Three-Mode Analysis in Practice

Pieter M. Kroonenberg

Department of Education, Leiden University
kroonenb@fsw.leidenuniv.nl

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Part 1

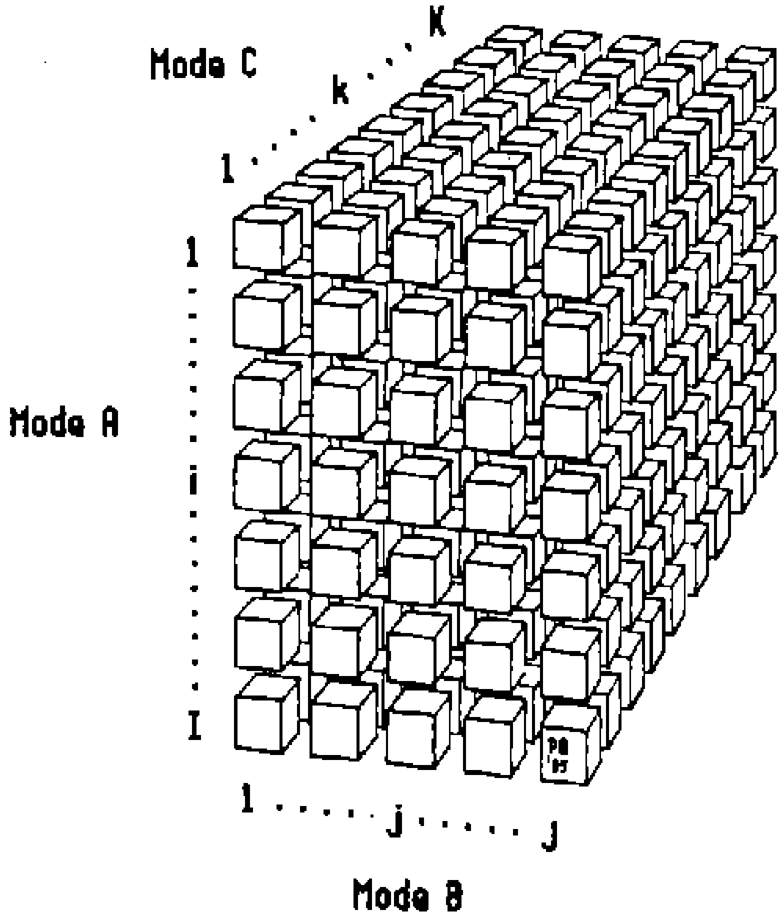
Introduction Three-Way Data

Three-Way Data Array

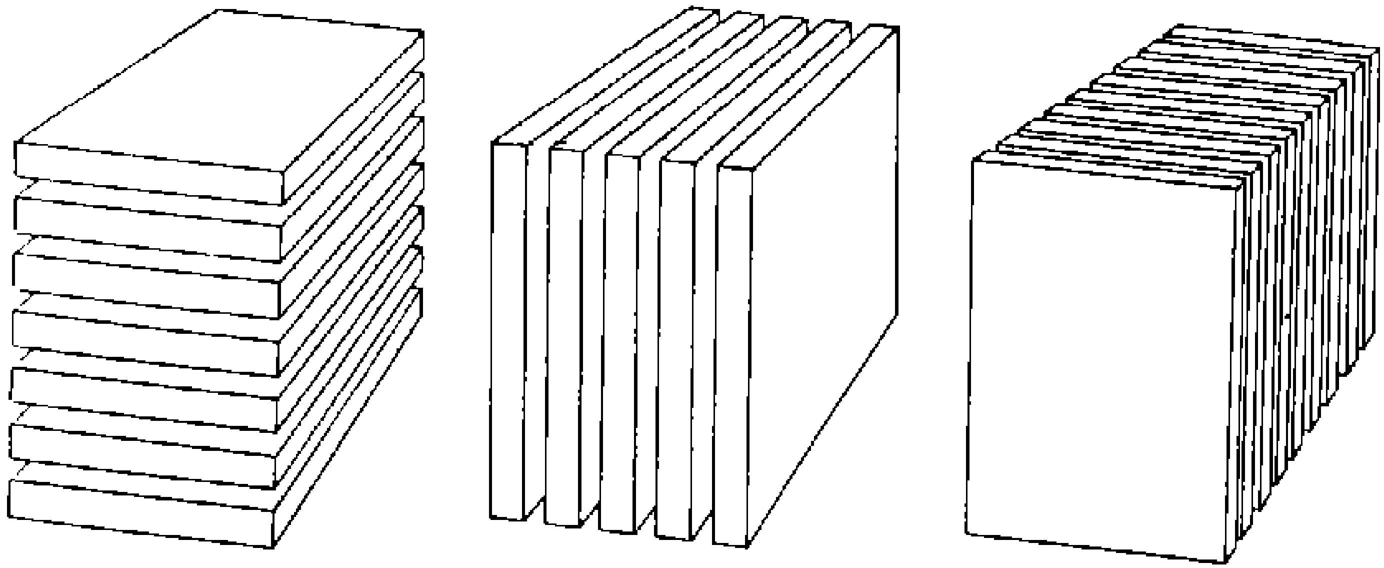
$\underline{\mathbf{X}}$

<u>underlining</u> *indicates* (three-way) array

- Mode A = first mode
  - ► $i = 1, \ldots, I$
- Mode B = second mode
  - ► $j = 1, \ldots, J$
- Mode C = third mode
  - ► $k = 1, \ldots, K$



Slices



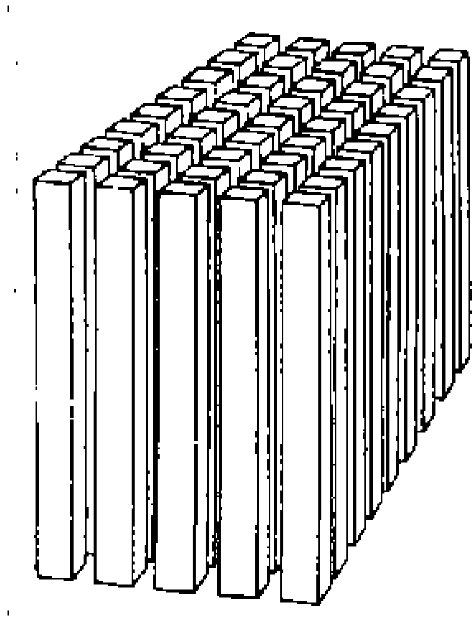
$\mathbf{X}_i$ Horizontal slices

$\mathbf{X}_j$ Lateral slices

$\mathbf{X}_k$ Frontal slices

Slices are matrices

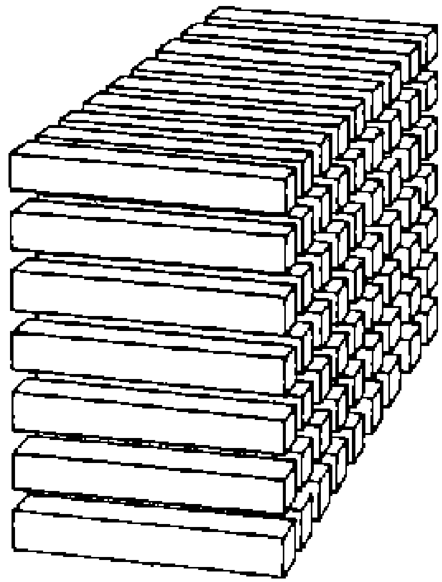
Fibers



$\mathbf{x}_{jk}$

Columns

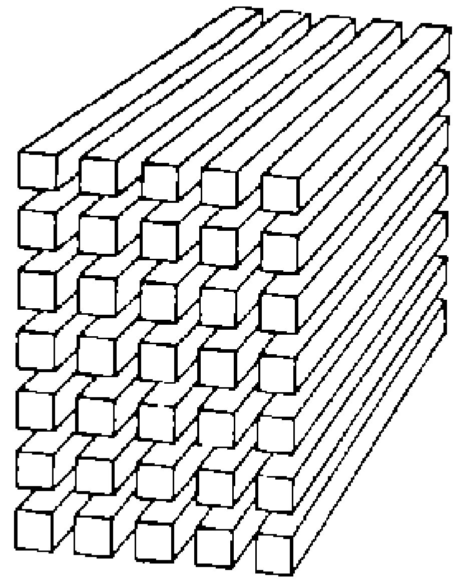
(column fibers)



$\mathbf{x}_{ik}$

Rows

(row fibers)



$\mathbf{x}_{ij}$

Tubes

(depth fibers)

Fibers are vectors

AThree-Mode Research Design

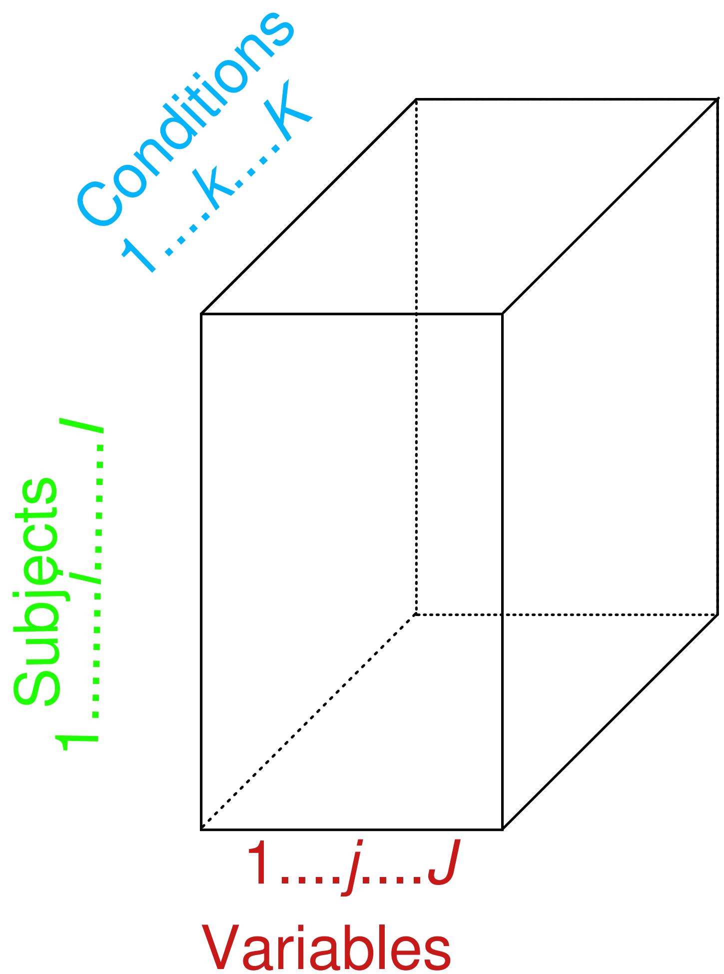
In personality, attitude, marketing, sensory perception, semantic differential and many other kinds of research, the opinions of subjects are collected on several different topics, concepts or in different situations or under different conditions using several variables, scales, or questions.

THREE-MODE DATA

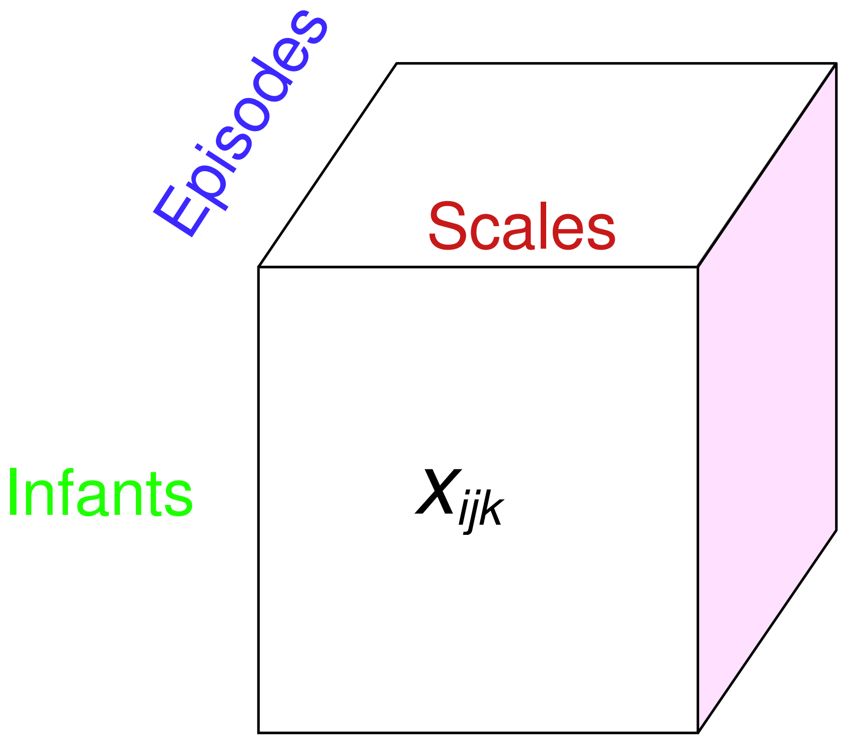
- Profile Data
  - I Subjects
  - J Variables
  - K Conditions
- Rating Data
  - I Concepts
  - J Scales
  - K Subjects
- Similarity Data
  - J' Scales
  - J Scales
  - K Subjects

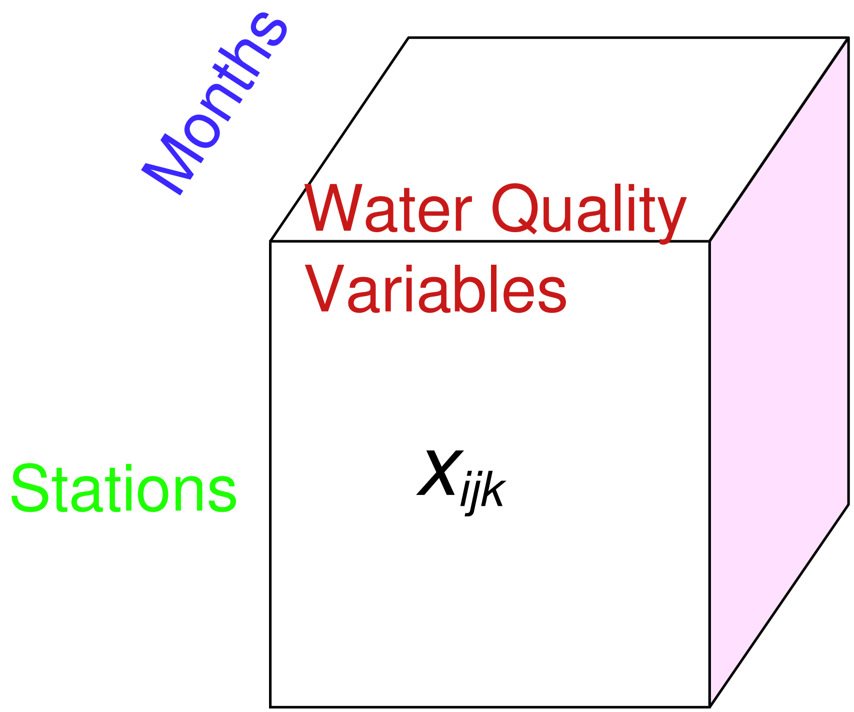
Some Three-Way Designs

Three-Mode Profile Data



Examples Three-Mode Profile Data



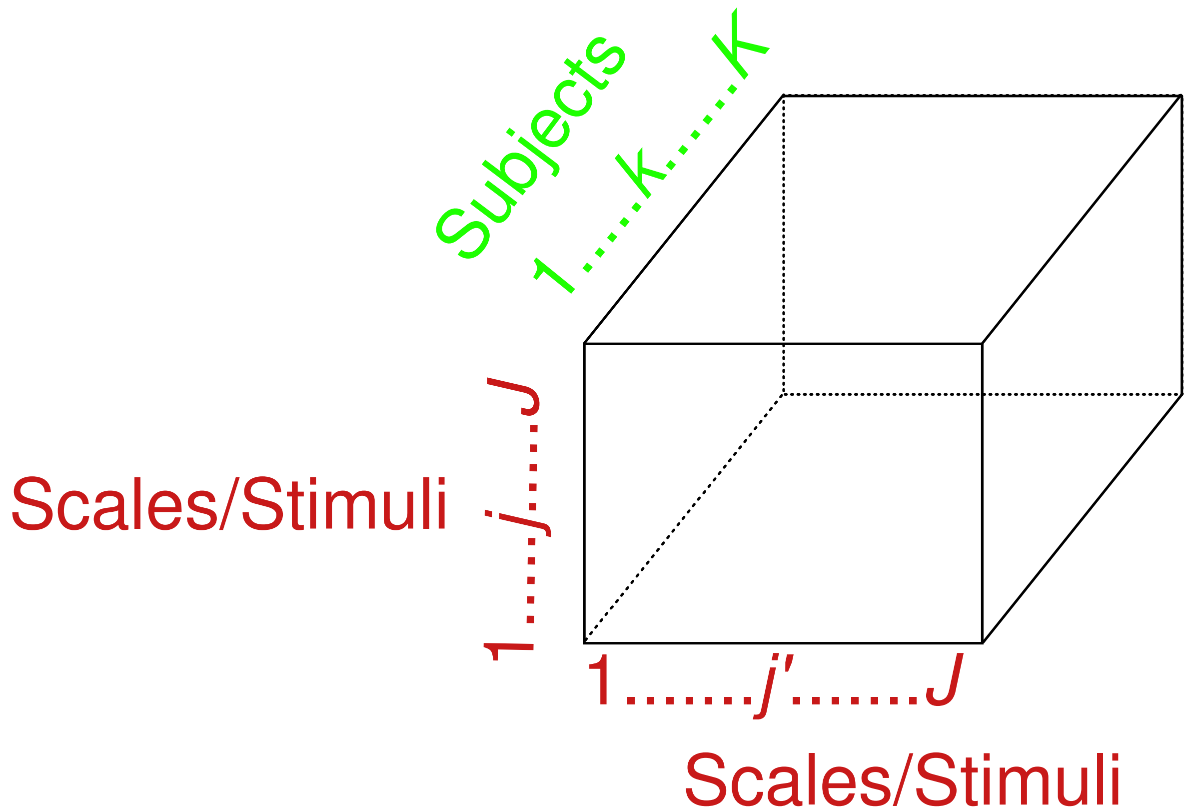


x_{ijk} score on scale j (avoidance) by infant i (Marie) during episode k (infant alone in room)

x_{ijk} score on variable j (oxygen) at station i (upstream) in month k (January)

Similarity (or correlation) data

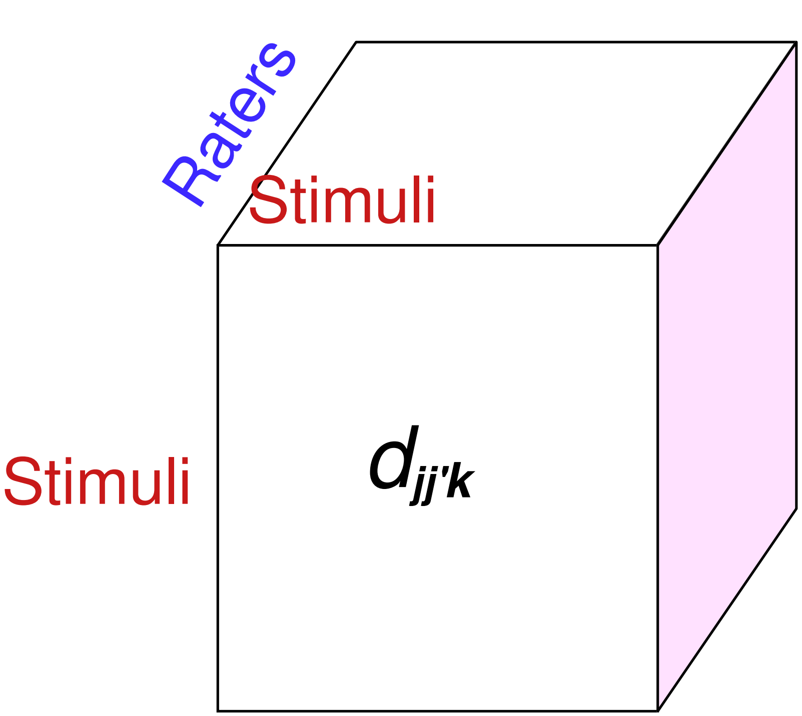
(derived data)

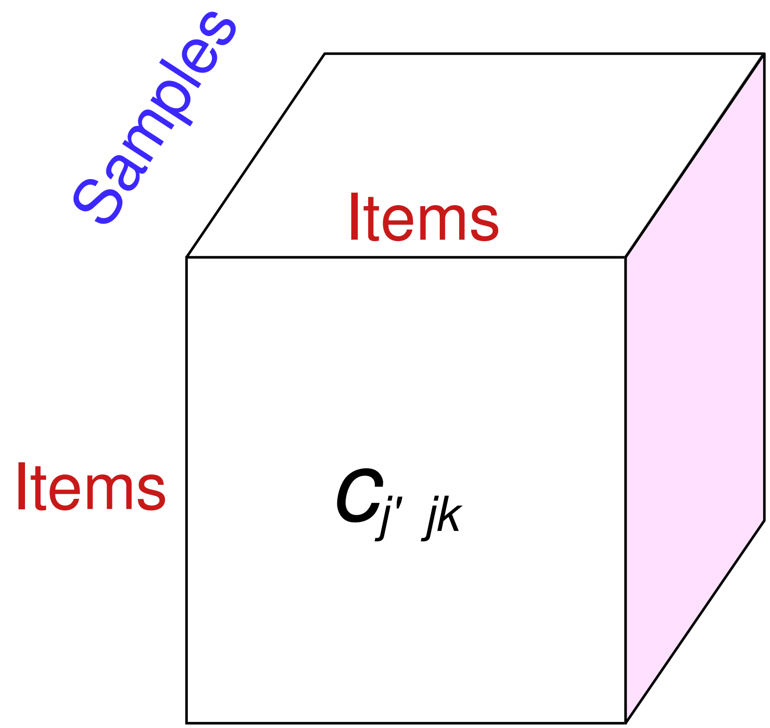


$s_{jj'}$ similarity between stimuli j' and j

$r_{jj'}$ correlation between scales j' and j

Examples Similarity and Correlation Data





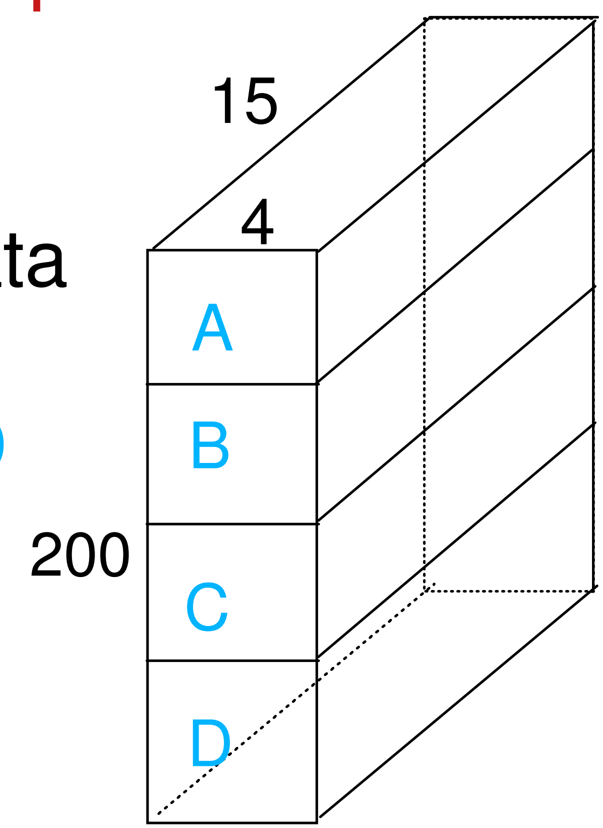
$d_{jj'k}$ = similarity rating of item j (inari soba) and item j' (tempura ramen) by rater k (Murakami sensei)

$c_{j'jk}$ correlation between item j (Mazes of IQ test) and item j' (Digit span of same IQ test) in sample k (Age group 14)

Improving inspection methods for surface roughness of metals

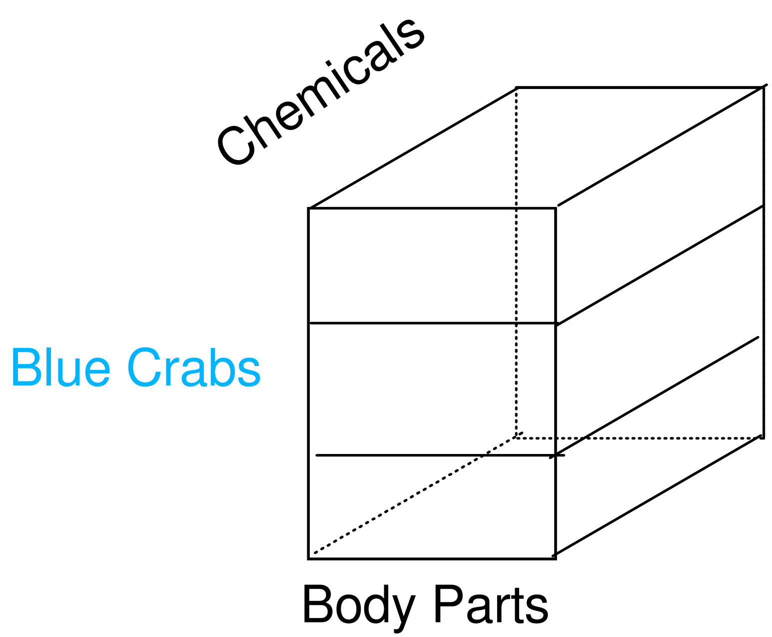
Example from IPRI, Tsukuba, Japan

- Profile Data
  - ► 200 inspectors rated 15 loaves on 4 types of roughness
  - ► 200 x 4 x 15 three-mode profile data
  - ► 4 types of inspectors; A,B,C and D



Example Blue Crabs

- Blue crabs are nice to eat, but not if they are diseased due to toxic substances in their body
- Gemperline et al. (*Analytical Chemistry*, 1992)
  - Study of the presence of various chemicals in several parts of the crabs bodies at three locations



Partial Results: Blue Crab Analysis

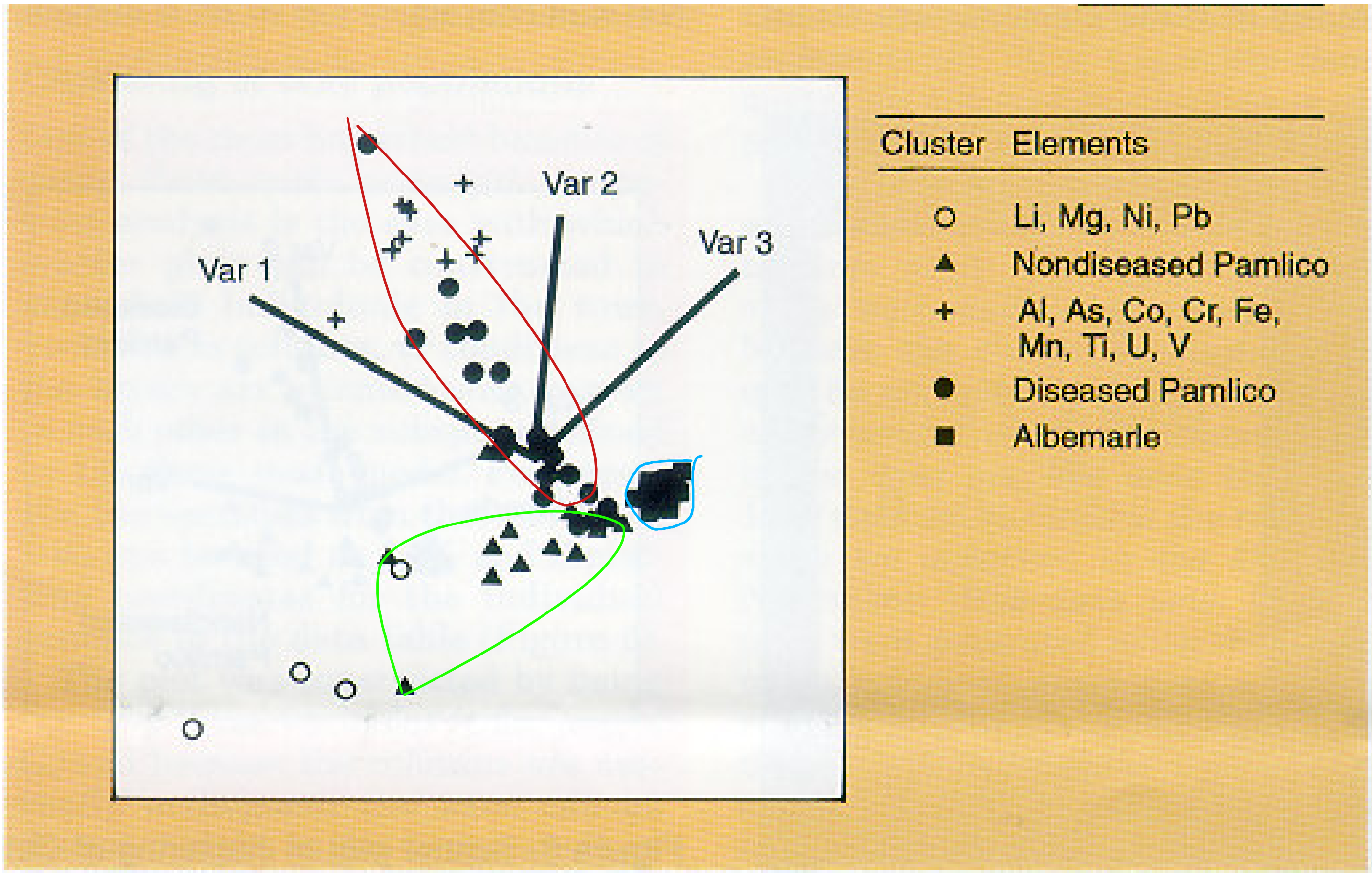


Figure 8. Joint plot showing showing clustering of elements by crab population for the 1989 data set.

Diseased Pamlico crabs contribute a large amount of variance to the variables Al, As, Co, Cr, Fe, Mn, Ti, U, and V. Nondiseased Pamlico crabs contribute a large amount of variance to the variables Li, Mg, Ni, and Pb. Other elements are omitted from the plot because they did not appear to cluster near any of the crab populations.

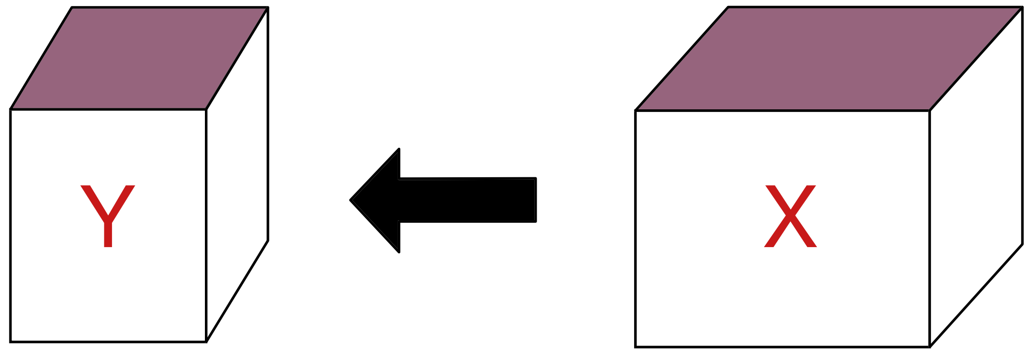
Structures for Arrays

Dependence and Interdependence

Dependence Structures

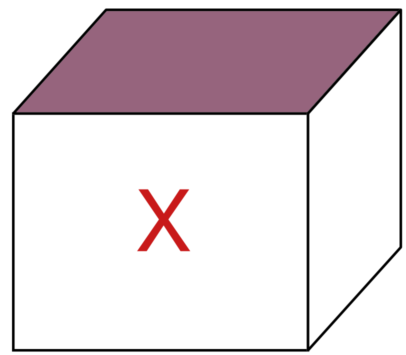
Two kinds of variables:

- criterion variables - **Y**
- predictor variables - **X**



One single type of variables

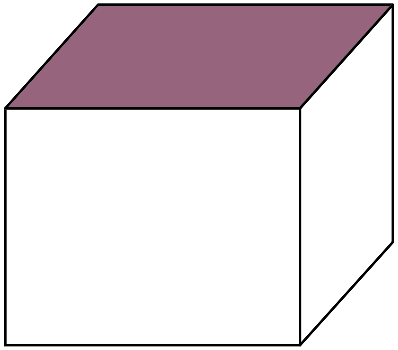
Interdependence Structures



Interdependence
(fully crossed)

Repeated Measures Data

- Fully crossed data: All subjects have scores on all variables at all occasions (except for missing data)
- Generally: Three-mode three-way
- Often used for direct modelling

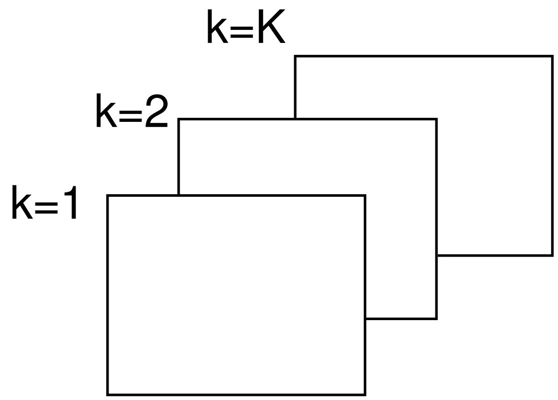


Interdependence

Cross-sectional

Multi-Set Data

- Different samples each generate a matrix
- "Scores" comparable within each matrix or matrix conditional
- "Scores" are often correlations, covariances, similarities, etc. or Two-mode three-way data



Interdependence

Derived Three-Way Data

Examples

- Sets of correlation (or covariance matrices), derived from profile data
- Frequency counts => Multiway contingency tables
- "Indirect" similarity data derived from profile data

Part 2

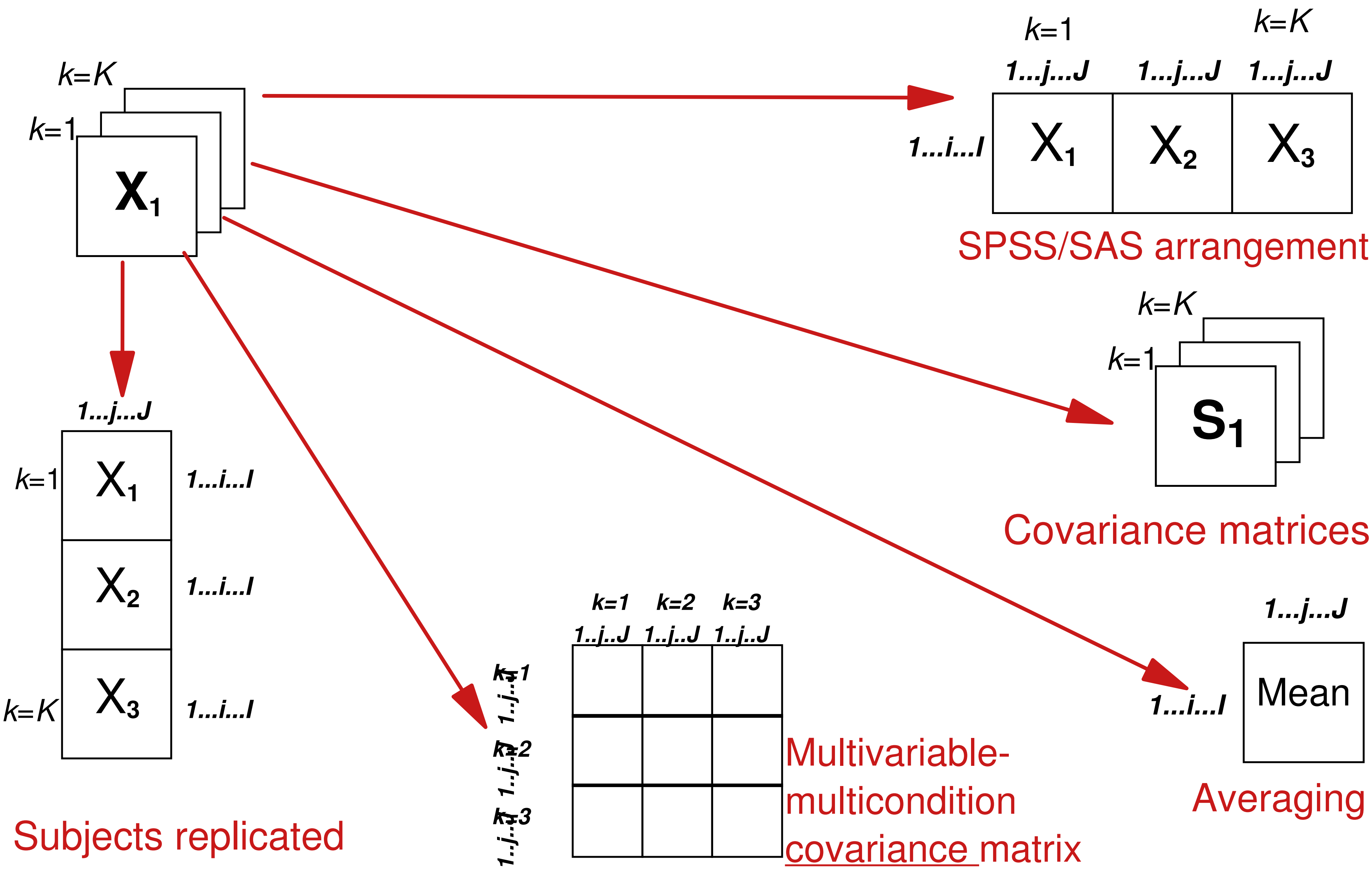
Modelling Three-Mode Data

Types of Analysis Techniques

Stochastic-Nonstochastic- Parameter estimation

- Stochastic Techniques
  - Use of distributional assumptions
  - Subjects are replications and not necessarily interesting as individuals
- Data-Analytic Techniques
  - 'Population' techniques
  - Subject are interesting as individuals: Interest in individual differences
- Parameter estimation
  - A (physical) model is known to apply and estimates of the parameters of the model are of primary interest.

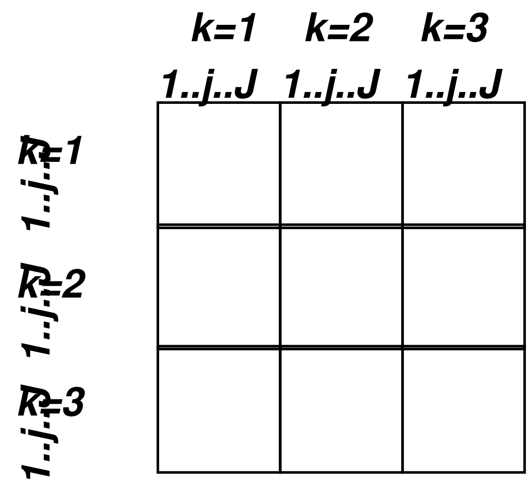
Traditional Approaches to Profile Data



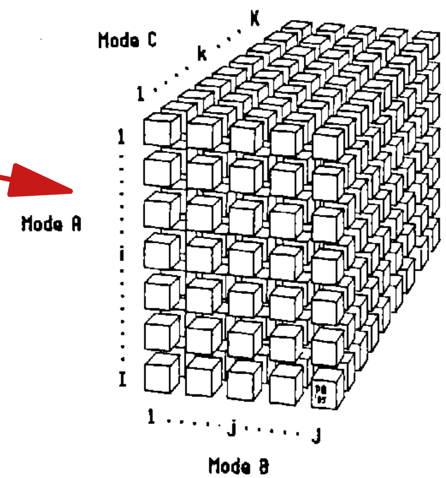
Stochastic Models

- Repeated measures multivariate analysis of variance

- Structural equations modelling on multivariable-multicondition matrix
  (=multitrait-multimethod matrix)



- Three-way analysis of variance without replications (one observation per cell)



Multivariate Repeated Measures Data

$$\begin{array}{c|c|c|c|} & k=1 & & k=K \\ & 1\ldots j\ldots J & 1\ldots j\ldots J & 1\ldots j\ldots J \\ \hline 1\ldots i\ldots I & X_1 & X_2 & X_3 \\ \hline \end{array}$$

SPSS/SAS arrangement

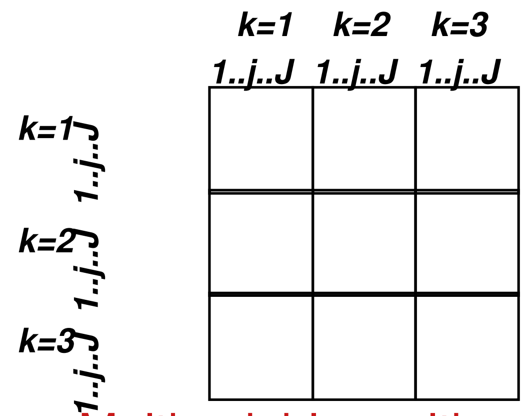
Repeated measures analysis of variance
with of without a design on the subject mode

- interpretation of significant multivariate trends
- interpretation of significant univariate trends
- interpretation of significance between group effects (if design is available on subjects)
- Little regard for individual differences, only as groups
- Problems with large interactions and complex structure in variables, lack of ordering in conditions

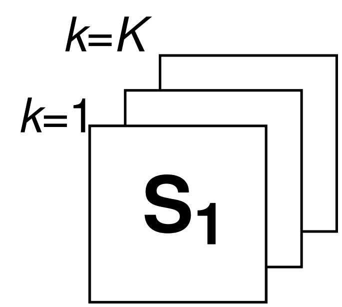
Covariances

(derived data)

- Structural equation modelling of *multivariable- multicondition matrix*
- Structural equation modelling of *set of covariance matrices*
  - if a good model fit, easy interpretation (*a priori* known)
  - needs large amounts of data for testing of models
  - strong assumptions about distributions and variable structure
  - No regard for individual differences

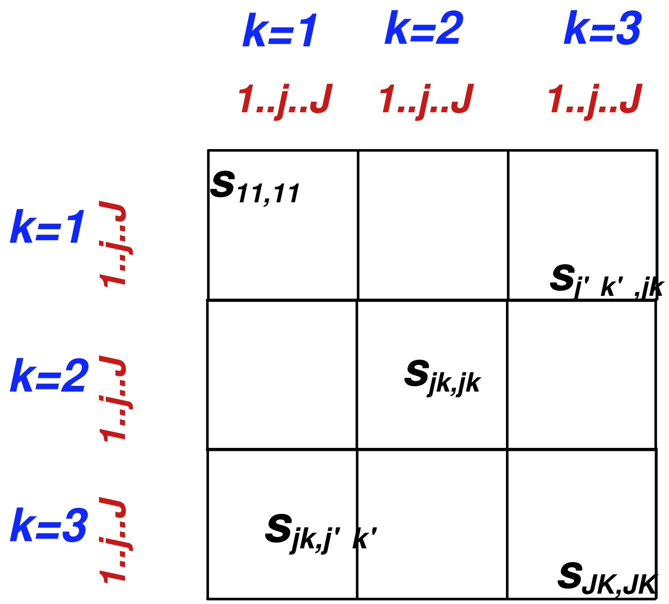


Multivariable-multicondition covariance matrix



Set of covariance matrices

Multimode Covariance Matrix



$s_{jk,jk}$ = *variance of variable j measured at time k*

$s_{j'k',jk}$ = *covariance of variable j measured at time k with variable j' measured ar time k'*

Common Nonstochastic Models

- Tucker2 model
  - Three-mode principal component analysis with extended core array
- Tucker3 model
  - Three-mode principal component analysis with full core array
- Parafac model
  - Parallel factors model [actually component model] with superdiagonal core array

Two-Mode PCA: Problem

variables

subjects $\mathbf{X} = \mathbf{A}\,\mathbf{P'}$ loadings for variables

scores for subjects

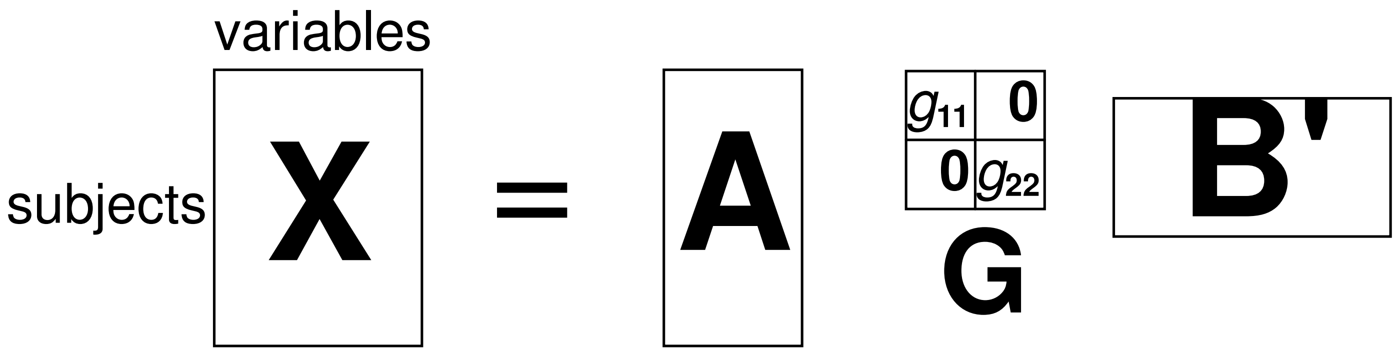
subjects

variables $\mathbf{X'} = \mathbf{Q}\,\mathbf{B'}$ 'loadings' for subjects

'scores' for variables

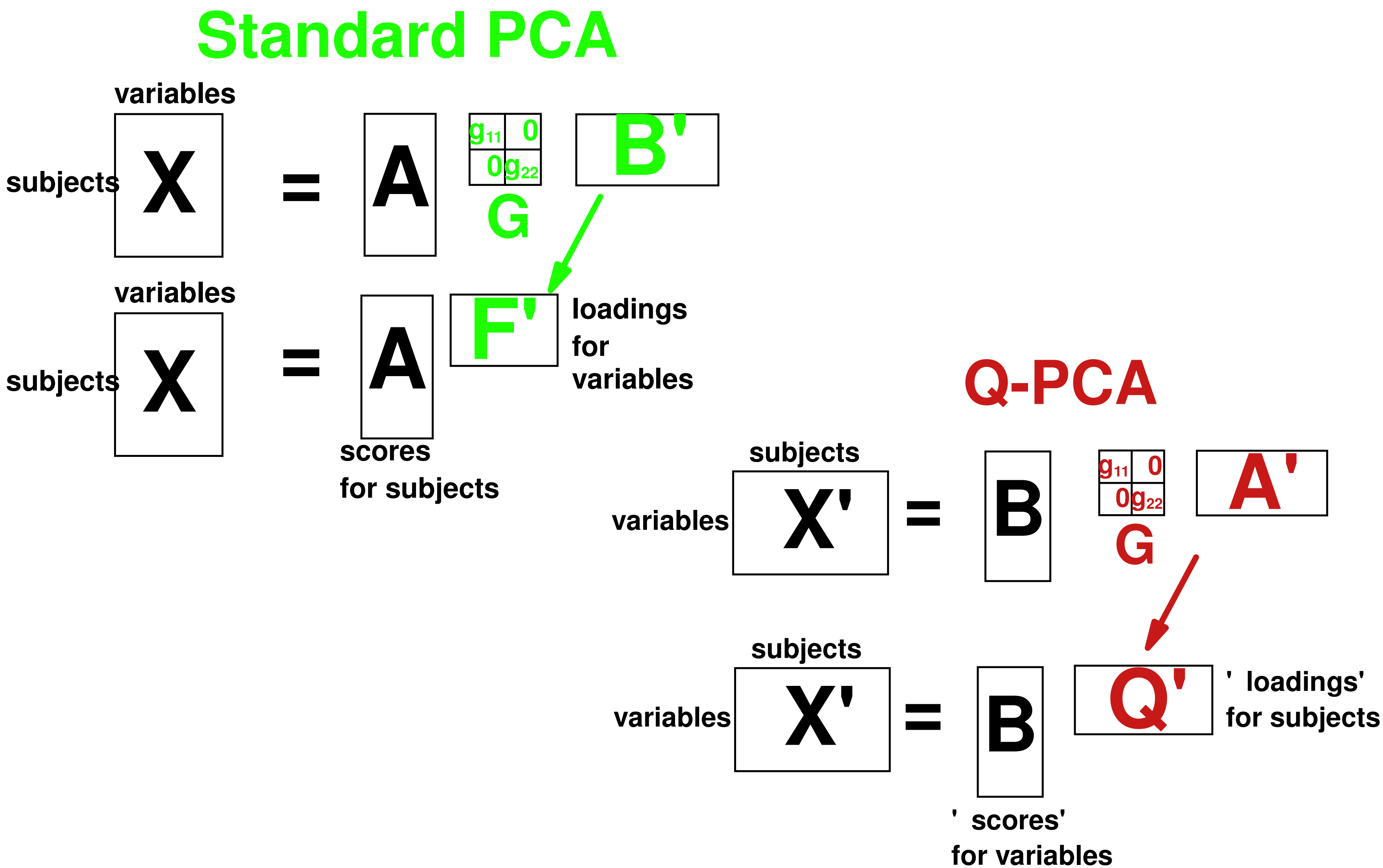
One data matrix: Two decompositions ????

Two-Mode PCA: Solutions
Singular Value Decomposition

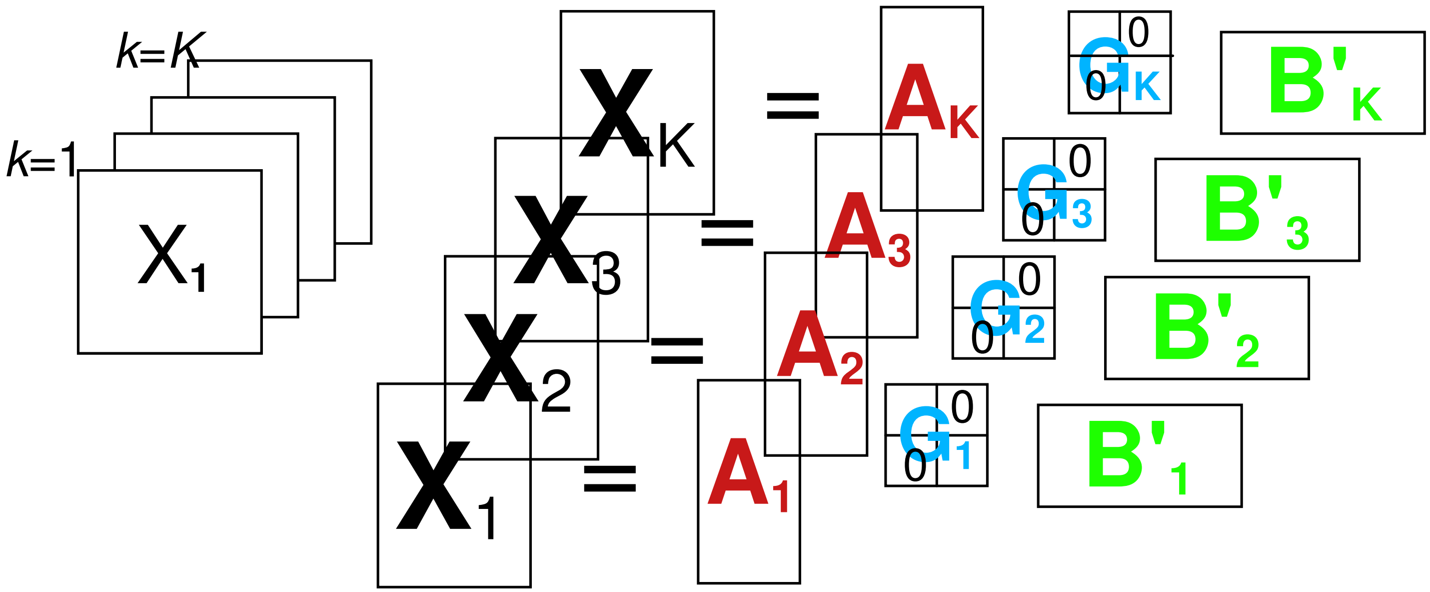


- The singular value decomposition is the basic structure of a matrix
- $\mathbf{A}'\mathbf{A} = \mathbf{I}$, $\mathbf{B}'\mathbf{B} = \mathbf{I}$, $\mathbf{G}$ = diagonal ($g_{12} = g_{21} = 0$)
- $\mathbf{P} = \mathbf{BG}$ & $\mathbf{Q} = \mathbf{AG}$
- First column of **A** is exclusively connected to first column of **B**, and the same for the second components, therefore they refer to the same component.
- $x_{ij} = \Sigma_s(a_{is}b_{js}g_{ss})$

SVD and PCA and Q-PCA

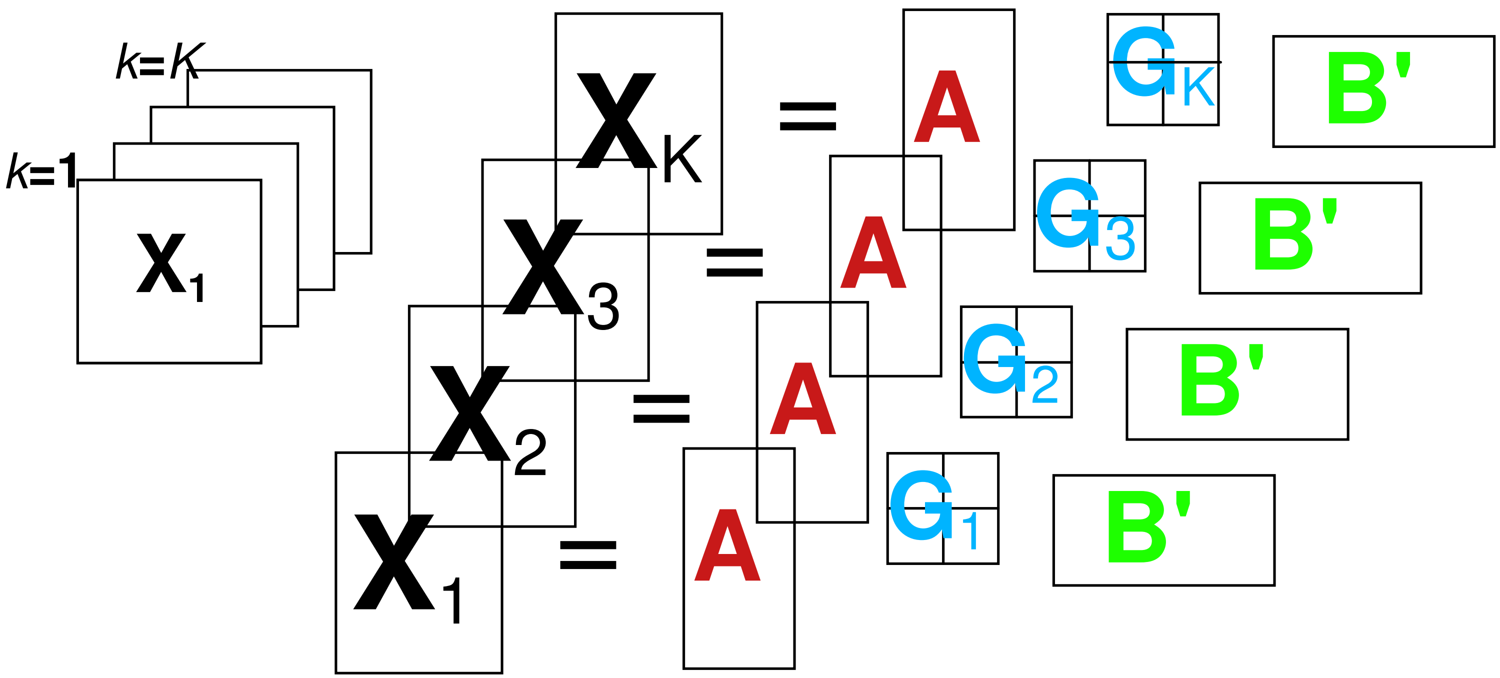


Three-Mode PCA: Replicated SVD



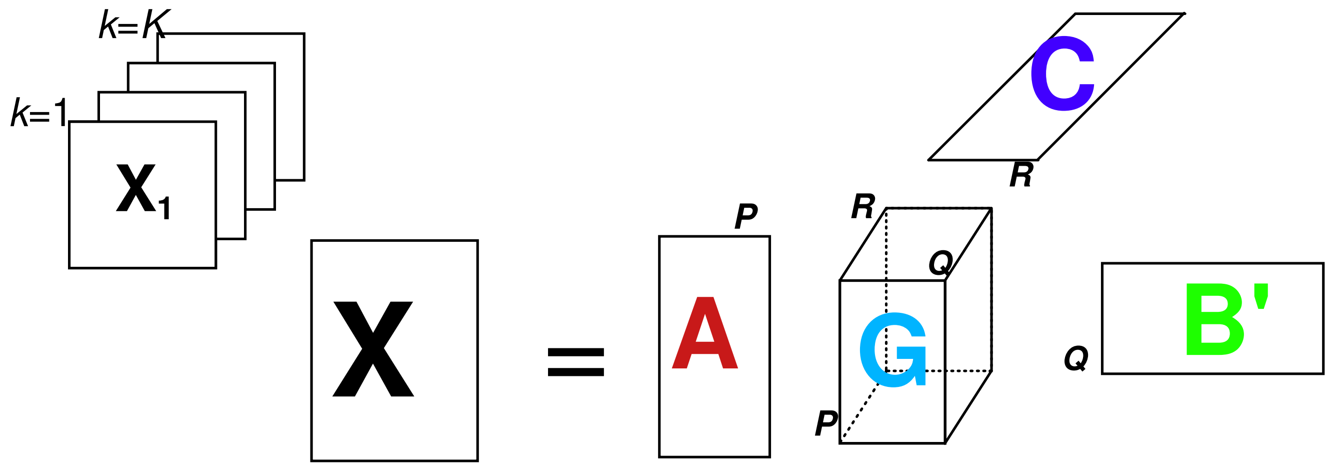
- Replicated SVD is not really a three-mode model.
- No restrictions.
- Independent solutions for each *k*.
- $x_{ijk} = \Sigma_s(a_{isk} b_{jsk} g_{ssk})$

Three-Mode PCA: Tucker2 Model



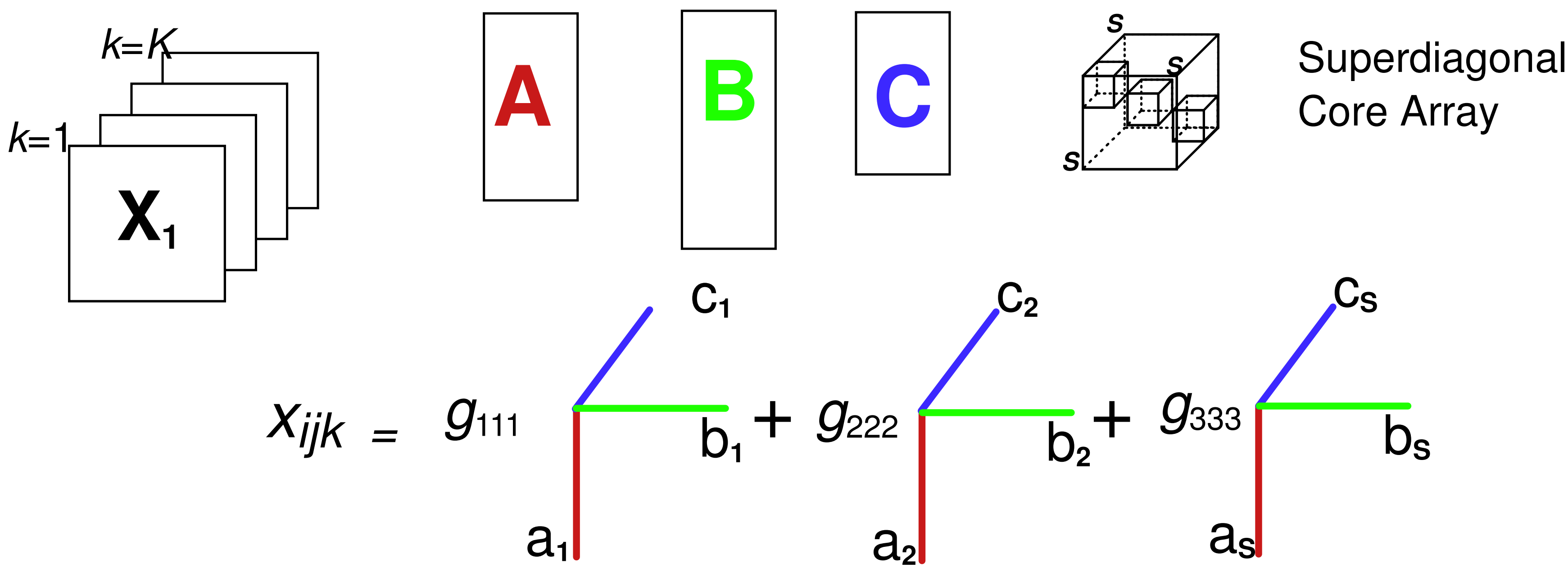
- True three-mode model with restrictions: Only one **A** and **B** for all subjects *k.*
- The singular value matrices $\mathbf{G}_k$ not diagonal anymore
- $x_{ijk} = \Sigma_p \, \Sigma_q (a_{ip} \, b_{jq} \, g_{pqk})$

Three-Mode PCA: Tucker3 Model



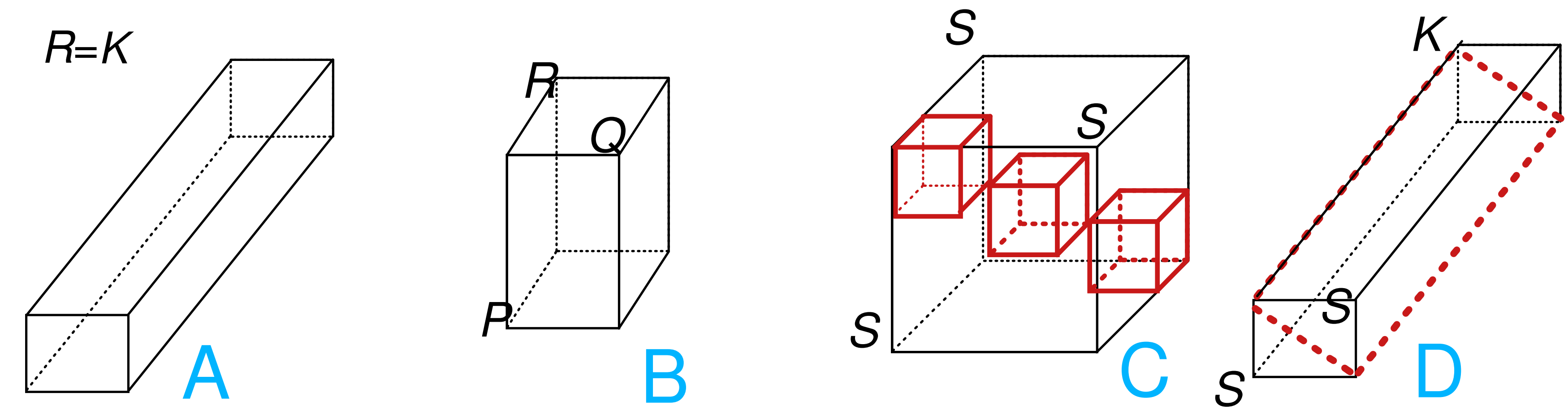
- True three-mode model with restrictions: One **A** and **B** and components **C** to describe the subjects.
- Singular values in core array **G** weight combinations of components.
- $x_{ijk} = \sum_p \sum_q \sum_r (a_{ip} b_{jq} c_{kr} g_{pqr})$

Three-Mode PCA: Parafac model



- True three-mode model with restrictions: One **A** and **B** and components **C** to describe the subjects.
- Singular values in core array **G** weight combinations of components. Core array is superdiagonal.
- First column of **A**, **B**, and **C** are exclusively linked to each other, therefore they refer to the same component.
- $x_{ijk} = \Sigma_s \, a_{is} \, b_{js} \, c_{ks} \, g_{sss}$

Three-Mode PCA: Core Arrays



Extended core array (R = K)

Full core array

Superdiagonal full core array
(S = P = Q = R)

Slice diagonal extended core array
(S = P = Q)

Three-Mode Analysis
Problems and Prospects

Pieter Kroonenberg

Department of Education, Leiden University
kroonenb@fsw.leidenuniv.nl

General

A highly subjective and partial list

- Some topics related to data which I think should be addressed or dismissed
- Areas of application
- Some interesting problems other people are working on which I find fascinating
- Interpretational issues

(Names generally indicate research **groups**)

Problems related to data

- Robustness
  - How robust are the outcomes to outlying observations?
  - How do we detect them?
  - There is a large literature on robust PCA, however robust methods seem to create outliers!
- Mixed measurement levels
  - How to treat sets of variables which can have any measurement level (ordinal, nominal, interval)? => optimal scaling? (Sands & Young, 1980)
- Statistical stability of parameter estimates
  - Bootstrap & Jackknife
    Bro, Kiers, Kroonenberg unpublished doodles

Areas of application (1)

- Is the development of three-mode analysis finished in the social and behavioural sciences?
  - may be not in psychophysics (ECG and EEG research)
- Vigorous development in chemistry and also signal processing and detection. Why?
  - because there are (physical) models rather than hypothesised components and emphasis on data reduction
- Data analysis in Agriculture
  - Interest in Genotype by Environment interaction for different attributes and Genotype by Location by Year interactions; thus in interaction in three-way analysis of variance

Areas of application (2)

- Tensor faces and other related work (Vasilescu)
- On-line three-mode analyses in process analysis and control in industrial (chemical) situations

  (Bro)
- Other applications ......

Technical areas of interest (1)

- Matters related to the rank of three-mode matrices, their relationships with sparse core arrays and uniqueness
  (Bro, Comon,Harshman, Kiers, Kruskal, Rocci, Sidiropoulos, Ten Berge and others(? - see Comon (2001)))
- Modelling interactions from three-way ANOVA
  - modelling multiplicatively two-way interactions and three-way interactions simultaneously but not completely

Technical areas of interest (2)

- Degeneracy of Parafac models
  (Harshman, Kiers, Paatero, Ten Berge)

- Multiway extensions: Proofs and properties
  - Is it 1,2, multi; 1,2,3, multi; 1,2,3,4, multi? (e.g. uniqueness proofs)
    (Bro, Harshman, Sidiropoulos)

- Three/Multiway general linear models (Multi-block models)
  - Development, use and interpretation
    (Bro, Smilde, Stahle, Vivien, Westerhuis)

Technical areas of interest (3)

- Comparisons with other techniques:
  canoncial correlation analysis, redudancy analysis, generalised Procrustes analysis
- Usefulness in multivariate longitudinal analysis
  (Multiset analysis, multivariate time series, repeated measures analysis)
- Usefulness of three-mode (confirmatory) factor analysis (structural equation modelling) and similar component models
  (Stochastic modelling: Bentler, Bloxom, Kroonenberg, Oort, Wansbeek)

Technical areas of interest (4)

- Notational and representational issues in the multiway context
  (Alsberg, Burdick, Harshman, Wansbeek)
  Note: do not forget the book by Magnus and Neudecker (Wiley)

Interpretational issues

- Using constraints to improve interpretation
  (Bro,Kiers, Krijnen, Ten Berge)
- Graphical procedures for interpreting all three modes together
  (Kiers, Kroonenberg)
- Model selection
  (Bro, Kiers, Kroonenberg, Van Mechelen)

- How to get people to use these methods?
- Are they useful enough outside the main application areas?
- How to explain the results to the uninitiated?