# Examples on Variable Selection in PCA in Sensory Descriptive and Consumer Data

**Per Lea, Frank Westad, Margrethe Hersleth**
**MATFORSK, Ås, Norway**

**Harald Martens**
**KVL, Copenhagen, Denmark**

**6th Sensometrics Meeting**
**Dortmund, July 31 - August 2, 2002**

# Outline of presentation

- Introduction
- Theory: Methods
- Practice: Applications
- Summary

# Background

- Increasing number of measurements/data sources

- Not enough professional data analysts in the world
  Þ YOU have to analyse your own data

  - Choice of method(s)
  - Safe use of the methods
  - Interpret - draw conclusions
  - How to present results to colleagues, client, boss….

# Multivariate modelling - Important aspects

- Outlier detection and their influence on the model
- Validation and model dimensionality
- Interpretation of model parameters and underlying structures
- Variable selection

Þ Estimation of uncertainty is vital in all these matters!

> “A number without any associated uncertainty is close to a random number”
>
> - Peter Wentzell, Halifax, Canada

# Bilinear models

- One block of data (“X”)
  - Assume a model which is linear in scores and loadings; extracted in terms of *factors* (so-called latent variables)
  - The scores are linear combinations of the original variables
  - Example: Principal Component Analysis (PCA)

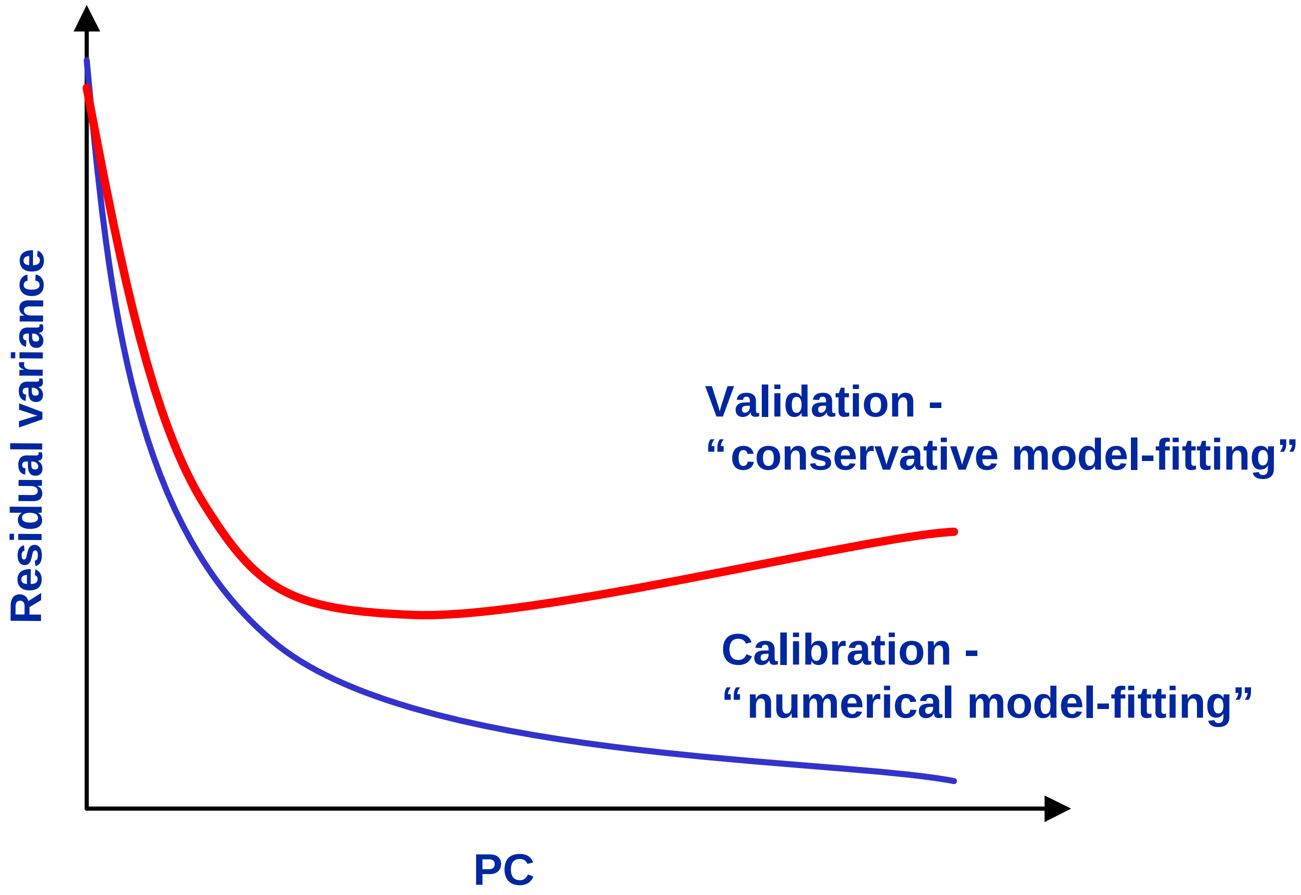
- Two blocks of data (“X and Y”)
  - Regression methods which decompose the matrices in terms of factors/components
  - Examples:
    - Principal Component Regression (PCR)
    - Partial Least squares Regression (PLSR)

# Validation

- Data-model based
  - Cross-validation (one set of objects)
    - We can validate by taking “one product out”,”one day out”, “one judge out”, “one consumer category out” etc.
  - Test set validation (two or more set of objects)

- System/process based
  - Validate on country level
  - Between different panels
  - … and more

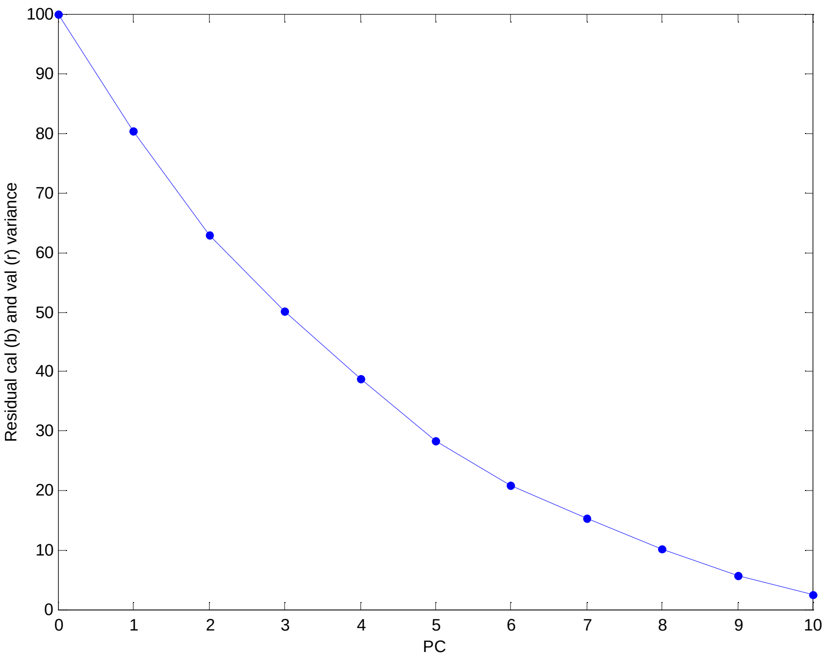
# Residual variance - validation

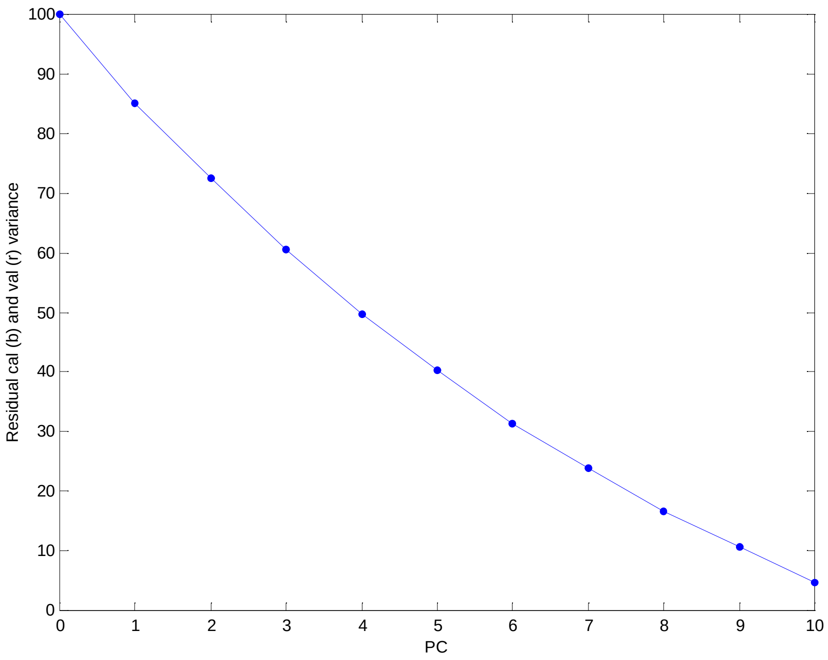


# Validation is essential

## Consumer questionnaire attitudes (103 ´11) Residual variance

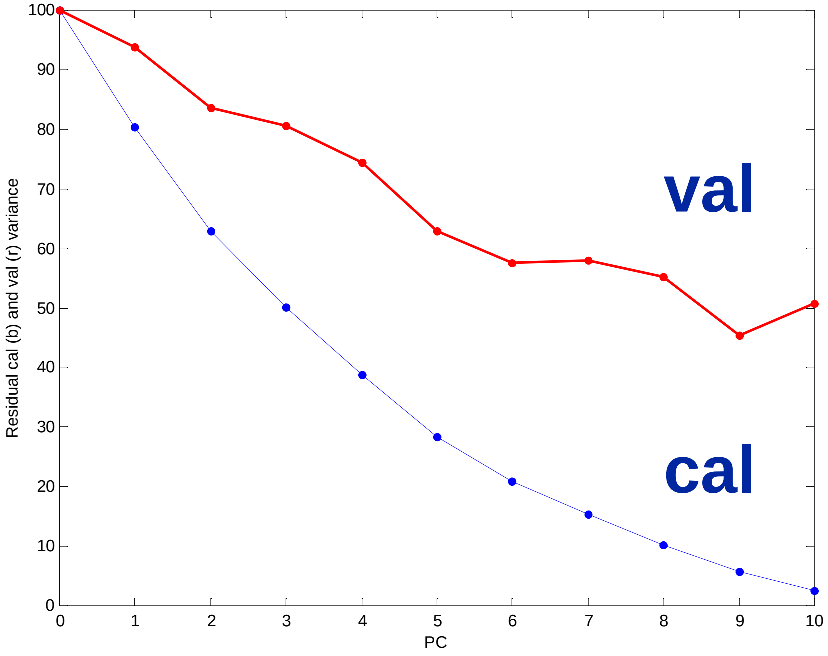
## Random numbers (103 ´11) Residual variance



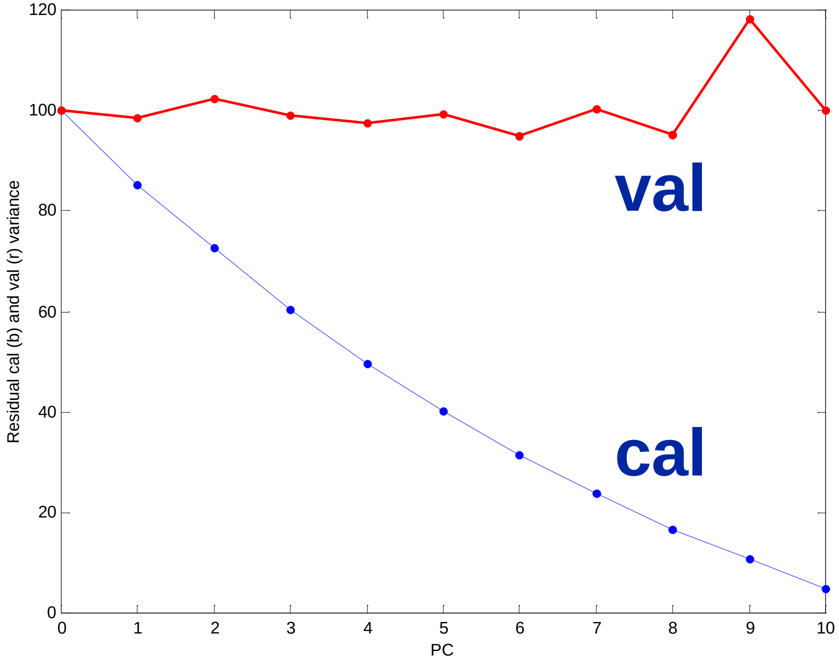


# Validation is essential

## Consumer questionnaire Attitudes (103 ´11) Residual variance



## Random numbers (103 ´11) Residual variance



# Rank

- Optimal number of dimensions
- What do we mean by rank
  - Numerical rank
  - Statistical rank
  - Application specific rank (using background knowledge)

# How to find the *correct* rank in PCA

- **Some possible approaches:**
  - **Bartlett’s test**
  - **SCREE plot**
  - **Broken stick**
  - **Keep all eigenvalues > 1 (Kaiser’s test) (Warning: do not use this one!)**
  - **Sum of PCs explaining > 95% of the variance**
  - **Cross validation**
  - **Human interpretation**

# Significance of loadings in PCA

- PCA is often applied as an explorative tool
- Important issues:
  - The number of relevant components
  - Which variables are significant on the components
- Resampling methods such as jack-knifing and bootstrapping are valuable tools for estimation of uncertainties in multivariate models
- Some other approaches:
  - Keep loadings > 0.3
  - Keep loadings > specified value based on number of samples (from tables based on simulations)
  - Keep subset of variables to preserve the overall information

# Uncertainty estimates

- Objectives
  - To estimate uncertainties in the model parameters
  - Reflect the *actual* data structure (outliers, skewness)

- Some approaches for estimation (Efron and Tibshirani)
  - Jackknifing/Cross validation (JK/CV)
  - Bootstrapping

- Cross-validation for individual segments might give components that are mirrored or flipped

  Þ Restricted Procrustes rotation

# Uncertainty estimates

**The variance of the model parameters can be estimated by jack-knifing**

**Example: Loadings,** *p*

$$s^2(p) = \left( \sum_{m=1}^{M} (p - p_m)^2 \right) \left( {(M-1)} \big/ {M} \right)$$

***M* = the number of segments**

***$s^2$(p)* = estimated uncertainty (variance) of *p***

***p* = the loading using all *N* objects**

***$p_m$*= the loading using all objects except the object(s) left out in cross validation segment *m*.**

# Uncertainty estimates

- A univariate t-test is performed for each element $p_k$ in the loading vector relative to the square root of it's estimated uncertainty, s($p$)
- Use the estimates for an approximate confidence interval for each variable
- The method seems robust for various cross validation schemes (number of segments, repeated random selection)

# PCA of sensory data

- Should one scale sensory data or not?
  - If not, the variables which are spanned the most will dominate
  - If scaled, small numerical differences might (erroneously) influence the result

- To reveal if scaling should be used or not, plot correlation loadings
- The correlation loadings are the correlations between the variables and the PC's

$$r_{\mathrm{ka}} = p_{\mathrm{ka}} \sqrt{\mathbf{t}_{\mathrm{a}}^{\mathrm{T}}\mathbf{t}_{\mathrm{a}}} \Big/ \sqrt{\mathbf{e}_{0,\mathrm{k}}^{\mathrm{T}}\mathbf{e}_{0,\mathrm{k}}}$$

PCA model: X = TP' + E

How much is explained in PC a?

Variance before modeling starts

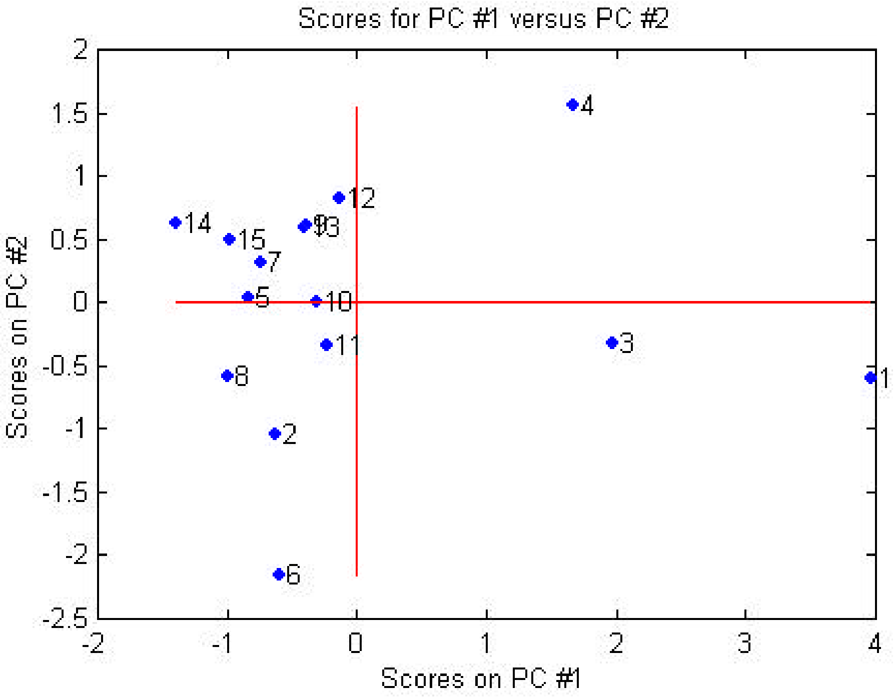
# Example 1: PCA on sensory descriptive data

- Product: Vanilla ice-cream
- 15 samples
- 18 sensory attributes
- Employ PCA: Three components are relevant

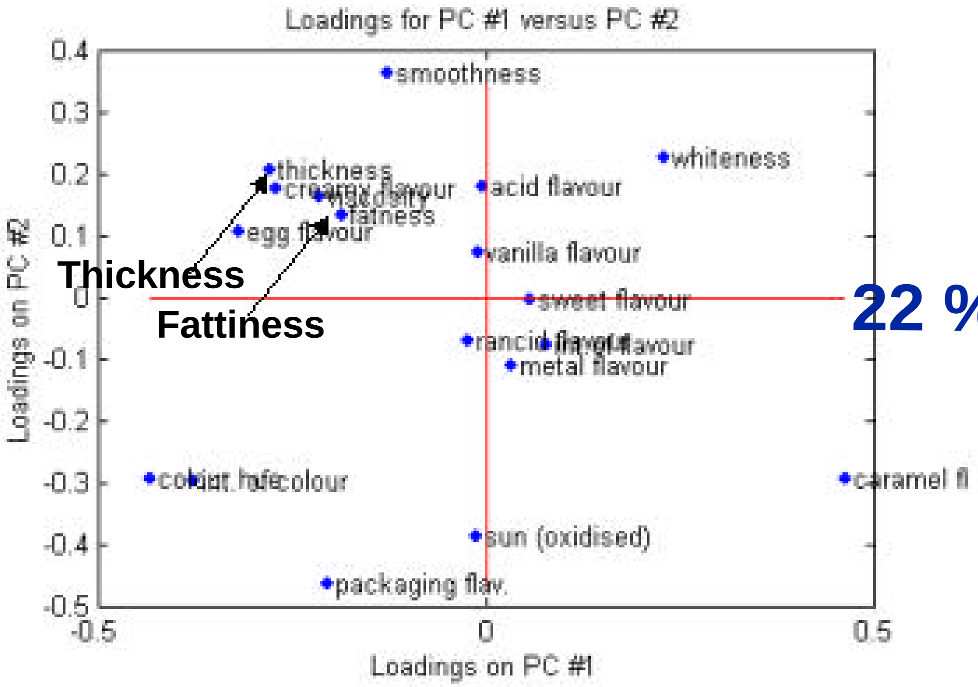
# Scores and loadings

## Vanilla Ice-cream; 15 products - 18 attributes

22 %



55%



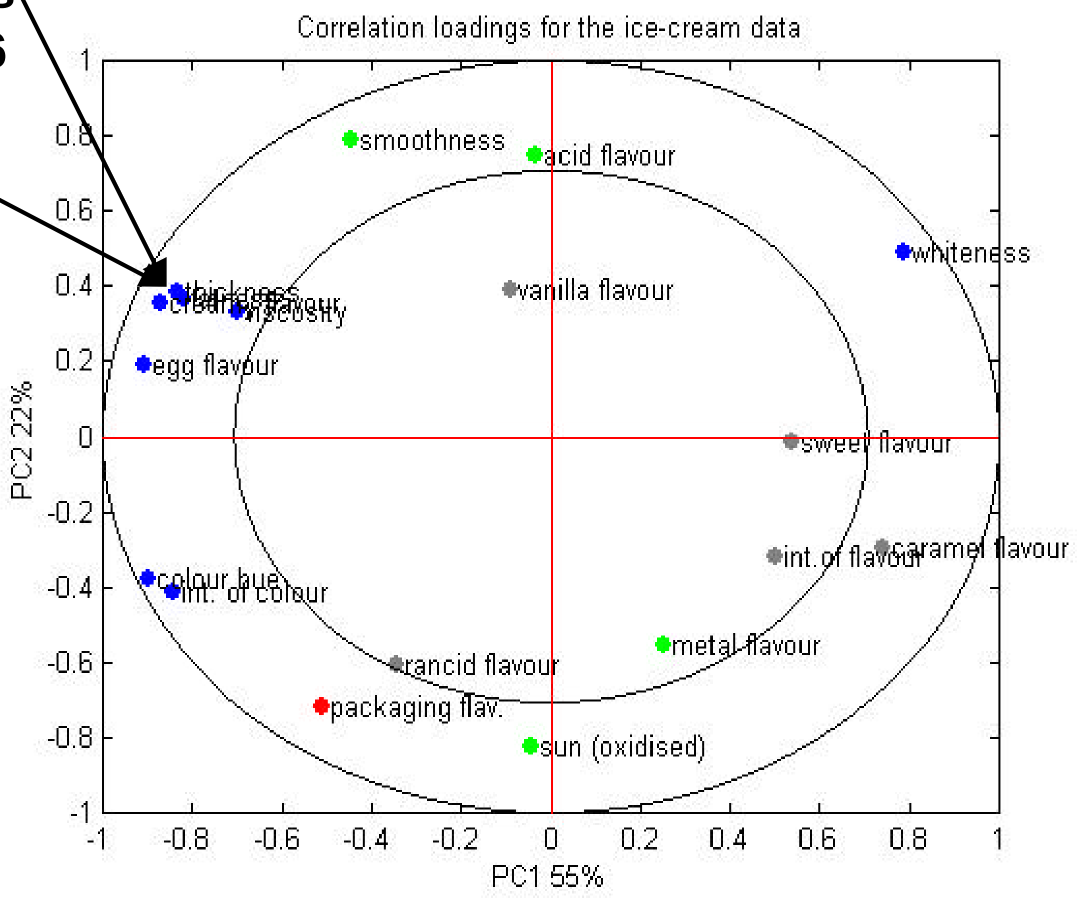
22 %

55%

# Correlation loadings

## Ice-cream

Correlation between thickness and fattiness: 0.96



Significant on PC 1

Significant on PC 2

Significant on both

Not significant

# How can we judge if the estimates are *correct*?

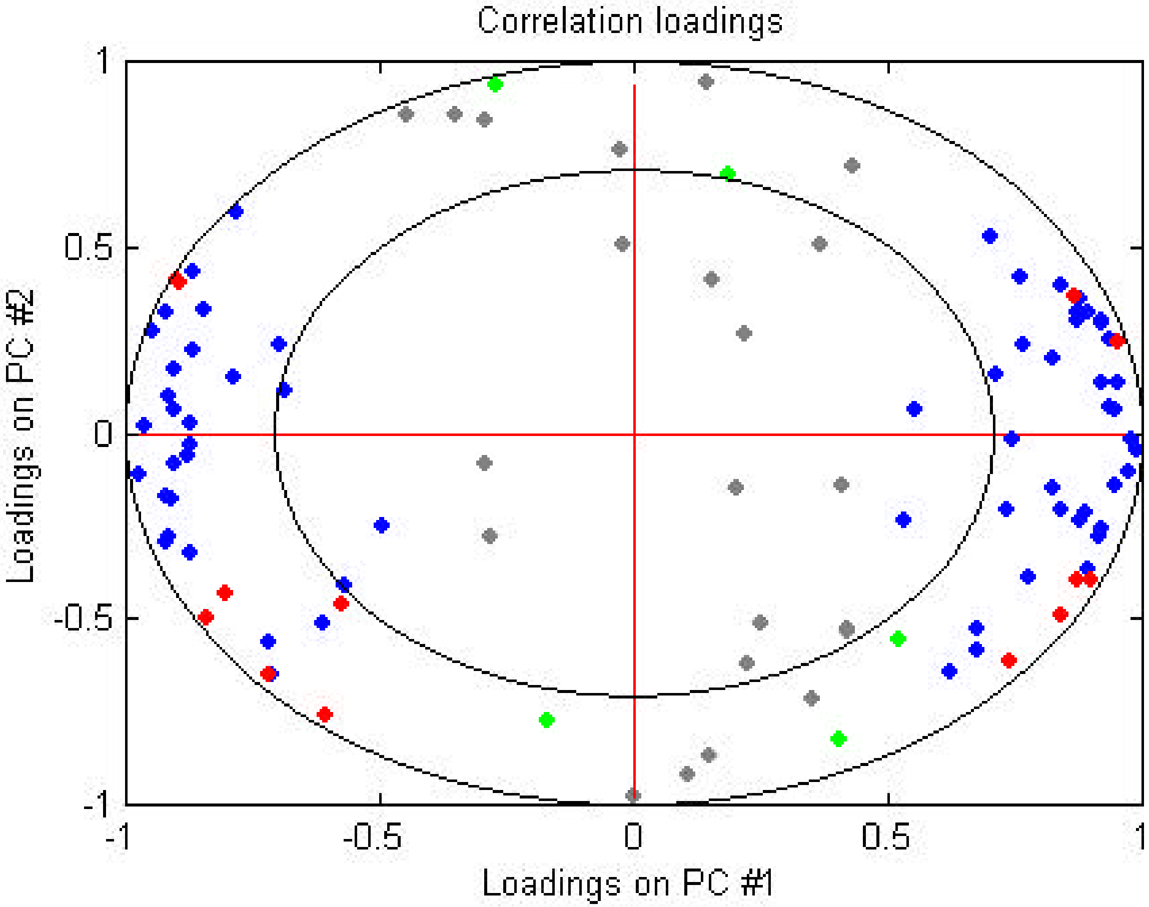
- Compare to ANOVA when “truth is known”
  - Pizza product
  - 8 samples from a $2^3$ factorial design, 29 sensory attributes
  - Analyse the data with ANOVA and PCA
- Results
  - Significant effects for 16 of the attributes (ANOVA)
  - 16 attributes significant on PC1, PC2, PC3 in the JK PCA
  - 14 of these were the same as for ANOVA

# Example

- Mozzarella cheese
- 6 products for consumer test
- 105 consumers
- 3 components were found to be relevant
- Which consumers are informative? (Significance level 20%)

# Correlation loadings

## Mozzarella Cheese; 6 products - 105 consumers



Significant on PC 1
Significant on PC 2
Significant on both
Not significant

# Summary

- Significance tests in PCA make interpretation easier
- Correlation loadings reveal the correlation structure also when variables are not scaled
- Validation is essential to assess the model dimensionality
- Restricted Procrustes is used to avoid rotation in cross-validation (flipping, mirroring)