | CE | BA | B | LI | W | NB | RB | U | TH | TA | AS | CS | SN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 94 | 36 | 3520 | 29 | 53 | 14.6 | 24.6 | 540 | 758 | 11.8 | 38 | 715 | 5 | 1.62 | 14.28 | 2.6 | 48 | 44 |
| 2 | 94 | 45 | 3020 | 43 | 34 | 28.1 | 94.0 | 640 | 785 | 15.5 | 31 | 624 | 4 | 4.81 | 10.26 | 5.4 | 73 | 48 |
| 3 | 81 | 46 | 3800 | 43 | 33 | 28.8 | 108.7 | 280 | 647 | 14.43 | 31 | 669 | 7 | 5.2 | 11.51 | 206.4 | 68 | 54 |
| 4 | 75 | 40 | 3320 | 27 | 26 | 15.2 | 38.5 | 330 | 627 | 18.66 | 36 | 683 | 1 | 2.69 | 12.72 | 65.1 | 58 | 57 |
| 5 | 60 | 35 | 2040 | 31 | 25 | 21.2 | 76.0 | 860 | 317 | 11.02 | 19 | 542 | 11 | 3.69 | 9.13 | 84.7 | 29 | 34 |
| 6 | 77 | 31 | 2920 | 29 | 29 | 17.2 | 58.3 | 360 | 592 | 16.78 | 37 | 748 | 8 | 2.83 | 17.86 | 80.5 | 66 | 69 |
| 7 | 56 | 134 | 4020 | 19 | 32 | 16.2 | 18.0 | 70 | 442 | 16.71 | 43 | 869 | 20 | 1.75 | 19.9 | 2592.3 | 44 | 70 |
| 8 | 65 | 127 | 2840 | 19 | 15 | 9.3 | 32.0 | 50 | 423 | 16.75 | 53 | 782 | 21 | 1.43 | 20.05 | 1045.0 | 45 | 64 |
| 9 | 81 | 130 | 3600 | 21 | 38 | 17.9 | 39.0 | 40 | 517 | 19.85 | 44 | 889 | 8 | 2.23 | 15.51 | 463.8 | 56 | 76 |
| 10 | 69 | 118 | 3200 | 41 | 33 | 25.9 | 94.3 | 200 | 686 | 29 | 27 | 674 | 10 | 4.49 | 11.12 | 119.7 | 85 | 63 |
| 12 | 96 | 107.5 | 6880 | 20 | 100 | 8.3 | 38.0 | 40 | 488 | 10.74 | 51 | 840 | 13 | 1.17 | 25.95 | 256.2 | 51 | 101 |
| 13 | 88 | 112 | 3800 | 19 | 24 | 12.9 | 28.9 | 40 | 594 | 10.89 | 53 | 935 | 13 | 1.83 | 26.8 | 210.2 | 60 | 74 |
| 14 | 58 | 115 | 6160 | 38 | 32 | 21.7 | 76.0 | 310 | 520 | 37.85 | 32 | 601 | 13 | 3.75 | 10.61 | 588.1 | 50 | 60 |
| 15 | 45 | 113 | 4280 | 45 | 30 | 27.1 | 99.9 | 320 | 666 | 11.1 | 28 | 638 | 7 | 5 | 8.11 | 57.5 | 71 | 49 |
| 16 | 19 | 120 | 4520 | 17 | 34 | 8.1 | 11.4 | 40 | 526 | 10.01 | 45 | 822 | 13 | 0.79 | 20.12 | 46.5 | 46 | 72 |
| 17 | 24 | 116 | 4240 | 26 | 36 | 18.0 | 43.1 | 120 | 333 | 13.12 | 37 | 675 | 18 | 2.52 | 11.2 | 235.3 | 50 | 57 |
| 18 | 93 | 100 | 3520 | 24 | 34 | 13.4 | 23.7 | 40 | 440 | 9.93 | 43 | 812 | 8 | 1.6 | 18.94 | 279.4 | 39 | 59 |
| 19 | 92 | 93 | 4960 | 19 | 43 | 12.7 | 20.0 | 120 | 630 | 12.5 | 50 | 923 | 7 | 1.17 | 23.64 | 571.8 | 62 | 72 |
| 20 | 81 | 80 | 6440 | 18 | 37 | 9.4 | 11.8 | 50 | 586 | 12.67 | 46 | 895 | 13 | 1.21 | 25.6 | 288.8 | 55 | 77 |
| 21 | 79 | 69 | 3240 | 40 | 34 | 26.9 | 101.0 | 40 | 397 | 22 | 33 | 612 | 18 | 4.73 | 8.43 | 1010.7 | 38 | 58 |
| 22 | 79 | 60 | 3300 | 41 | 37 | 23.0 | 129.9 | 560 | 684 | 9.9 | 35 | 679 | 11 | 4.2 | 13.57 | 16.9 | 102 | 55 |
| 23 | 92 | 57 | 3720 | 43 | 32 | 24.0 | 81.0 | 340 | 832 | 10.75 | 33 | 703 | 6 | 4.75 | 15.53 | 58.8 | 113 | 63 |

# A Factor Analysis example - PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

The correlation matrix

| | F | ZR | SR | CE | BA | B | LI | W | NB | RB | U | TH | TA |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| F | | -0.50221 | 0.30731 | -0.54151 | -0.42093 | -0.28885 | 0.19875 | 0.15289 | 0.46813 | 0.58401 | 0.012455 | -0.53583 | 0.50934 |
| ZR | -0.50221 | | 0.055172 | 0.95109 | 0.86482 | 0.4027 | 0.13749 | -0.056488 | -0.71756 | -0.78795 | 0.012894 | 0.95715 | -0.76939 |
| SR | 0.30731 | 0.055172 | | 0.062507 | 0.066011 | -0.082219 | -0.076446 | -0.18118 | 0.041973 | 0.0027489 | 0.014244 | -0.0051581 | 0.10591 |
| CE | -0.54151 | 0.95109 | 0.062507 | | 0.86814 | 0.35716 | 0.03861 | -0.037515 | -0.72012 | -0.77759 | 0.07226 | 0.96249 | -0.77617 |
| BA | -0.42093 | 0.86482 | 0.066011 | 0.86814 | | 0.42212 | 0.056067 | 0.079535 | -0.76312 | -0.75126 | 0.10691 | 0.88669 | -0.77485 |
| B | -0.28885 | 0.4027 | -0.082219 | 0.35716 | 0.42212 | | 0.11569 | -0.10935 | -0.57752 | -0.55081 | -0.20643 | 0.40807 | -0.53463 |
| LI | 0.19875 | 0.13749 | -0.076446 | 0.03861 | 0.056067 | 0.11569 | | -0.059215 | 0.076383 | 0.2815 | -0.63521 | 0.081594 | 0.10293 |
| W | 0.15289 | -0.056488 | -0.18118 | -0.037515 | 0.079535 | -0.10935 | -0.059215 | | -0.12996 | -0.0084492 | 0.15031 | -0.044045 | -0.096932 |
| NB | 0.46813 | -0.71756 | 0.041973 | -0.72012 | -0.76312 | -0.57752 | 0.076383 | -0.12996 | | 0.81782 | -0.030427 | -0.7507 | 0.89426 |
| RB | 0.58401 | -0.78795 | 0.0027489 | -0.77759 | -0.75126 | -0.55081 | 0.2815 | -0.0084492 | 0.81782 | | -0.18664 | -0.79942 | 0.88746 |
| U | 0.012455 | 0.012894 | 0.014244 | 0.07226 | 0.10691 | -0.20643 | -0.63521 | 0.15031 | -0.030427 | -0.18664 | | 0.0092227 | -0.11037 |
| TH | -0.53583 | 0.95715 | -0.0051581 | 0.96249 | 0.88669 | 0.40807 | 0.081594 | -0.044045 | -0.7507 | -0.79942 | 0.0092227 | | -0.79443 |
| TA | 0.50934 | -0.76939 | 0.10591 | -0.77617 | -0.77485 | -0.53463 | 0.10293 | -0.096932 | 0.89426 | 0.88746 | -0.11037 | -0.79443 | |
| AS | 0.20773 | -0.32656 | -0.093352 | -0.21183 | -0.24763 | -0.34152 | -0.24679 | 0.29603 | 0.26883 | 0.32194 | 0.46611 | -0.30133 | 0.22816 |
| CS | 0.072648 | 0.29065 | -0.036181 | 0.25418 | 0.29177 | 0.10383 | 0.75412 | -0.09801 | -0.079188 | 0.080846 | -0.37248 | 0.30078 | -0.067257 |
| SN | 0.73552 | -0.59186 | 0.15903 | -0.60059 | -0.47931 | -0.47726 | 0.28084 | 0.15559 | 0.56749 | 0.78645 | 0.019273 | -0.5946 | 0.62395 |

# A Factor Analysis example - PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

PC eigenvalues: how much of the original variance is captured by each PC

Principal components analysis

Summary | Scatter plot | Scores | Loadings plot | Loadings | Scree plot

| PC | Eigenvalu | % variance |
|---|---|---|
| 1 | 7.24719 | 45.295 |
| 2 | 2.60592 | 16.287 |
| 3 | 1.56877 | 9.8048 |
| 4 | 1.28902 | 8.0563 |
| 5 | 0.960919 | 6.0057 |
| 6 | 0.64666 | 4.0416 |
| 7 | 0.477462 | 2.9841 |
| 8 | 0.293343 | 1.8334 |
| 9 | 0.279331 | 1.7458 |
| 10 | 0.172708 | 1.0794 |
| 11 | 0.15083 | 0.94269 |
| 12 | 0.117418 | 0.73386 |
| 13 | 0.0919825 | 0.57489 |
| 14 | 0.0480764 | 0.30048 |
| 15 | 0.0286725 | 0.1792 |
| 16 | 0.0217038 | 0.13565 |

Matrix: Correlation

Groups: Disregard

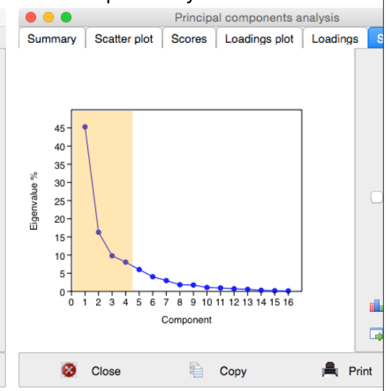
Missing values: Mean value imputatic

Bootstrap N: 0

Recompute

Detach tab

Close | Copy | Print




# A Factor Analysis example - PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

A variable's communality tells you how much of its variance is explained by your factors. In this case, for 4 factors:

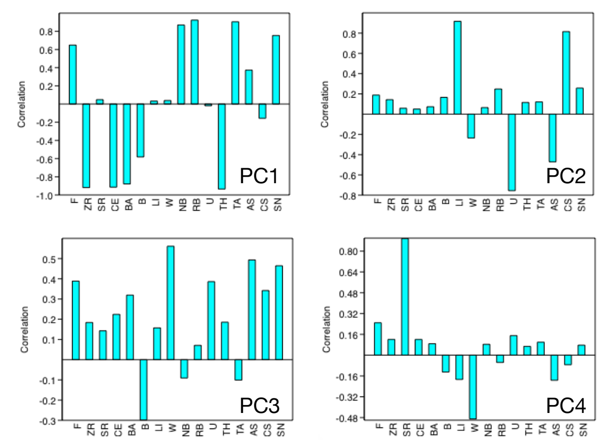
Communalities

| | Initial | Extraction |
|---|---|---|
| F | 1.000 | .728 |
| ZR | 1.000 | .944 |
| SR | 1.000 | .698 |
| CE | 1.000 | .905 |
| BA | 1.000 | .901 |
| B | 1.000 | .675 |
| LI | 1.000 | .899 |
| W | 1.000 | .710 |
| NB | 1.000 | .790 |
| RB | 1.000 | .923 |
| U | 1.000 | .624 |
| TH | 1.000 | .935 |
| TA | 1.000 | .860 |
| AS | 1.000 | .723 |
| CS | 1.000 | .820 |
| SN | 1.000 | .873 |

# A Factor Analysis example - PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

Variable loadings



# A Factor Analysis example - PAST

## The Sn-W mineralized granite of Regoufe (Portugal)

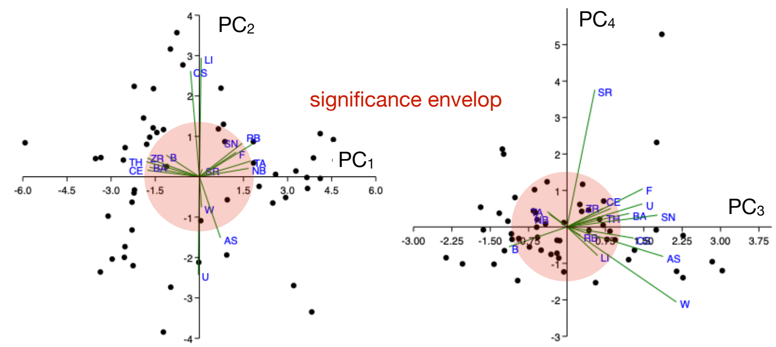
| Summary / Scatter plot / **Scores** / Loadings plot / Loadings | PC 1 | PC 2 | PC 3 | PC 4 |
|---|---|---|---|---|
| 2 | 0.82047 | 1.2982 | -1.6875 | 0.54203 |
| 3 | -2.2156 | 2.2375 | -0.19651 | -0.72032 |
| 4 | -1.5725 | 1.2107 | 0.83885 | -0.11722 |
| 5 | 0.64699 | 1.1837 | -0.96398 | -1.4718 |
| 6 | -2.5503 | -1.9959 | -2.3628 | -0.84471 |
| 7 | 0.86607 | 0.86924 | -0.16158 | -0.85254 |
| 8 | 3.8211 | -3.347 | 2.8373 | -0.95335 |
| 9 | 3.2064 | -2.6937 | 0.55837 | -1.5285 |
| 10 | 2.5915 | 0.058918 | 0.78231 | -0.34281 |
| 11 | -1.2186 | 1.1672 | 2.1411 | -1.2177 |
| 12 | 5.0685 | 0.46625 | 1.8525 | 5.2839 |
| 13 | 3.8793 | 0.46543 | -0.14352 | -0.37514 |
| 14 | 0.04771 | -1.0882 | 3.0333 | -1.1993 |
| 15 | -1.8972 | 1.454 | 0.42957 | -0.093339 |
| 16 | 3.6772 | -0.28991 | -0.61238 | 0.39277 |
| 17 | 0.93084 | -1.9372 | 0.25046 | 0.61637 |
| 18 | 2.4969 | -0.64977 | -1.1553 | 0.15791 |
| 19 | 4.1089 | 1.0677 | 0.28669 | 0.42668 |
| 20 | 4.6143 | 0.41045 | 0.71639 | 0.70874 |
| 21 | -0.9729 | -2.7342 | 2.2684 | -0.23563 |
| 22 | -1.559 | 2.1812 | 0.63526 | 0.21126 |
| 23 | -0.76501 | 3.5679 | 0.93892 | -0.35468 |

The scores for each sample on the different factors

# A Factor Analysis example - PAST

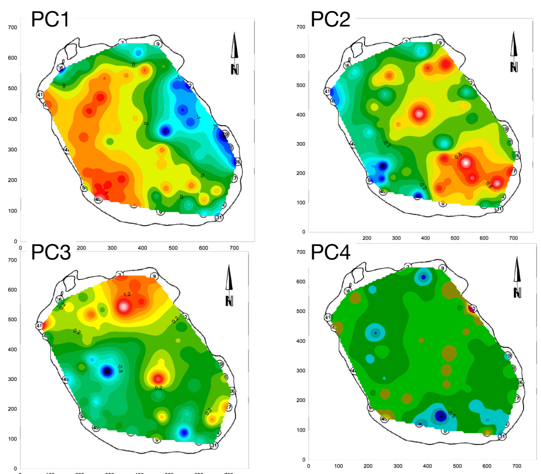
## The Sn-W mineralized granite of Regoufe (Portugal)

Bi-plot: combines the data loadings on the PCs and the variable scores on the PCs




# A Factor Analysis example

## The Sn-W mineralized granite of Regoufe (Portugal)




Tentative interpretation:

PC1: inverse of degree of greisinisation and albitisation

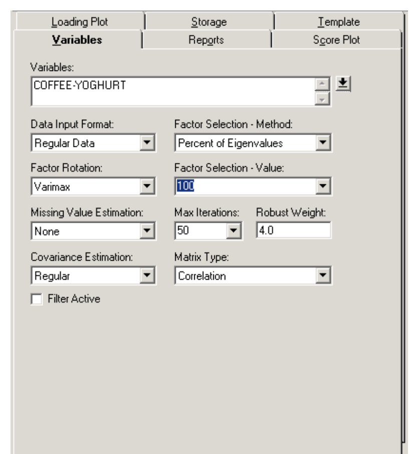
PC2: deuteric alteration

PC3: ore-related elements

PC4: different levels within the granite magma body

# Factor Analysis vs. Cluster Analysis

## the data set: the eating habits of Europe




**variables:** the original variables as input

**rotation:** you can tell NCSS to perform a PC rotation such as Varimax or none

**missing values:** if you have these you have to tell NCSS how to deal with them: row-wise exclusion, replace by mean or estimate from correlations

**matrix type:** correlation or covariance

**factor selection:** start by selecting % eigenvalues and setting this to 100%: gives you all PCs. Can then decide that only first 4 are meaningful and change this

# Principle component analysis - PCA

## output: the eating habits of Europe

**Descriptive Statistics Section**

| Variables | Count | Mean | Standard Deviation | Communality |
|---|---|---|---|---|
| Coffee | 16 | 77.5 | 25.76561 | 1.000000 |
| Nescafe | 16 | 39.25 | 23.14735 | 1.000000 |
| Tea | 16 | 78.5 | 18.54005 | 1.000000 |
| Sweetener | 16 | 17.1875 | 11.02252 | 1.000000 |
| Biscuits | 16 | 60.875 | 19.18637 | 1.000000 |
| Pack_soup | 16 | 49 | 15.42725 | 1.000000 |
| Tin_soup | 16 | 18.4375 | 20.2154 | 1.000000 |
| Frozen_fish | 16 | 21.875 | 13.98034 | 1.000000 |
| Frozen_veg | 16 | 15.875 | 12.78997 | 1.000000 |
| Fresh_apples | 16 | 66.8125 | 17.58112 | 1.000000 |
| Tin_fruit | 16 | 41.9375 | 23.25645 | 1.000000 |
| Jam | 16 | 55.1875 | 22.59268 | 1.000000 |
| Garlic | 16 | 42.3125 | 34.67702 | 1.000000 |
| Butter | 16 | 75.8125 | 20.91002 | 1.000000 |
| Margerine | 16 | 69 | 26.73076 | 1.000000 |
| Olive_oil | 16 | 54.1875 | 28.8426 | 1.000000 |
| Yoghurt | 16 | 20.625 | 18.34076 | 1.000000 |

# Principle component analysis - PCA

## output: the eating habits of Europe

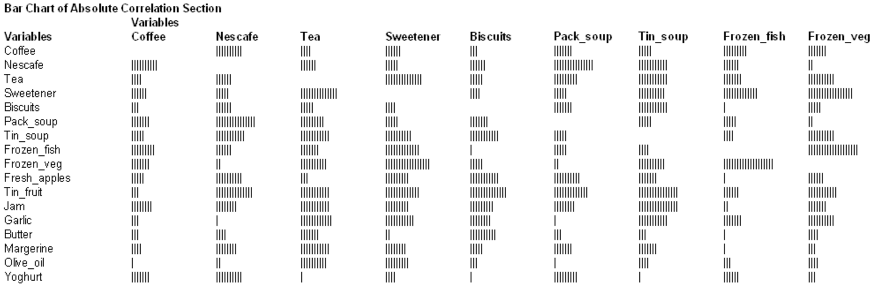
**Correlation Section**

| Variables | Variables Coffee | Nescafe | Tea | Sweetener | Biscuits | Pack_soup | Tin_soup | Frozen_fish | Frozen_veg | Fre |
|---|---|---|---|---|---|---|---|---|---|---|
| Coffee | 1.000000 | -0.451482 | -0.154771 | 0.267487 | -0.106133 | -0.302228 | -0.238387 | 0.409759 | 0.315186 | |
| Nescafe | -0.451482 | 1.000000 | 0.290961 | 0.228696 | 0.259018 | 0.727154 | 0.506803 | -0.291814 | -0.064515 | |
| Tea | -0.154771 | 0.290961 | 1.000000 | 0.669251 | 0.209905 | 0.441225 | 0.523398 | 0.320735 | 0.478507 | |
| Sweetener | 0.267487 | 0.228696 | 0.669251 | 1.000000 | 0.186738 | 0.226212 | 0.495064 | 0.617516 | 0.814964 | |
| Biscuits | -0.106133 | 0.259018 | 0.209905 | 0.186738 | 1.000000 | 0.313521 | 0.548802 | 0.029017 | 0.232484 | |
| Pack_soup | -0.302228 | 0.727154 | 0.441225 | 0.226212 | 0.313521 | 1.000000 | 0.244120 | -0.243882 | -0.085481 | |
| Tin_soup | -0.238387 | 0.506803 | 0.523398 | 0.495064 | 0.548802 | 0.244120 | 1.000000 | 0.189154 | 0.474401 | |
| Frozen_fish | 0.409759 | -0.291814 | 0.320735 | 0.617516 | 0.029017 | -0.243882 | 0.189154 | 1.000000 | 0.905160 | |
| Frozen_veg | 0.315186 | -0.064515 | 0.478507 | 0.814964 | 0.232484 | -0.085481 | 0.474401 | 0.905160 | 1.000000 | |
| Fresh_apples | 0.241139 | 0.480764 | 0.133454 | 0.423680 | 0.538291 | 0.480530 | 0.335071 | 0.030005 | 0.285694 | |
| Tin_fruit | -0.100075 | 0.694902 | 0.546490 | 0.646054 | 0.672017 | 0.613927 | 0.740128 | 0.269813 | 0.530707 | |
| Jam | -0.385434 | 0.383235 | 0.538513 | 0.410780 | 0.431766 | 0.366096 | 0.729504 | 0.088306 | 0.339465 | |
| Garlic | 0.110990 | 0.033616 | -0.593807 | -0.520098 | -0.351444 | 0.015203 | -0.546658 | -0.322249 | -0.473994 | |
| Butter | -0.140384 | 0.154920 | 0.302403 | 0.094169 | 0.455585 | 0.114699 | 0.133634 | 0.043929 | 0.186117 | |
| Margerine | -0.174813 | 0.387019 | 0.534448 | 0.351163 | 0.233069 | 0.319930 | 0.300657 | 0.031041 | 0.148003 | |
| Olive_oil | 0.022293 | 0.075116 | -0.480293 | -0.432305 | -0.139580 | -0.049143 | -0.183091 | -0.111702 | -0.197097 | |
| Yoghurt | 0.313610 | 0.497244 | 0.003725 | 0.196254 | 0.011225 | 0.409263 | 0.036074 | -0.259675 | -0.144018 | |

# Principle component analysis - PCA

## output: the eating habits of Europe

**Bar Chart of Absolute Correlation Section**

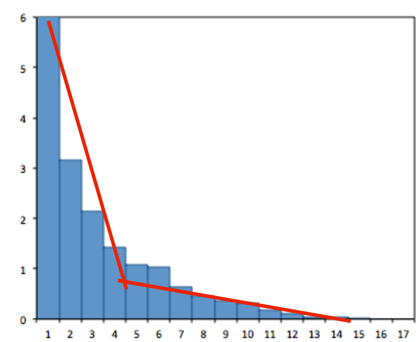



# Principle component analysis - PCA

## output: the eating habits of Europe

**Eigenvalues**

<table>
<tr><th>No.</th><th>Eigenvalue</th><th>Individual Percent</th><th>Cumulative Percent</th><th>Scree Plot</th></tr>
<tr><td>1</td><td>6.020081</td><td>35.41</td><td>35.41</td><td>||||||||</td></tr>
<tr><td>2</td><td>3.156737</td><td>18.57</td><td>53.98</td><td>||||</td></tr>
<tr><td>3</td><td>2.139819</td><td>12.59</td><td>66.57</td><td>|||</td></tr>
<tr><td>4</td><td>1.425082</td><td>8.38</td><td>74.95</td><td>||</td></tr>
<tr><td>5</td><td>1.078415</td><td>6.34</td><td>81.29</td><td>||</td></tr>
<tr><td>6</td><td>1.037413</td><td>6.10</td><td>87.40</td><td>||</td></tr>
<tr><td>7</td><td>0.642829</td><td>3.78</td><td>91.18</td><td>|</td></tr>
<tr><td>8</td><td>0.465207</td><td>2.74</td><td>93.92</td><td>|</td></tr>
<tr><td>9</td><td>0.368342</td><td>2.17</td><td>96.08</td><td>|</td></tr>
<tr><td>10</td><td>0.319876</td><td>1.88</td><td>97.96</td><td>|</td></tr>
<tr><td>11</td><td>0.172239</td><td>1.01</td><td>98.98</td><td>|</td></tr>
<tr><td>12</td><td>0.106809</td><td>0.63</td><td>99.60</td><td>|</td></tr>
<tr><td>13</td><td>0.037875</td><td>0.22</td><td>99.83</td><td>|</td></tr>
<tr><td>14</td><td>0.026913</td><td>0.16</td><td>99.99</td><td>|</td></tr>
<tr><td>15</td><td>0.002364</td><td>0.01</td><td>100.00</td><td>|</td></tr>
<tr><td>16</td><td>0.000000</td><td>0.00</td><td>100.00</td><td></td></tr>
<tr><td>17</td><td>0.000000</td><td>0.00</td><td>100.00</td><td></td></tr>
</table>




now rerun the routine for up to 4 principle components

# Principle component analysis - PCA

## output: the eating habits of Europe

**Descriptive Statistics Section**

| Variables | Count | Mean | Standard Deviation | Communality |
|---|---|---|---|---|
| Coffee | 16 | 77.5 | 25.76561 | 0.825747 |
| Nescafe | 16 | 39.25 | 23.14735 | 0.826203 |
| Tea | 16 | 78.5 | 18.54005 | 0.712119 |
| Sweetener | 16 | 17.1875 | 11.02252 | 0.885670 |
| Biscuits | 16 | 60.875 | 19.18637 | 0.638357 |
| Pack_soup | 16 | 49 | 15.42725 | 0.712475 |
| Tin_soup | 16 | 18.4375 | 20.2154 | 0.687004 |
| Frozen_fish | 16 | 21.875 | 13.98034 | 0.848950 |
| Frozen_veg | 16 | 15.875 | 12.78997 | 0.936613 |
| Fresh_apples | 16 | 66.8125 | 17.58112 | 0.781884 |
| Tin_fruit | 16 | 41.9375 | 23.25645 | 0.929247 |
| Jam | 16 | 55.1875 | 22.59268 | 0.706079 |
| Garlic | 16 | 42.3125 | 34.67702 | 0.839802 |
| Butter | 16 | 75.8125 | 20.91002 | 0.386488 |
| Margerine | 16 | 69 | 26.73076 | 0.404393 |
| Olive_oil | 16 | 54.1875 | 28.8426 | 0.682256 |
| Yoghurt | 16 | 20.625 | 18.34076 | 0.874905 |

# Principle component analysis - PCA

## output: the eating habits of Europe - coefficients

**Bar Chart of Absolute Eigenvectors after Varimax Rotation**

<table>
<tr><th></th><th>Factors</th><th></th><th></th><th></th></tr>
<tr><th>Variables</th><th>Factor1</th><th>Factor2</th><th>Factor3</th><th>Factor4</th></tr>
<tr><td>Coffee</td><td>||</td><td>||||||</td><td>|||||||||||</td><td>|||</td></tr>
<tr><td>Nescafe</td><td>|||||</td><td>|||||||||</td><td>|</td><td>|</td></tr>
<tr><td>Tea</td><td>|||||||</td><td>||</td><td>|||</td><td>||||</td></tr>
<tr><td>Sweetener</td><td>|||||||</td><td>|||||</td><td>|||||</td><td>||||</td></tr>
<tr><td>Biscuits</td><td>|||||</td><td>|||</td><td>|</td><td>|||||||||</td></tr>
<tr><td>Pack_soup</td><td>|||||</td><td>||||||||</td><td>|</td><td>|||</td></tr>
<tr><td>Tin_soup</td><td>|||||||</td><td>|</td><td>|||</td><td>||||</td></tr>
<tr><td>Frozen_fish</td><td>|||</td><td>|||||||||</td><td>||||</td><td>|||</td></tr>
<tr><td>Frozen_veg</td><td>||||||</td><td>||||||||</td><td>||||</td><td>||||</td></tr>
<tr><td>Fresh_apples</td><td>|||||</td><td>||||</td><td>||||||||</td><td>|</td></tr>
<tr><td>Tin_fruit</td><td>||||||||</td><td>|||</td><td>|||</td><td>||||</td></tr>
<tr><td>Jam</td><td>|||||||</td><td>|</td><td>||||||</td><td>|</td></tr>
<tr><td>Garlic</td><td>||||||</td><td>|||||</td><td>|||||||</td><td>|||</td></tr>
<tr><td>Butter</td><td>|||</td><td>||</td><td>|</td><td>|||||||||</td></tr>
<tr><td>Margerine</td><td>|||||</td><td>|</td><td>||||</td><td>||||</td></tr>
<tr><td>Olive_oil</td><td>||||</td><td>||||</td><td>||||</td><td>|||||||||||</td></tr>
<tr><td>Yoghurt</td><td>||</td><td>||||||</td><td>|||||||||</td><td>||||||||</td></tr>
</table>

# Principle component analysis - PCA

## output: the eating habits of Europe - correlations

**Bar Chart of Absolute Factor Loadings after Varimax Rotation**

<table>
<tr><th></th><th>Factors</th><th></th><th></th><th></th></tr>
<tr><th>Variables</th><th>Factor1</th><th>Factor2</th><th>Factor3</th><th>Factor4</th></tr>
<tr><td>Coffee</td><td>||||||||||||||||</td><td>||||</td><td>|||||||</td><td>|||||||</td></tr>
<tr><td>Nescafe</td><td>||||||||</td><td>||||||||||||||</td><td>|||||</td><td>||||||||</td></tr>
<tr><td>Tea</td><td>||||</td><td>|||</td><td>||||||||||||||||</td><td>||||</td></tr>
<tr><td>Sweetener</td><td>||||||||||||||</td><td>|||||||</td><td>||||||||||||</td><td>|||</td></tr>
<tr><td>Biscuits</td><td>|</td><td>||||</td><td>||||</td><td>||||||||||||||||</td></tr>
<tr><td>Pack_soup</td><td>|||||||</td><td>||||||||||||||</td><td>||||||</td><td>||||||</td></tr>
<tr><td>Tin_soup</td><td>||</td><td>|||</td><td>||||||||||||</td><td>||||||||||||</td></tr>
<tr><td>Frozen_fish</td><td>||||||||||||||||||</td><td>||||||</td><td>||||</td><td>|||</td></tr>
<tr><td>Frozen_veg</td><td>|||||||||||||||||</td><td>||</td><td>||||||||</td><td>|||||||</td></tr>
<tr><td>Fresh_apples</td><td>||||||</td><td>|||||||||||||||</td><td>|</td><td>||||||||</td></tr>
<tr><td>Tin_fruit</td><td>|||||</td><td>|||||||||||</td><td>||||||||</td><td>||||||||||||||</td></tr>
<tr><td>Jam</td><td>||</td><td>||</td><td>|||||||||||||||</td><td>||||||||</td></tr>
<tr><td>Garlic</td><td>||||</td><td>|||||</td><td>|||||||||||||||||</td><td>||||</td></tr>
<tr><td>Butter</td><td>|</td><td>|</td><td>|</td><td>|||||||||||||</td></tr>
<tr><td>Margerine</td><td>||</td><td>||||</td><td>||||||||||||</td><td>||||</td></tr>
<tr><td>Olive_oil</td><td>|||</td><td>||</td><td>|||||||||||||||</td><td>|||||||</td></tr>
<tr><td>Yoghurt</td><td>||</td><td>|||||||||||||||||||</td><td>||</td><td>|||||</td></tr>
</table>

# Principle component analysis - PCA

## output: the eating habits of Europe

**Factor Structure Summary after Varimax Rotation**

| Factors | | | |
|---|---|---|---|
| **Factor1** | **Factor2** | **Factor3** | **Factor4** |
| Frozen_fish | Yoghurt | Garlic | Biscuits |
| Frozen_veg | Fresh_apples | Tea | Tin_fruit |
| Coffee | Nescafe | Olive_oil | Butter |
| Sweetener | Pack_soup | Jam | Tin_soup |
| | Tin_fruit | Sweetener | |
| | | Margerine | |
| | | Tin_soup | |

## Principle component analysis - PCA

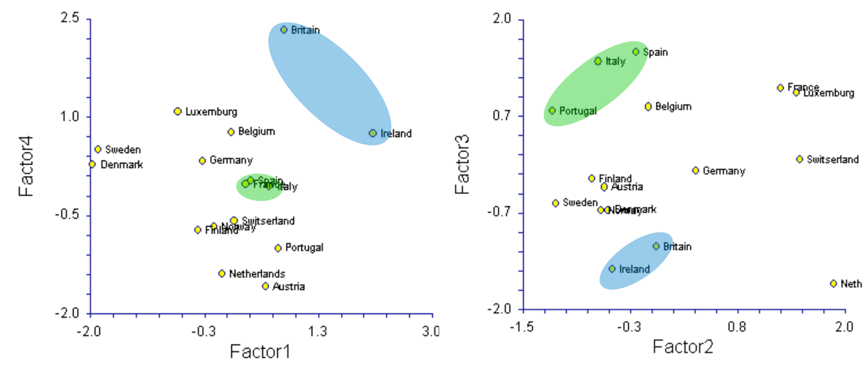
### output: the eating habits of Europe - new row transformation

Factor Score after Varimax Rotation

| | Factors | | | |
|---|---|---|---|---|
| Row | Factor1 | Factor2 | Factor3 | Factor4 |
| 1 | -0.3644 | 0.3788 | -0.0904 | 0.3360 |
| 2 | 0.6165 | -0.6782 | 1.4195 | -0.0599 |
| 3 | 0.2665 | 1.2995 | 1.0593 | -0.0254 |
| 4 | -0.0786 | 1.8754 | -1.6456 | -1.3972 |
| 5 | 0.0605 | -0.1348 | 0.7957 | 0.7732 |
| 6 | -0.7204 | 1.4754 | 0.9845 | 1.0832 |
| 7 | 0.8281 | -0.0470 | -1.1348 | 2.3280 |
| 8 | 0.7444 | -1.1724 | 0.7406 | -1.0016 |
| 9 | 0.5602 | -0.6078 | -0.3117 | -1.5889 |
| 10 | 0.0995 | 1.5130 | 0.0692 | -0.5877 |
| 11 | -1.8878 | -1.1434 | -0.5359 | 0.4995 |
| 12 | -1.9707 | -0.5770 | -0.6248 | 0.2745 |
| 13 | -0.1946 | -0.6459 | -0.6321 | -0.6754 |
| 14 | -0.4299 | -0.7455 | -0.1961 | -0.7278 |
| 15 | 0.3406 | -0.2631 | 1.5489 | 0.0244 |
| 16 | 2.1301 | -0.5269 | -1.4462 | 0.7452 |

## Principle component analysis - SIMCA

### output: the eating habits of Europe




## PLS-R and PLS-DA

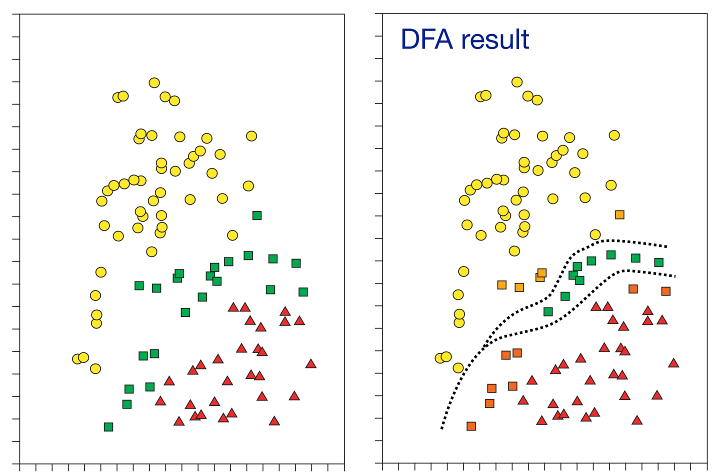
### An extension to eigenvector methods with a dependent variable

PCA and FA re-cast the **independent variable** matrix into a new coordinate system aligned with the directions of **maximum variance** with the aim of separating noise from information, reducing the dimensionality of your data, and identify processes

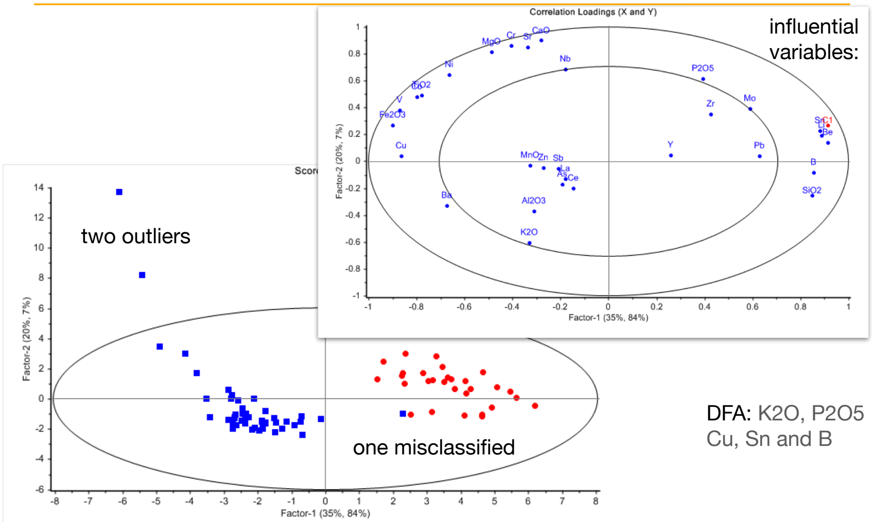
PLS-R and PLS-DA re-cast the **independent variable** matrix into a new coordinate system aligned with a **dependent variable** ( Y = $f$(**X**) ) with the aim of classification (-DA) or quantification of a regression model (-R), for example for calibration.

> You can of course do a DA or R based on the original variables, but you here make the assumption that there are directions in your data that better line up with Y than the original variables —> you obtain those from a PCA-style transformation of your data

## PLS-DA example with the Unscrambler



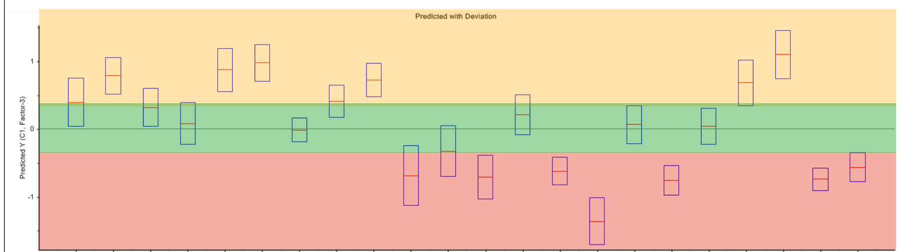
## PLS-DA example with the Unscrambler




**DFA:** K2O, P2O5
Cu, Sn and B

## PLS-DA example with the Unscrambler

predictions from the PLS model for the unknowns:




## PLS-DA example with the Unscrambler