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New computational properties for Hierarchical Principal Component Analysis (HPCA) and its relation to PARAFAC Model

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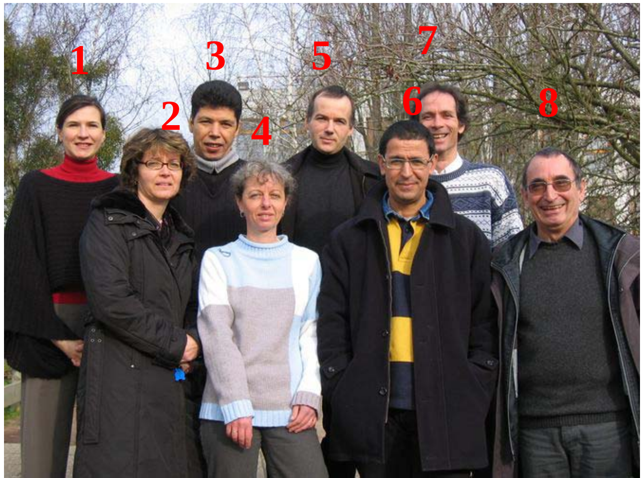
Sensometric-chemometric group



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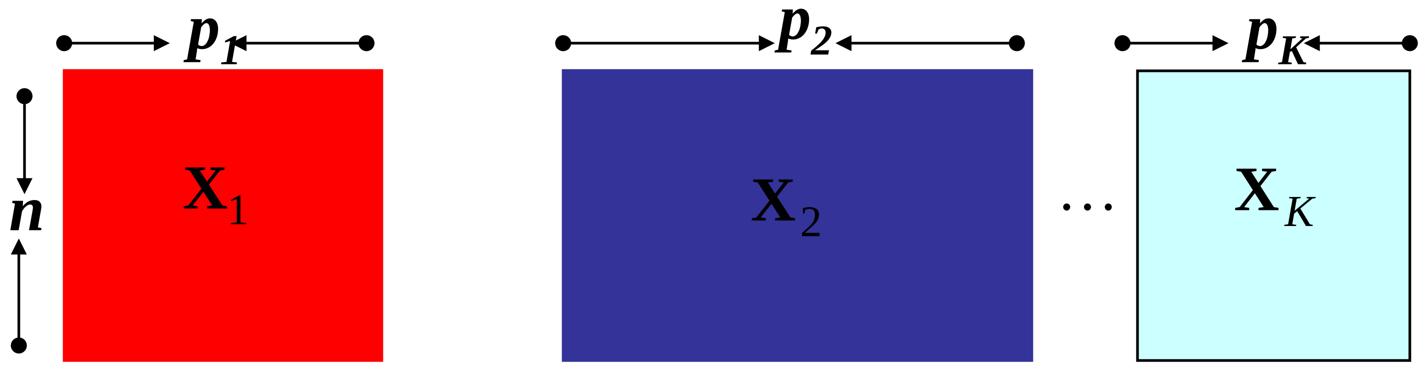
Summary

- Introduction
  - Multiblock data sets.
  - Four Principles for Multiblock Methdology.
  - Overview of some Multiblock Methods.
- Hierarchical Principal Component Analysis.
  - Brief presentation of HPCA.
  - Motivation.
- Computational Results
  - Monotony properties of HPCA procedure.
  - Convergence properties of HPCA procedure.
- Relations between HPCA and PARAFAC
  - Equivalence between HPCA and CCSWA .
  - Simulation Study : HPCA/CCSWA procedures.
- Conclusions.

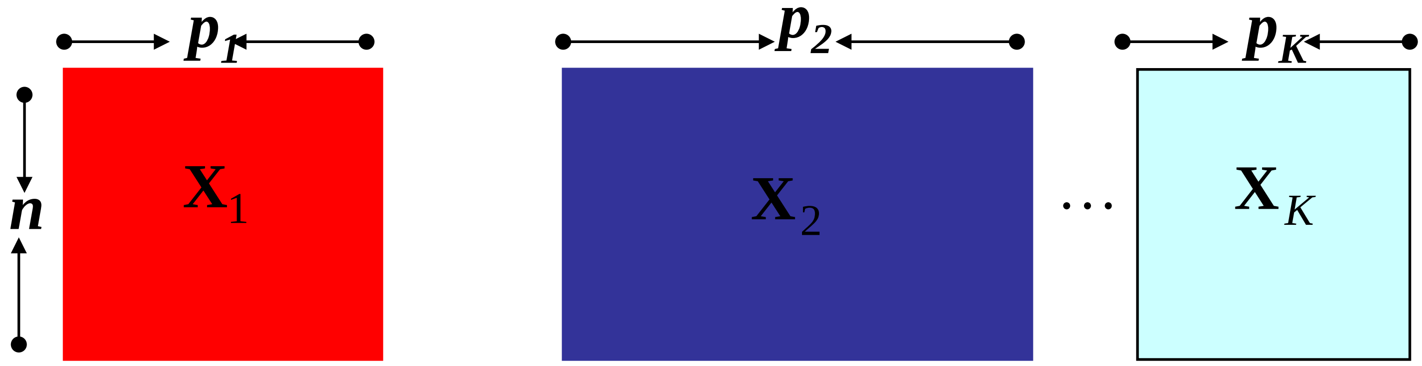
Multiblock Data sets



Different types of multivariate data are collected from corresponding samples.

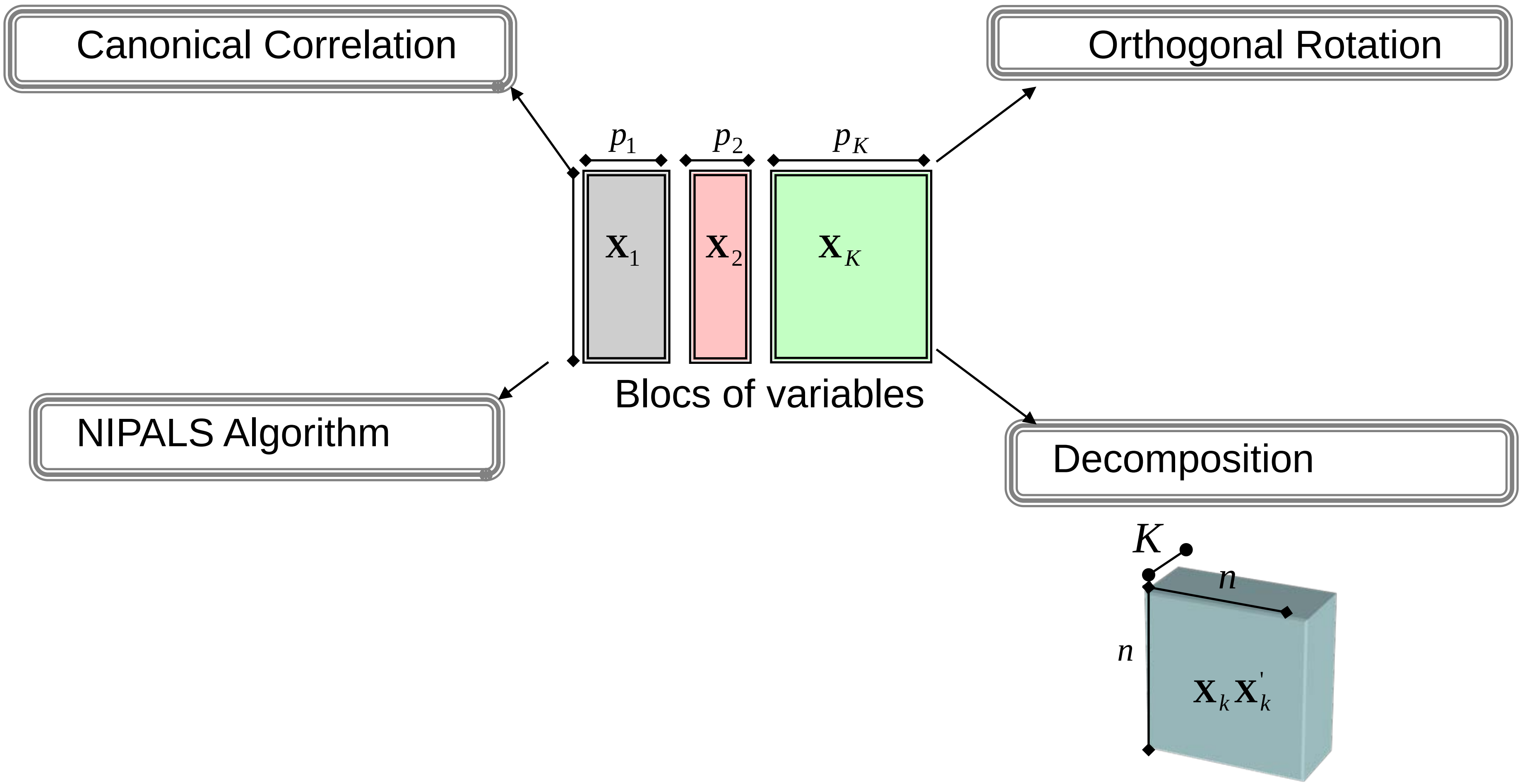
- Applications.
  - Ecology
  - Biospectroscopy
  - Functional Genomics
  - Sensory sciences
  - Ect….

Aim of Multiblock Analysis

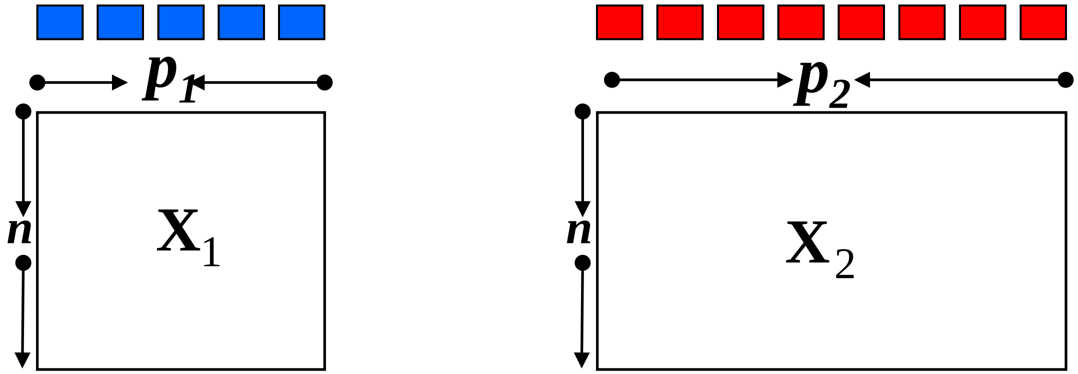


- To find relationships between data blocks.
- To summarize simultaneously the relevant information between blocks.
- To identify the within block patterns which define the so-called relevant information.

Principles for Multiblock Methodology



Canonical correlation Analysis (CCA)



- Considers (linear) relationships between two groups of variables.
- Multivariate extension of correlation analysis

Hotelling H. (1936). Biometrika, 28, 321-377.

Principle of CCA

- Given
  - a linear combination of ***X1*** variables:

$$\mathbf{z}_1 = t_1^{(1)}\mathbf{x}_1^{(1)} + t_2^{(1)}\mathbf{x}_2^{(1)} + \ldots + t_p^{(1)}\mathbf{x}_p^{(1)}$$

  - a linear combination of ***X2*** variables:

$$\mathbf{z}_2 = t_1^{(2)}\mathbf{x}_1^{(2)} + t_2^{(2)}\mathbf{x}_2^{(2)} + \ldots + t_q^{(2)}\mathbf{x}_q^{(2)}$$

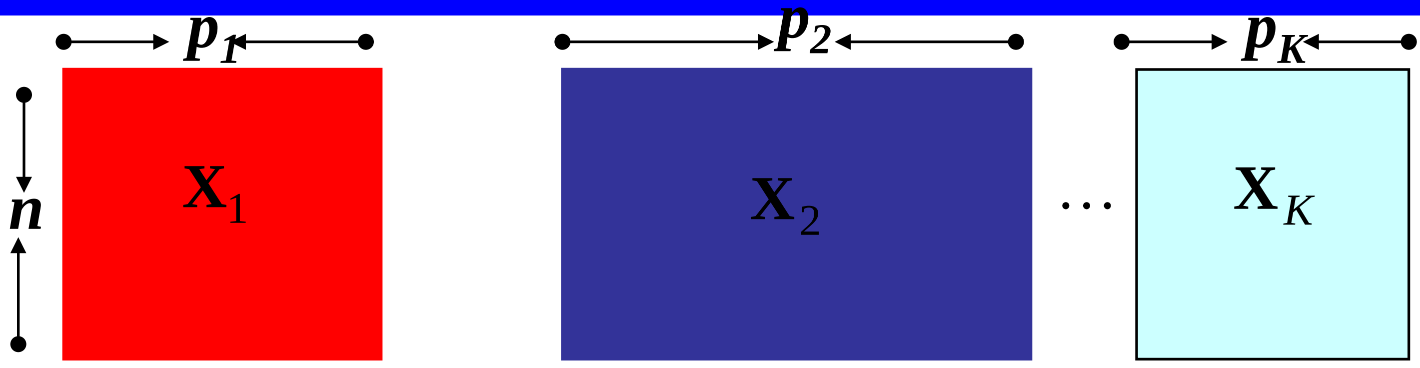
- The first **canonical correlation** is $corr\left(\tilde{\mathbf{z}}_1, \tilde{\mathbf{z}}_2\right)$

$$corr\left(\tilde{\mathbf{z}}_1, \tilde{\mathbf{z}}_2\right) = \underset{\mathbf{z}_1, \mathbf{z}_2}{Max}\, corr\left(\mathbf{z}_1, \mathbf{z}_2\right)$$

- **canonical variates** are $\left(\tilde{\mathbf{z}}_1, \tilde{\mathbf{z}}_2\right)$

Hotelling H. (1936). Biometrika, 28, 321-377.

Generalized Canonical Correlation Analyses



$$SUMCOR \Rightarrow Max \sum_{i \neq j \; i,j=1}^{K} corr\left(\mathbf{z}_i, \mathbf{z}_j\right)$$

Horst, P. (1961). Psychometrika, 26, 129-149.

$$MAXVAR \Rightarrow Max \quad \lambda\left(\left\lfloor corr\left(\mathbf{z}_i, \mathbf{z}_j\right)\right\rfloor\right)$$

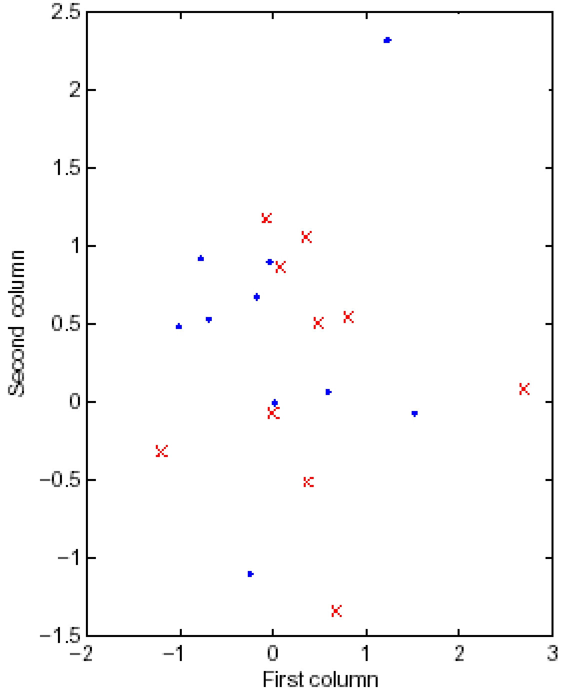
Horst, P. (1965). New York: Holt, Rinehart & Winston.

Carroll, J.D. (1968).Proceeding of the 76th Convention of the American Psychological Association, 3, 227-228

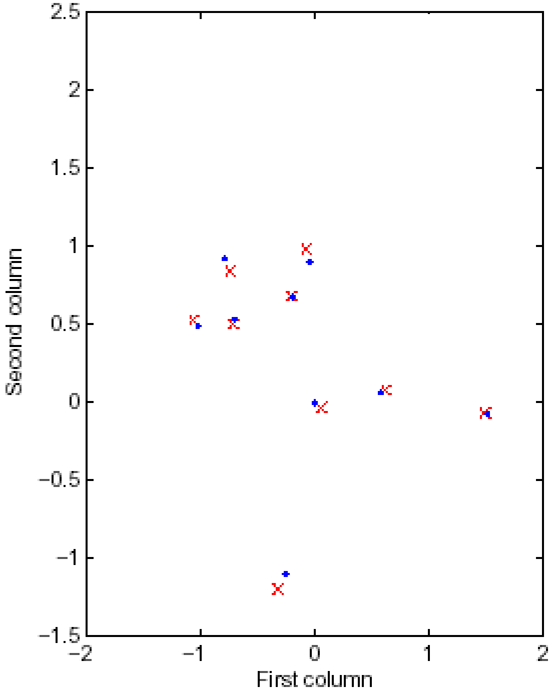
$$SSQCOR \Rightarrow Max \sum_{i \neq j \; i,j=1}^{K} corr^2\left(\mathbf{z}_i, \mathbf{z}_j\right)$$

Kettenring, J.R. (1971). Biometrika. 58, 433-451.

Orthogonal Rotation Principle

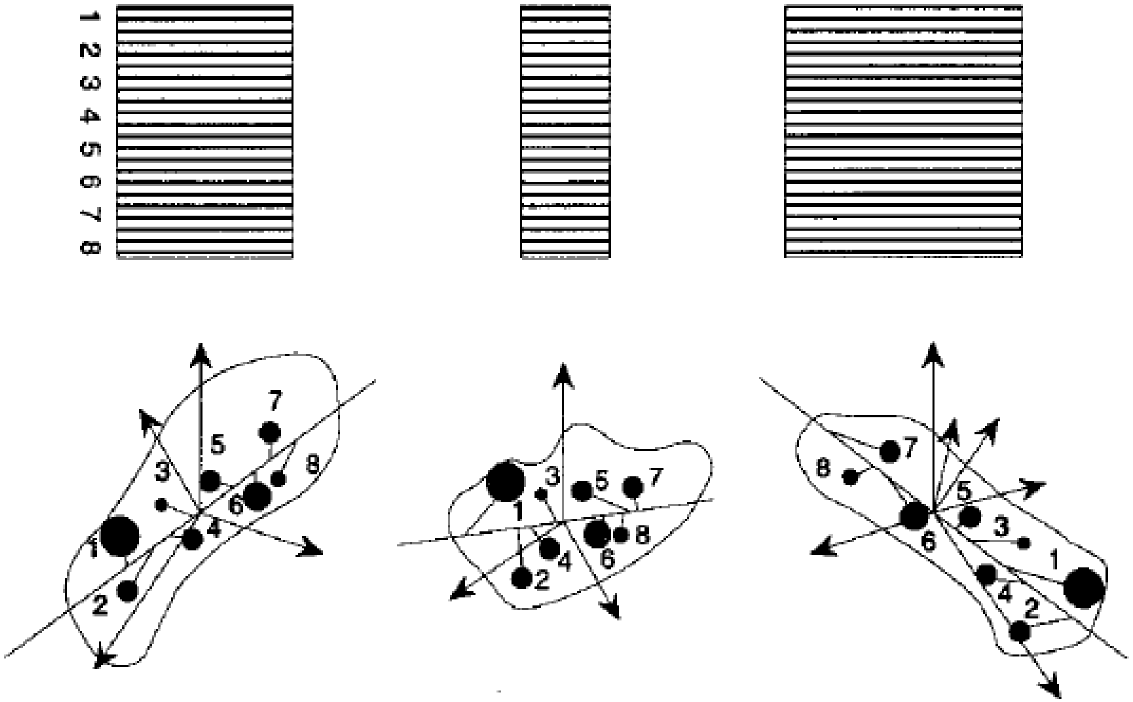


Before orthogonal Rotation



After orthogonal Rotation

Generalized Orthogonal Rotation



Generalized Orthogonal Rotation

- Model 1.

$$\underset{\mathbf{T}_i'\mathbf{T}_i=\mathbf{I}_p}{Min} \sum_{i<j}^{K} tr\left[\left(\mathbf{X}_i\mathbf{U}_i - \mathbf{X}_j\mathbf{U}_j\right)'\left(\mathbf{X}_i\mathbf{U}_i - \mathbf{X}_j\mathbf{U}_j\right)\right]$$

Ten Berge, (1977). Psychometrika,42,267-276

- Model 2.

$$\underset{\mathbf{T}_i'\mathbf{T}_i=\mathbf{I}_p}{Min} \sum_{i<j}^{K} tr\left[\left(s_i\mathbf{X}_i\mathbf{U}_i - s_j\mathbf{X}_j\mathbf{U}_j\right)'\left(s_i\mathbf{X}_i\mathbf{U}_i - s_j\mathbf{X}_j\mathbf{U}_j\right)\right]$$

$$\sum_{i,j=1}^{K} s_i^2 tr\left(\mathbf{X}_i'\mathbf{X}_i\right) = \sum_{i=1}^{K} tr\left(\mathbf{X}_i'\mathbf{X}_i\right)$$

Gower (1975). Psychometrika,40,33-51

Remark

One general procedure (monotony convergence) to compute solutions of the various optimization problems generated by these several methods

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www.elsevier.com/locate/csda

Analysis of K sets of data, with differential emphasis on agreement between and within sets

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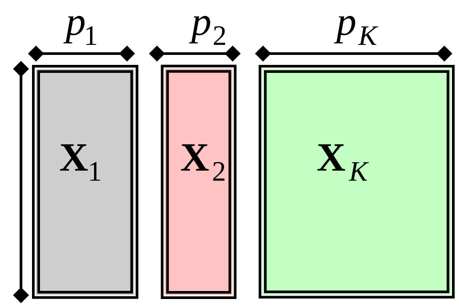
Canonical Correlation

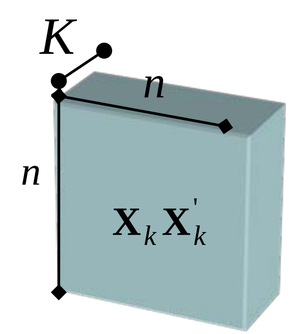
Orthogonal Rotation



Blocs of variables

NIPALS Algorithm

Decomposition



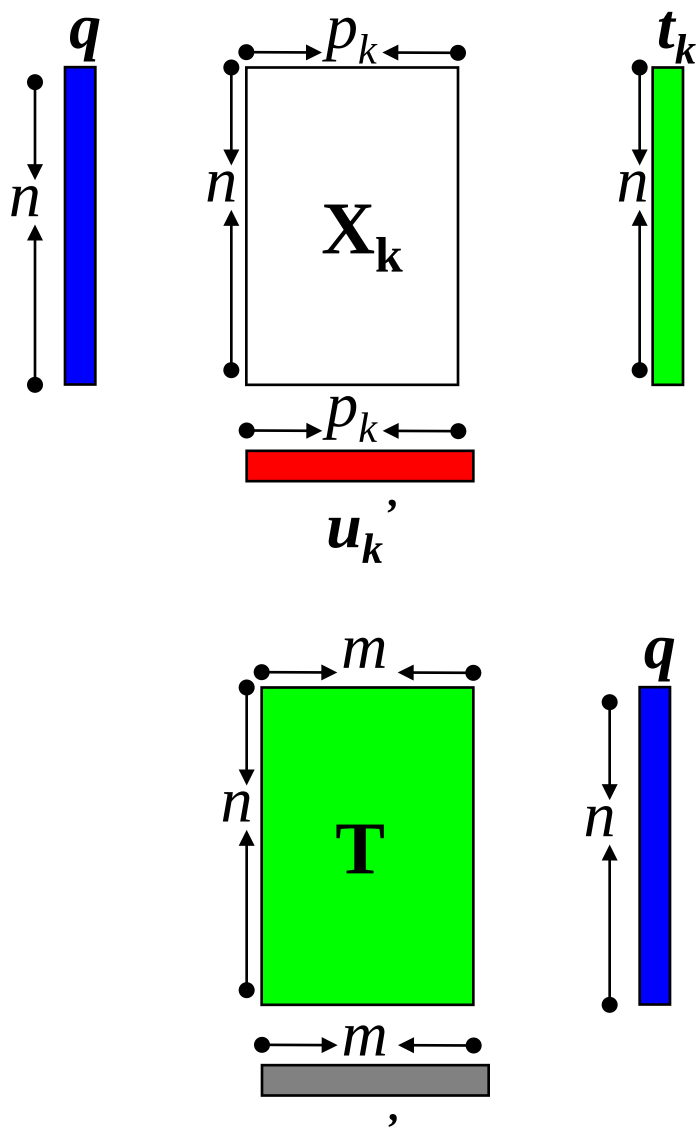
Hierarchical Principal Component Analysis (HPCA)

- HPCA can be considered as an intuitive extension of NIPALS for PCA to more than one Block.
- HPCA is a Multiblock Method
- HPCA has been introduced by Wold et al(1996).
    - *Wold S, Tjessem K. J. Chemometrics 1996;10:463-482*
- HPCA has been compared to some other Multiblock methods.
    - *Westerhuis JA, Kourti T, Macgregor JF. J. Chemometrics 1998;12:301-321*
    - *Smilde AK, Westerhuis JA, De Jong S. J. Chemometrics 2003;17:323-337*
- HPCA introduces
    - Block scores and Block Loadings→ to find the within block patterns
    - Super Matrix, Super loadings and Global scores→ to summarize the relevant information between the blocks

Hierarchical Principal Component Analysis (HPCA)

- $\mathbf{q} \leftarrow \mathbf{q} / \sqrt{\mathbf{q}'\mathbf{q}}$
- $\mathbf{u}_k \leftarrow \mathbf{X}_k'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{t}_k \leftarrow \mathbf{X}_k\mathbf{u}_k$
- $\mathbf{T} \leftarrow \begin{bmatrix} \mathbf{t}_1 & \mathbf{t}_2 & \cdots & \mathbf{t}_K \end{bmatrix}$
- $\mathbf{w} \leftarrow \mathbf{T}'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{q} \leftarrow \mathbf{T}\mathbf{q}$

$$\mathbf{X}_k = \mathbf{X}_k - \mathbf{q}\,\mathbf{q}'\,\mathbf{X}_k$$



Motivation

Lack of knowledge about the properties of HPCA.

– Convergence properties are unknown.

– An optimization criterion for HPCA is not known.

(Smilde AK, Westerhuis JA, De Jong S. J. Chemometrics 2003;17:323-337)

– The link to others multiblock methods is no clear.

Notations

- $\mathbf{q} \leftarrow \mathbf{q} / \sqrt{\mathbf{q}'\mathbf{q}}$
- $\mathbf{u}_k \leftarrow \mathbf{X}_k'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{t}_k \leftarrow \mathbf{X}_k\mathbf{u}_k$
- $\mathbf{T} \leftarrow [\mathbf{t}_1 \quad \mathbf{t}_2 \quad \cdots \quad \mathbf{t}_K]$
- $\mathbf{w} \leftarrow \mathbf{T}'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{q} \leftarrow \mathbf{T}\mathbf{q}$

$$\mathbf{u}_k^{(1)},\ \mathbf{u}_k^{(2)},\ldots,\mathbf{u}_k^{(s)}$$

$$\mathbf{t}_k^{(1)},\ \mathbf{t}_k^{(2)},\ \ldots,\mathbf{t}_k^{(s)}$$

$$\mathbf{q}^{(1)},\ \mathbf{q}^{(2)},\ldots,\mathbf{q}^{(s)}$$

$$\mathbf{w}^{(1)},\mathbf{w}^{(2)},\ldots,\mathbf{w}^{(s)}$$

$w_k^{(s)}$ denotes the k^th^ component of $\mathbf{w}^{(s)}$

$\mathbf{x}_k^{(j)}$ denotes the j^th^ variable of $\mathbf{X}_k$

Compact form of HPCA

- $\mathbf{q} \leftarrow \mathbf{q} / \sqrt{\mathbf{q}'\mathbf{q}}$
- $\mathbf{u}_k \leftarrow \mathbf{X}_k'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{t}_k \leftarrow \mathbf{X}_k\mathbf{u}_k$
- $\mathbf{T} \leftarrow \begin{bmatrix} \mathbf{t}_1 & \mathbf{t}_2 & \cdots & \mathbf{t}_K \end{bmatrix}$
- $\mathbf{w} \leftarrow \mathbf{T}'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{q} \leftarrow \mathbf{T}\mathbf{q}$

↔

Property 1

$$\sum_{k=1}^{K} w_k^{(s)} \mathbf{X}_k \mathbf{X}_k' \mathbf{q}^{(s)} = \lambda^{(s)} \mathbf{q}^{(s+1)}$$

$$w_k^{(s)} = \mathbf{q}^{(s)'} \mathbf{X}_k \mathbf{X}_k' \mathbf{q}^{(s)}$$

$$\left\| \mathbf{q}^{(s)} \right\| = \left\| \mathbf{q}^{(s+1)} \right\| = 1$$

Monotony properties of HPCA : basic properties

$n^4 \times \left[\sum_{j=1}^{p_k} \mathrm{cov}^2\left(\mathbf{x}_k^{(j)}, \mathbf{q}^{(s)}\right) \right]^2$	• The square of total variance of block *k* explained by the global score vector • Relation between each block and the global score vector
$n^2 \times \mathrm{cov}^2\left(\mathbf{t}_k^{(s)}, \mathbf{q}^{(s)}\right)$	• Variance of the block score vector explained by the global score vector. • Relation between block score vector and global score vector
$\left\Vert \mathbf{X}_k \mathbf{X}_k' \right\Vert^2 - \left\Vert \mathbf{X}_k \mathbf{X}_k' - w_k^{(s)} \mathbf{q}^{(s)} \mathbf{q}^{(s)'} \right\Vert^2$	Rank one fit by super loading and global score of the matrix of scalars products.

Property 2

$$n^4 \times \left[\sum_{j=1}^{p_k} \mathrm{cov}^2\left(\mathbf{x}_k^{(j)}, \mathbf{q}^{(s)}\right) \right]^2 = n^2 \times \mathrm{cov}^2\left(\mathbf{t}_k^{(s)}, \mathbf{q}^{(s)}\right) = \left\Vert \mathbf{X}_k \mathbf{X}_k' \right\Vert^2 - \left\Vert \mathbf{X}_k \mathbf{X}_k' - w_k^{(s)} \mathbf{q}^{(s)} \mathbf{q}^{(s)'} \right\Vert^2$$

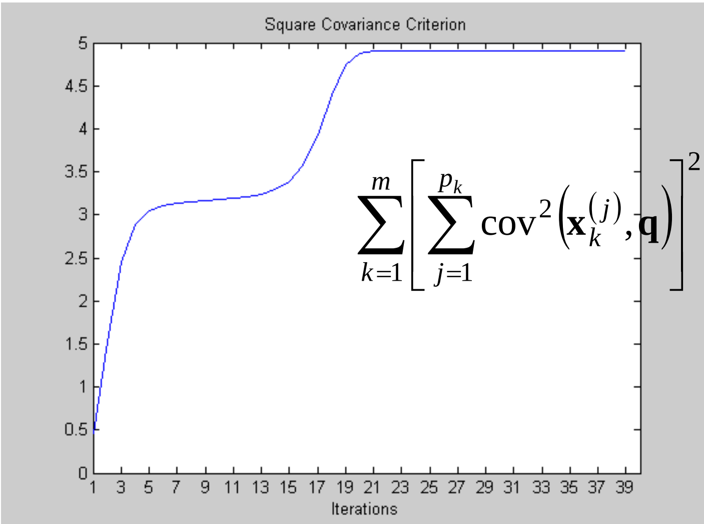
Property 3

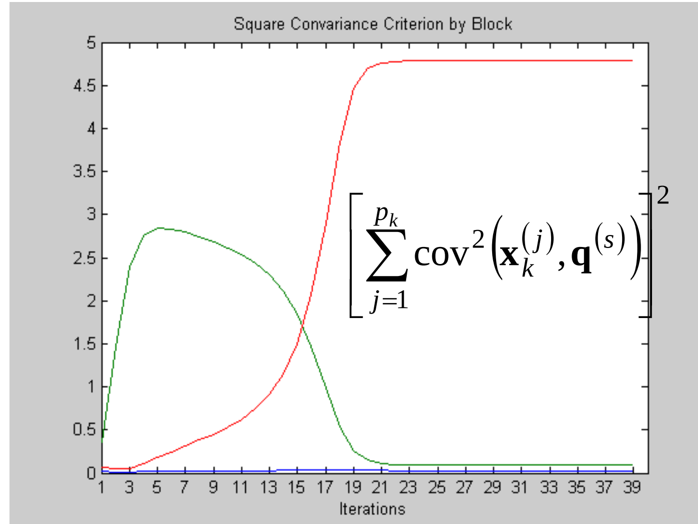
$$n^4 \times \sum_{k=1}^{m} \left[\sum_{j=1}^{p_k} \mathrm{cov}^2\left(\mathrm{x}_k^{(j)}, \mathrm{q}^{(s)}\right) \right]^2 = n^2 \times \sum_{k=1}^{m} \mathrm{cov}^2\left(\mathrm{t}_k^{(s)}, \mathrm{q}^{(s)}\right) = \sum_{k=1}^{m} \left\Vert \mathrm{X}_k \mathrm{X}_k' \right\Vert - \sum_{k=1}^{m} \left\Vert \mathrm{X}_k \mathrm{X}_k' - \mathrm{w}_k^{(s)} \mathrm{q}^{(s)} \mathrm{q}^{(s)'} \right\Vert^2$$

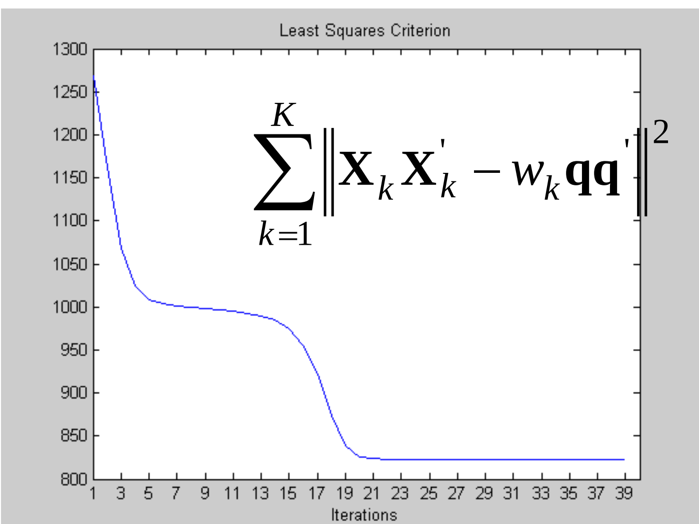
Monotony properties : Illustration using 3 blocks

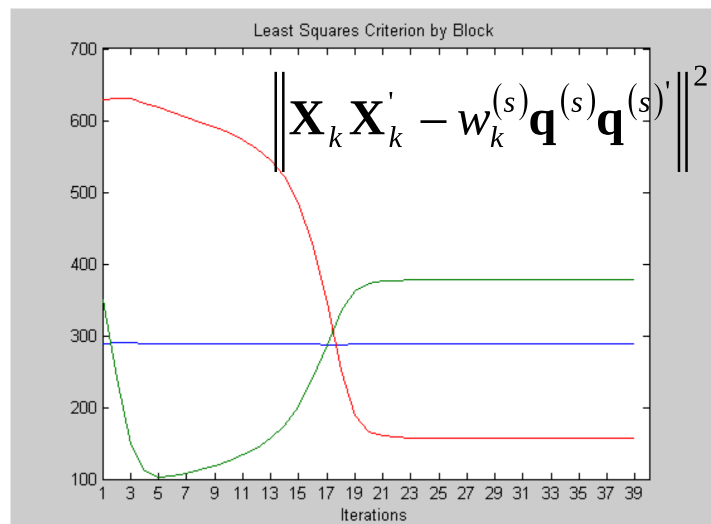
X_1			X_2			X3			
154	-3	-91	-147	51	62	106	-116	68	13
-35	57	-150	-57	1	-109	-75	-167	-67	-28
-14	-15	59	40	56	-192	-211	-37	123	-38
29	-47	135	-18	58	-151	-115	-105	-115	221
-114	-21	202	-187	-58	70	-1	26	38	-32
-82	84	-63	-172	220	-67	-131	-39	-103	155
88	-42	-65	14	40	15	296	134	-38	22
164	123	126	-70	56	202	-33	-1	38	4
-156	36	25	-145	-11	-107	-18	135	-89	51
-121	-20	19	89	111	180	-101	-19	73	158

Monotony properties : Illustration using 3 block









Main result:
Monotony properties of the HPCA procedure

Property 4

$$\sum_{k=1}^{m}\left[\sum_{j=1}^{p_k}\operatorname{cov}^2\left(\mathbf{x}_k^{(j)},\mathbf{q}^{(s)}\right)\right]^2 \leq \sum_{k=1}^{m}\left[\sum_{j=1}^{p_k}\operatorname{cov}^2\left(\mathbf{x}_k^{(j)},\mathbf{q}^{(s+1)}\right)\right]^2$$

Property 5

$$\sum_{k=1}^{K}\operatorname{cov}^2\left(\mathbf{X}_k\mathbf{u}_k^{(s)},\mathbf{q}^{(s)}\right)\leq \sum_{k=1}^{K}\operatorname{cov}^2\left(\mathbf{X}_k\mathbf{u}_k^{(s+1)},\mathbf{q}^{(s+1)}\right)$$

Property 6

$$\sum_{k=1}^{K}\left\|\mathbf{X}_k\mathbf{X}_k^{'} - w_k^{(s)}\mathbf{q}^{(s)}\mathbf{q}^{(s)'}\right\|^2 \geq \sum_{k=1}^{K}\left\|\mathbf{X}_k\mathbf{X}_k^{'} - w_k^{(s+1)}\mathbf{q}^{(s+1)}\mathbf{q}^{(s+1)'}\right\|^2$$

•*Hanafi, M Kohler, A (In progress)*

Consequence : monotony convergence of HPCA

Property 7

$$\sum_{k=1}^{m}\left[\sum_{j=1}^{p_k}\operatorname{cov}^2\left(\mathbf{x}_k^{(j)},\mathbf{q}^{(s)}\right)\right]^2 \xrightarrow[s\to\infty]{} a^{(*)}$$

Property 8

$$\sum_{k=1}^{K}\operatorname{cov}^2\left(\mathbf{X}_k\mathbf{u}_k^{(s)},\mathbf{q}^{(s)}\right) \xrightarrow[s\to\infty]{} a^{(*)}$$

Property 9

$$\sum_{k=1}^{K}\left\|\mathbf{X}_k\mathbf{X}_k^{'} - w_k^{(s)}\mathbf{q}^{(s)}\mathbf{q}^{(s)'}\right\|^2 \xrightarrow[s\to 0]{} \sum_{k=1}^{m}\left\|\mathbf{X}_k\mathbf{X}_k^{'}\right\|^2 - a^{(*)}$$

Remark

$$\sum_{k=1}^{m}\left[\sum_{j=1}^{p_k}\mathrm{cov}^2\left(\mathbf{x}_k^{(j)},\mathbf{q}^{(s)}\right)\right]^2 \xrightarrow[s\to\infty]{} a^{(*)}$$

$$\sum_{k=1}^{K}\mathrm{cov}^2\left(\mathbf{X}_k\mathbf{u}_k^{(s)},\mathbf{q}^{(s)}\right) \xrightarrow[s\to\infty]{} a^{(*)}$$

$$\sum_{k=1}^{K}\left\|\mathbf{X}_k\mathbf{X}_k' - w_k^{(s)}\mathbf{q}^{(s)}\mathbf{q}^{(s)'}\right\|^2 \xrightarrow[s\to 0]{} \sum_{k=1}^{m}\left\|\mathbf{X}_k\mathbf{X}_k'\right\|^2 - a^{(*)}$$

$$\not\Rightarrow \quad \mathbf{q}^{(s)} \xrightarrow[s\to\infty]{} \mathbf{q}^{(*)}$$

Perspective $\quad \mathbf{q}^{(s)} \overset{?}{\underset{s\to\infty}{\longrightarrow}} \mathbf{q}^{(*)}$

Criteria for HPCA

Property 10

$$\underset{\|\mathbf{q}\|=1}{Max} \sum_{k=1}^{m} \left[\sum_{j=1}^{p_k} \text{cov}^2\left(\mathbf{x}_k^{(j)}, \mathbf{q}\right) \right]^2$$

Property 11

$$\underset{\|\mathbf{q}\|=1}{Max} \sum_{k=1}^{K} \left(\mathbf{q}'\mathbf{X}_k\mathbf{X}_k'\mathbf{q}\right)^2$$

Property 12

$$\underset{\|\mathbf{q}\|=1}{Min} \sum_{k=1}^{K} \left\| \mathbf{X}_k\mathbf{X}_k' - w_k\mathbf{q}\mathbf{q}' \right\|^2$$

CCSWA

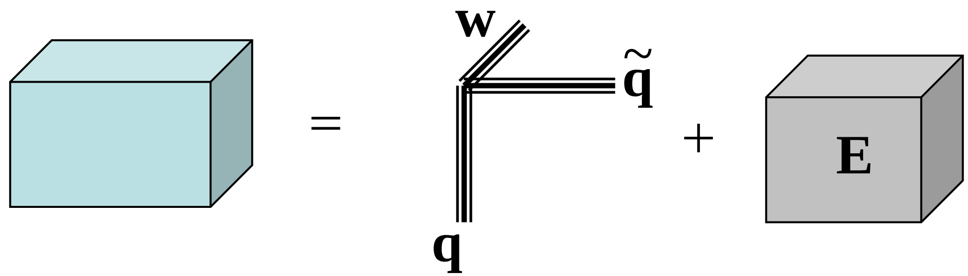
Common Components and specific Weights Analysis(CCSWA)

CCSWA has been investigated at different levels .

- *Qannari E. M,. Wakeling I., Courcoux Ph., MacFie M.F.(2000) Food Quality and Preference. 11, 151-154.*
- *Hanafi M., Qannari E. M,(2008). Revue de la Société Française de Statistique.(In french)*
- *Hanafi M., Mazerolles G., Dufour E., Qannari E. M. (2006). Journal of Chemometrics. Vol 20, 5, 172-183*
- *Qannari E. M., Courcoux Ph., Vigneau E. Food Quality and Preference .(2000). 12, 365-368.*
- *Pram Nielsen J., Bertrand D., Micklander E., Courcoux Ph., Munck L. .(2000) Journal of Near Infrared Spectroscopy. 9, 275 –285.*
- *Courcoux Ph., Devaux F., Bouchet B. .(2000) Chemometrics and Intelligent Laboratory Systems. 63, 57-68.*
- *Mazerolles G., Devaux F, Dufour E., Qannari E.M., Courcoux Ph. .(2002) Chemometrics and Intelligent Laboratory Systems. 63, 57-68.*
- *Mazerolles G., Hanafi M., Dufour E., Qannari E. M., Bertrand D. (2006). Chemometrics and Intelligent Laboratory Systems. 81, 41-49.*

HPCA and PARAFAC

$\mathbf{X}_k \mathbf{X}_k'$



$$\left(w_1^{(1)}, w_2^{(1)}, \ldots, w_k^{(1)}, \mathbf{q}^{(1)}, \tilde{\mathbf{q}}^{(1)}\right) \leftarrow \underset{\lambda_1, \lambda_2, \ldots, \lambda_K, \|\tilde{\mathbf{q}}\| = \|\mathbf{q}\| = 1}{Minimize} \sum_{k=1}^{K} \left\| \mathbf{X}_k \mathbf{X}_k' - w_k \mathbf{q} \tilde{\mathbf{q}}' \right\|^2$$

$$\left(\mathbf{q}^{(1)} = \tilde{\mathbf{q}}^{(1)}\right)$$

Ten Berge J. M. F., Kiers, H. A. L., Krijnen, W. P. (1993). *Journal of classification*. (10), 115-124.

HPCA-CCSWA = Best rank one approximation of PARAFAC
(symmetric case)

Simutation Study : HPCA - CCSWA

$$\left(w_1^{(*)}, w_1^{(*)}, \ldots, w_K^{(*)}, \mathbf{q}_1^{(*)}\right) \Rightarrow \underset{w_1, w_2, \ldots, w_K, \|\mathbf{q}\|=1}{Minimize} \sum_{k=1}^{K} \left\| \mathbf{X}_k \mathbf{X}_k' - w_k \mathbf{q}\mathbf{q}' \right\|^2$$

CCSWA

- $w_1, w_2, \ldots, w_K$
- $\mathbf{W} = \sum_{k=1}^{K} w_k \mathbf{X}_k \mathbf{X}_k'$
- *Extract* the first eigenvector $\mathbf{q}$ of $\mathbf{W}$
- $w_k = \mathbf{q}_k' \mathbf{X}_k \mathbf{X}_k' \mathbf{q} \quad (1 \le k \le m)$

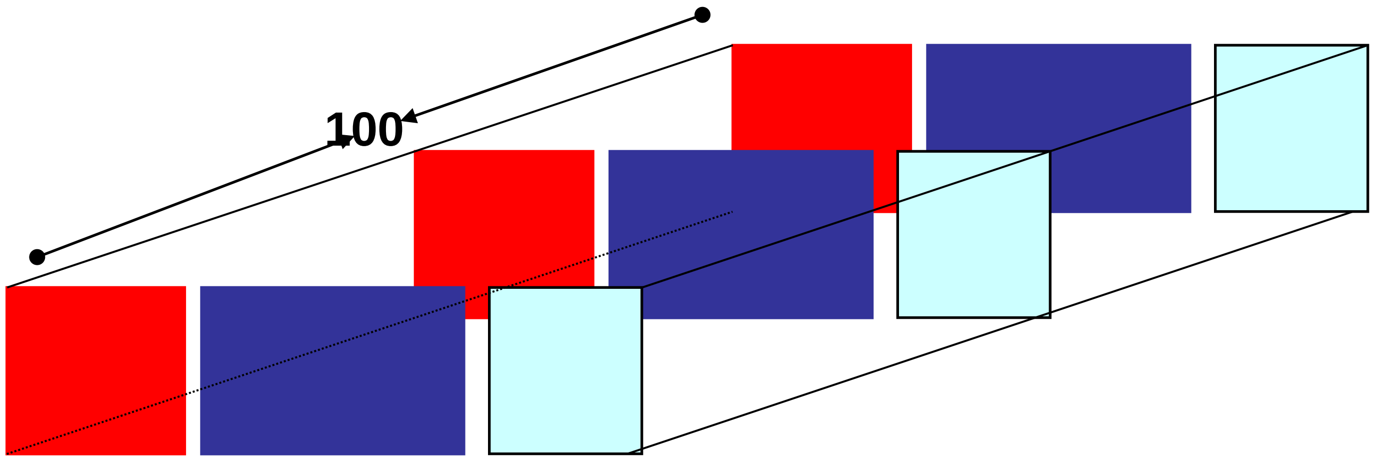
HPCA

- $\mathbf{q} \leftarrow \mathbf{q} / \sqrt{\mathbf{q}'\mathbf{q}}$
- $\mathbf{u}_k \leftarrow \mathbf{X}_k' \mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{t}_k \leftarrow \mathbf{X}_k \mathbf{u}_k$
- $\mathbf{T} \leftarrow [\mathbf{t}_1 \quad \mathbf{t}_2 \quad \cdots \quad \mathbf{t}_K]$
- $\mathbf{w} \leftarrow \mathbf{T}'\mathbf{q} / \mathbf{q}'\mathbf{q}$
- $\mathbf{q} \leftarrow \mathbf{T}\mathbf{q}$

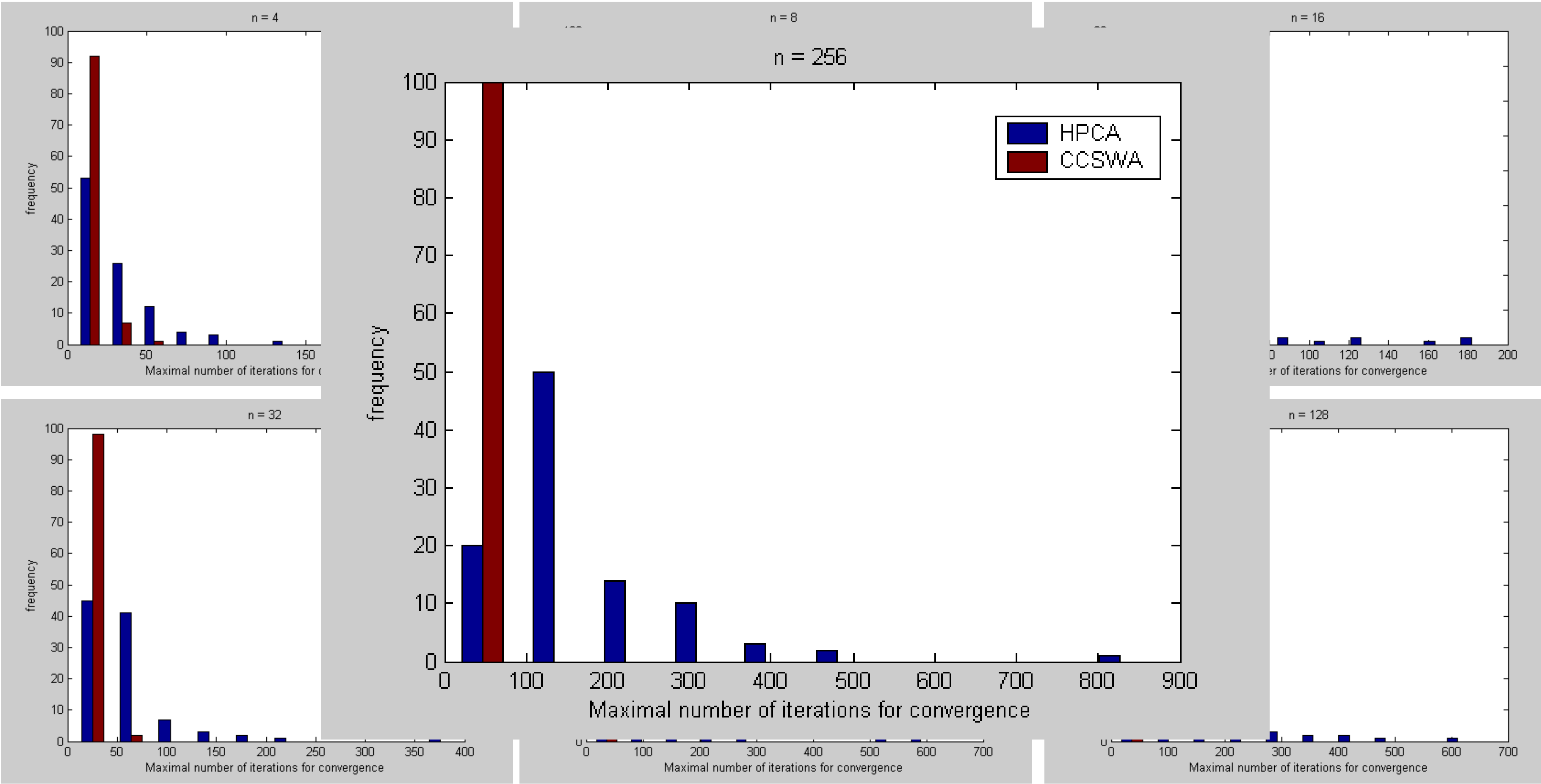
$$\sum_{k=1}^{K} \left\| \mathbf{X}_k \mathbf{X}_k' - w_k^{(s)} \mathbf{q}^{(s)} \mathbf{q}^{(s)'} \right\|^2 \ge \sum_{k=1}^{K} \left\| \mathbf{X}_k \mathbf{X}_k' - w_k^{(s+1)} \mathbf{q}^{(s+1)} \mathbf{q}^{(s+1)'} \right\|^2$$

Simulation Study

Experiments	1	2	3	4	5	6	7
n	4	8	16	32	64	128	256

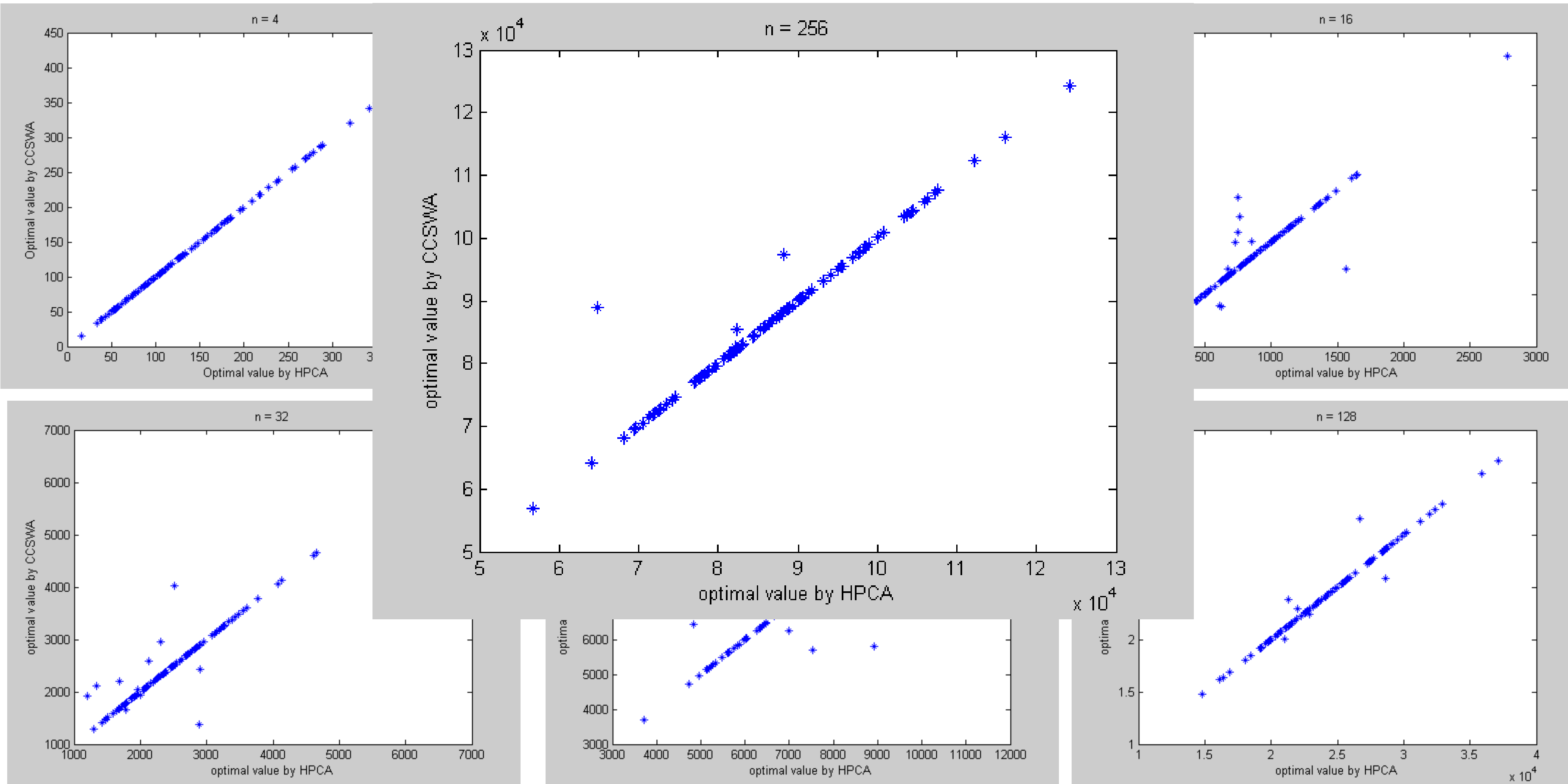


Speed of convergence



Speed of convergence ➔ CCSWA is much better than HPCA

Optimality of the obtained solutions



Optimality of solutions ➔ CCSWA is much better than HPCA

Optimality of the obtained solutions

100 different starting vectors

	369.86	526.89	535.19
CCSWA	11	43	56
HPCA	16	32	52

Conclusions

- Different monotony properties allow :
  - To understand how the different parameters are related to each other.
  - To formulate new convergence properties for the HPCA procedure.
  - To show that CCSWA and HPCA are the same methods.
  - HPCA/CSSWA can be seen as a particular case of PARAFAC model.

Conclusions

Gap between generalized canonical correlation/covariance methods and Parafac Model.

HPCP/CCSWA can be defined as :

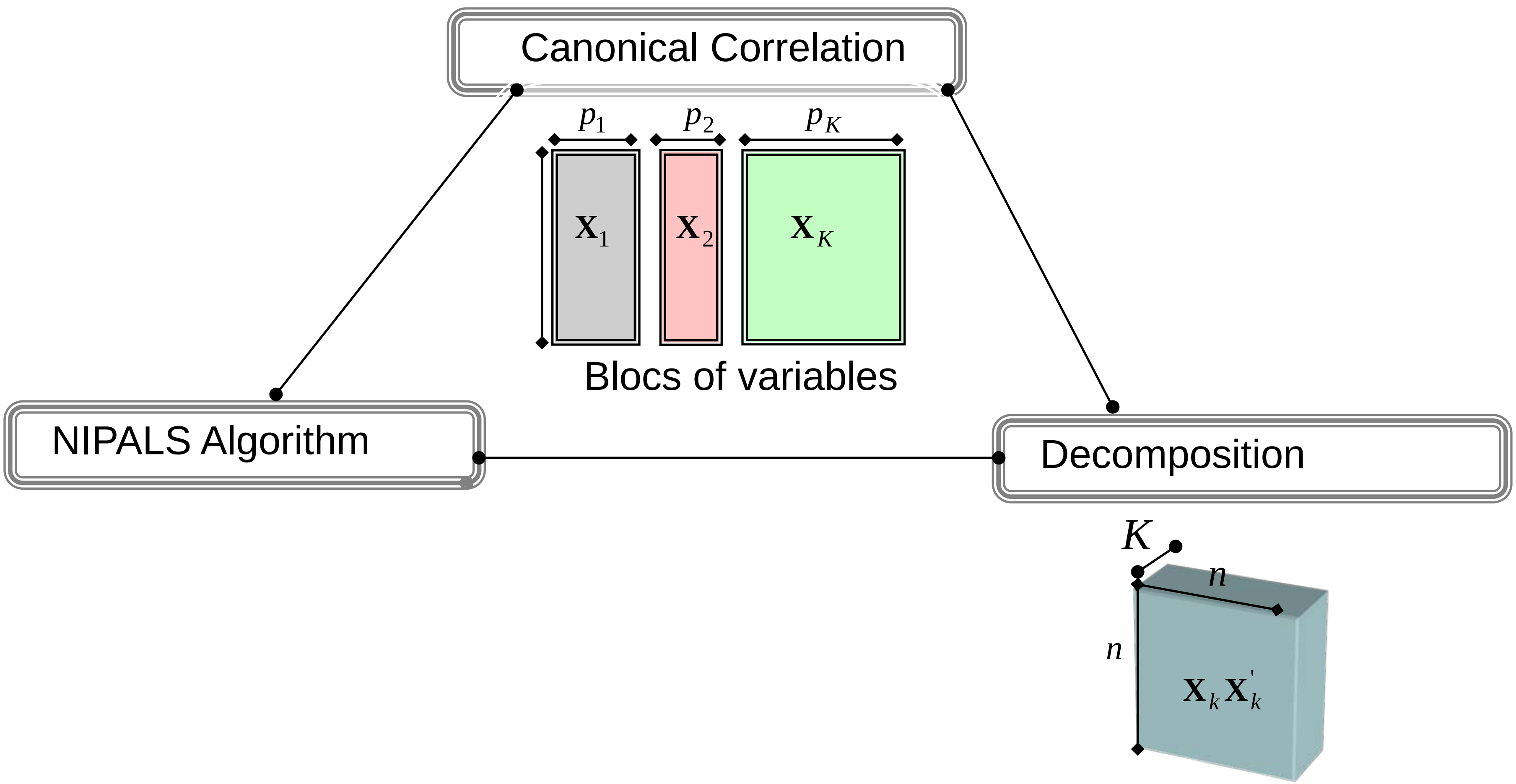
$$\underset{\|\mathbf{u}_k\|=\|\mathbf{q}\|=1}{Maximize} \sum_{k=1}^{m} \operatorname{cov}^4\left(\mathbf{X}_k \mathbf{u}_k , \mathbf{q}\right)$$

Hanafi M., Qannari E. M,(2008). Journal of French Statistical Society. [In Franch]

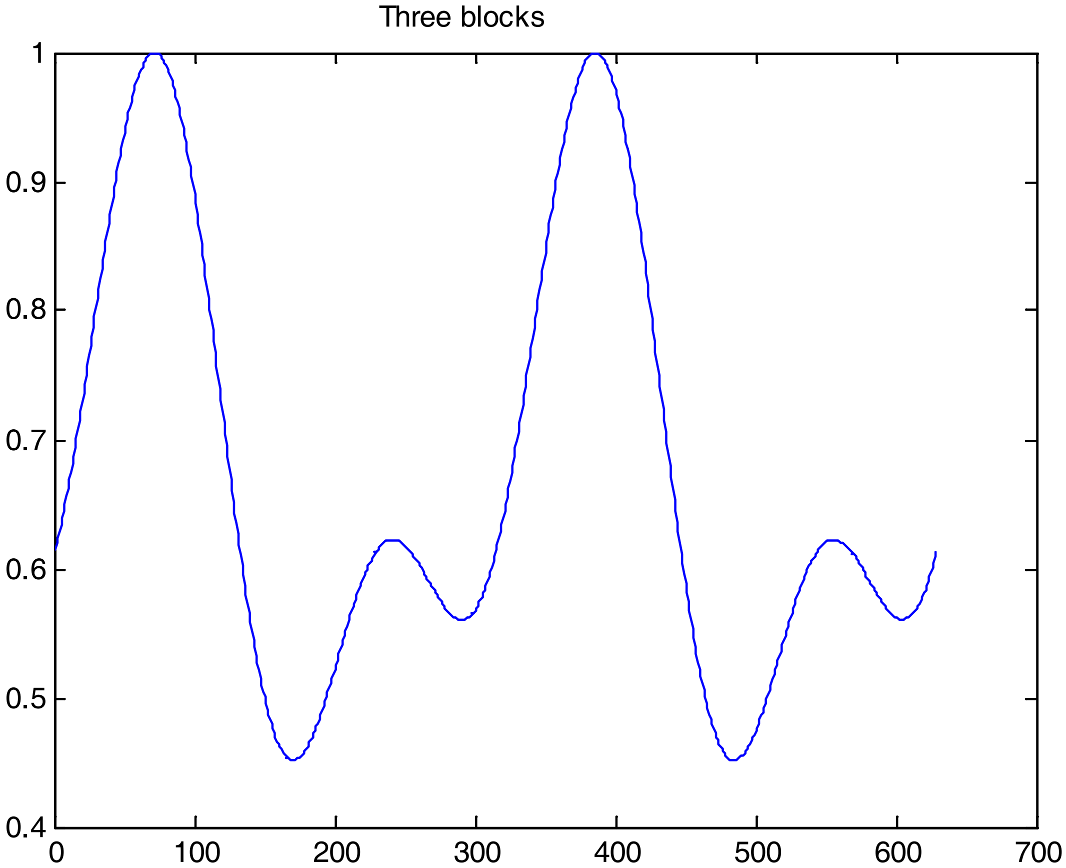
Hanafi M., Mazerolles G., Dufour E., Qannari E. M. (2006). Journal of Chemometrics. Vol 20, 5, 172-183

Conclusions

Gap between three principles



Consequence : Criteria for HPCA



S1 =

4	-1
-1	7

S2 =

27	16
16	22

S3 =

17	-14
-14	16

CCSWA

$$\left(w_1^{(1)}, w_2^{(1)}, \ldots, w_m^{(1)}, \mathbf{q}_1\right) \Rightarrow \underset{w_2, w_2, \ldots, w_m, \|\mathbf{q}\|=1}{Minimize} \sum_{k=1}^{K} \left\| \mathbf{X}_k \mathbf{X}_k^{'} - w_k \mathbf{q}\mathbf{q}' \right\|^2$$

$$\mathbf{X}_k^{(r)} = \mathbf{X}_k - \sum_{j<r} \mathbf{q}_j \mathbf{q}_j^{'} \mathbf{X}_k$$

$$\left(w_1^{(r)}, w_2^{(r)}, \ldots, w_m^{(r)}, \mathbf{q}_r\right) \Rightarrow \underset{w_1, w_2, \ldots, w_m, \|\mathbf{q}\|=1}{Minimize} \sum_{k=1}^{K} \left\| \mathbf{X}_k^{(r)} \mathbf{X}_k^{(r)'} - w_k \mathbf{q}\mathbf{q}' \right\|^2$$

Specific weights

Common components