Nway methods in process control

Nway methods for products quality control
and process analysers applied to batch process

GUIDELINES

1- Purposes, Industrial Requirements, Methods

2- Data, classical methods: PCA & PLS

3- Nway methods

4- Process Monitoring - PARAFAC 2

5- Chemical Reaction Monitoring - OPA

6- Regression - IV Tucker

Purposes

- to enhance the information from multivariate process data

  - NIR analysers or PI industrial database or multivariate lab. data)
- to enhance process understanding
  - detection of deviations, non-stable intermediates
  - changes in the chemical composition of the blending
  - end-point monitoring,
- to monitor the evolution of the process in real time
  - necessitates a summarizing (modeling) of the data
  - displaying batch control charts easily interpretable

Industry requires:

- Simple and different models
  (handled by different people)

- Graphic tools

- Stable predictions according to new samples

- Best detection of abnormalities

- Realistic modelling task

Industry requires:

• Real time quality control made during process or batch evolution (the upsets found earlier made possible corrections)

• models based on summarized adequate data measured on a representative set of good measurements : that mean an exploration of the data and easily interpretable control charts

• to forecast a result or to detect problems

Kinds of Process data :

1- Batch process : they have a finite duration and specific constraints (ex: viscosity measured during batch)

2- Whole Process variables that can be measured on-line : such as:

- operating process data i.e temperature, pression, flowrate, shaking
- spectroscopic process i.e NIR, Raman, UV, MIR

The methods bring up

- Methods

Explore 1 data set		Explore or regress 2 data sets	
PCA OPA	Parafac Parafac2 Tucker OPA 3D	PLS IV-PCA	n-PLS IV-Tucker
2 way	N way	2 way	N way

Concern several different arrays: simple, multiple, cube, Nway, multiple slices...

Aims of analysis could be :

-an exploration of the array X : detection of clusters, of typical sample(s) or outlier(s)

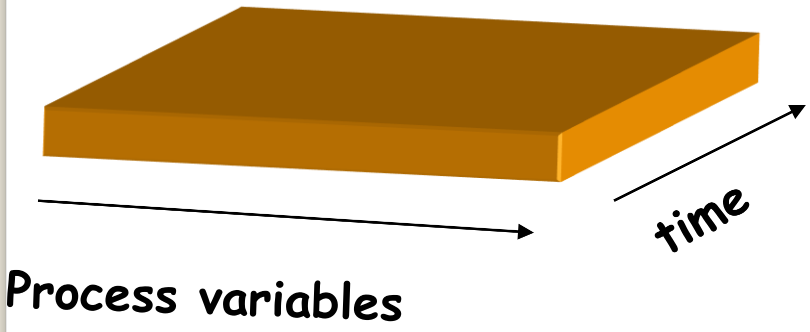
-a process understanding : how and what can we learn about the chemical reactions

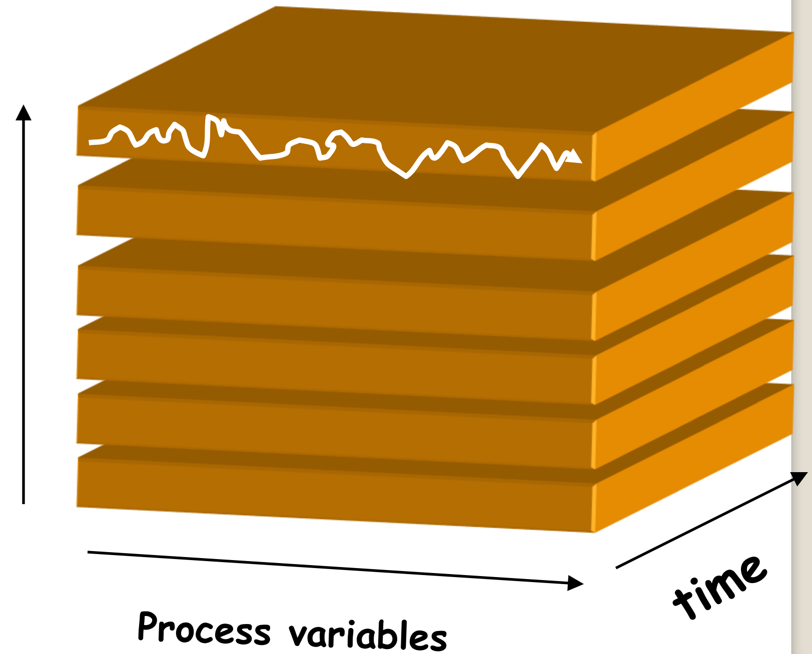
- a statistical process monitoring : detection of disturbances
-modelling one or more characteristics

- to involve both variations due to known causes and unknow causes

- to link the operating conditions with chemical reactions

Data

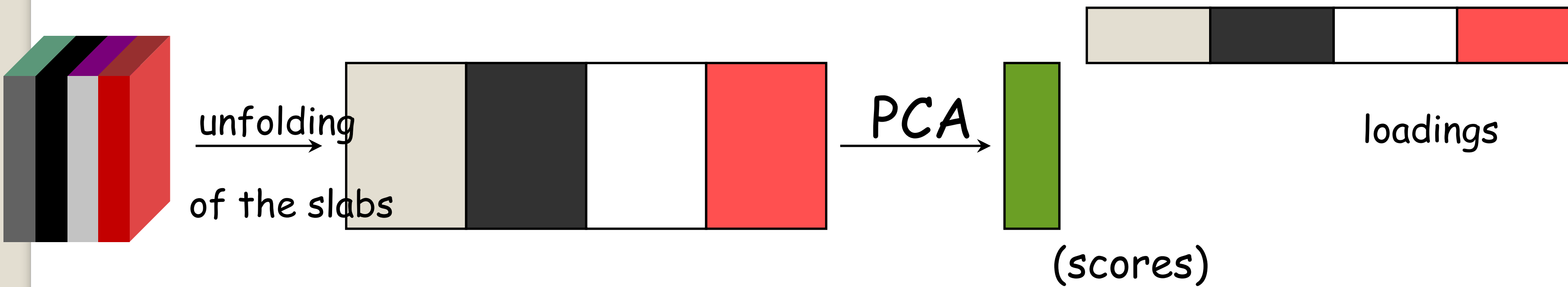




One batch

Series of batches

Data exploratory analysis



Y *Rank* 1 : $Y=(Y_{ij})$, Exist $a=(a_i)$ and $b=(b_j)$ such that $Y_{ij}=a_i b_j$

Advantages: simple to use based on eigen-structure properties. Usual data analysis are well known (PCA, PCR, PLS…)

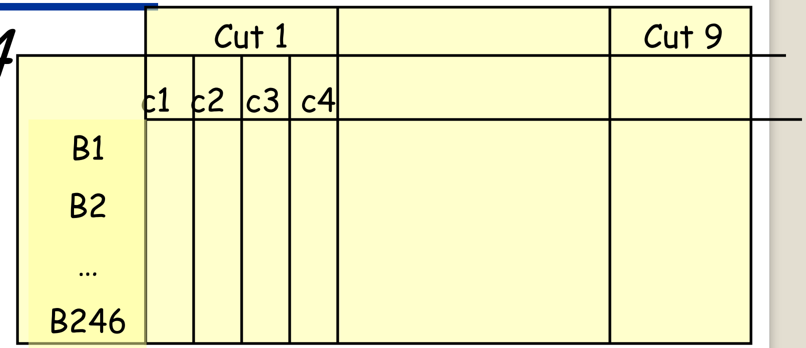
Drawbacks: sub-optimal. ***Some information is lost.***

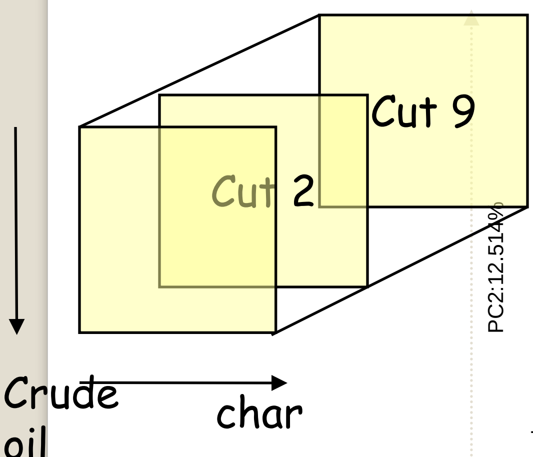
We lose the N-linear structure if exists

Remind: PCA analysis & PLS

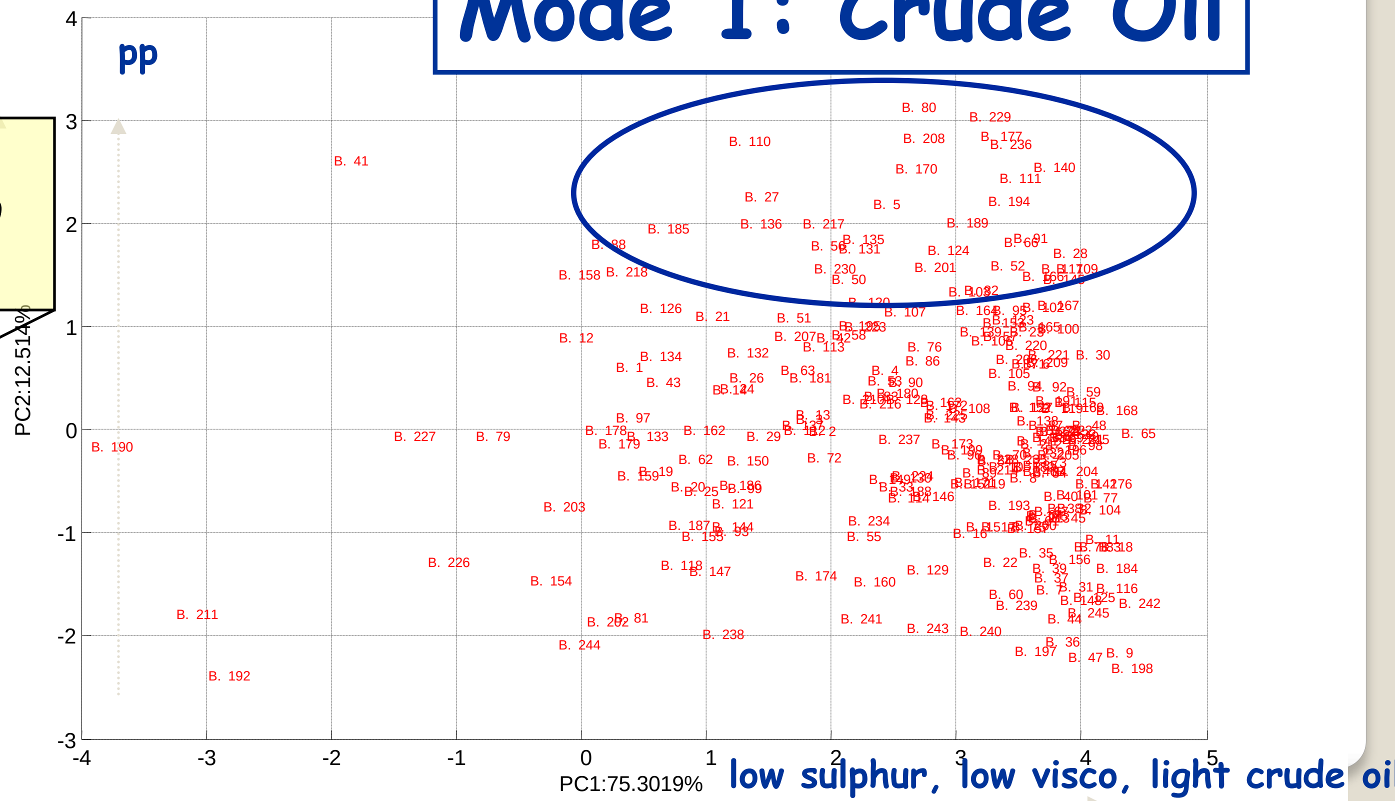
Data: 246 crude oil X 9 "cuts" x 4 characteristics

Array : 246 X 36 (unfolding per "cuts")





Mode 1: Crude Oil



Remind: PCA analysis & PLS

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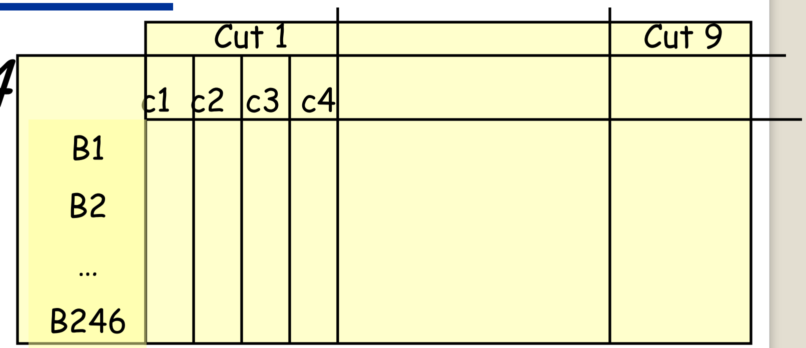
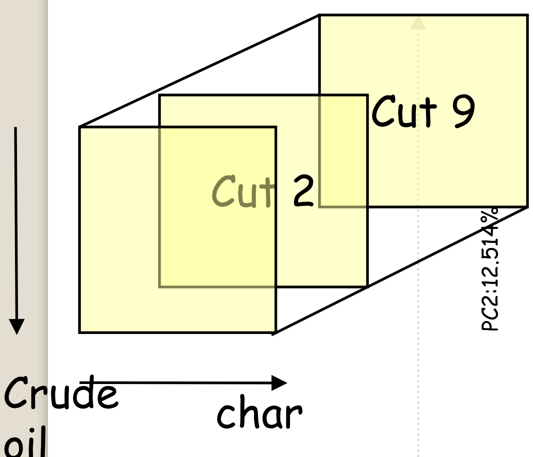
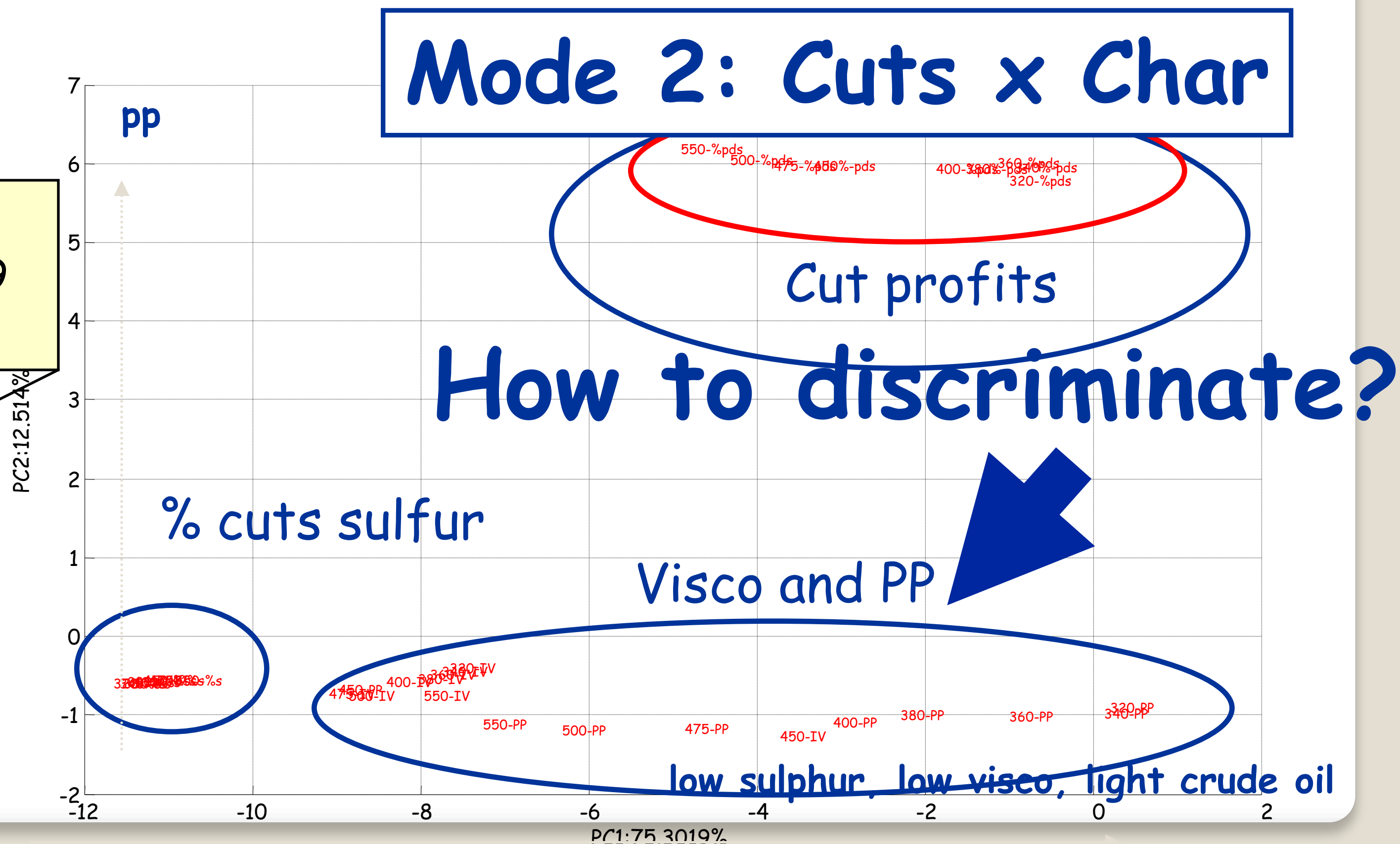


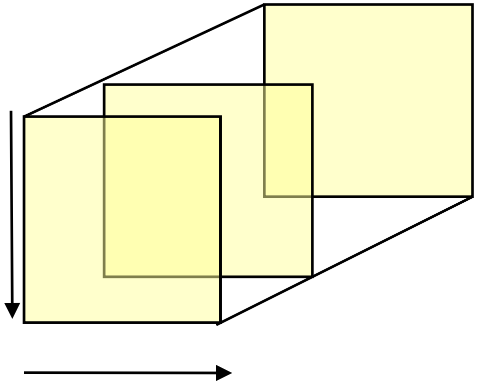




Remind: PCA analysis & PLS

Data:
Array :

Example of PLS ?

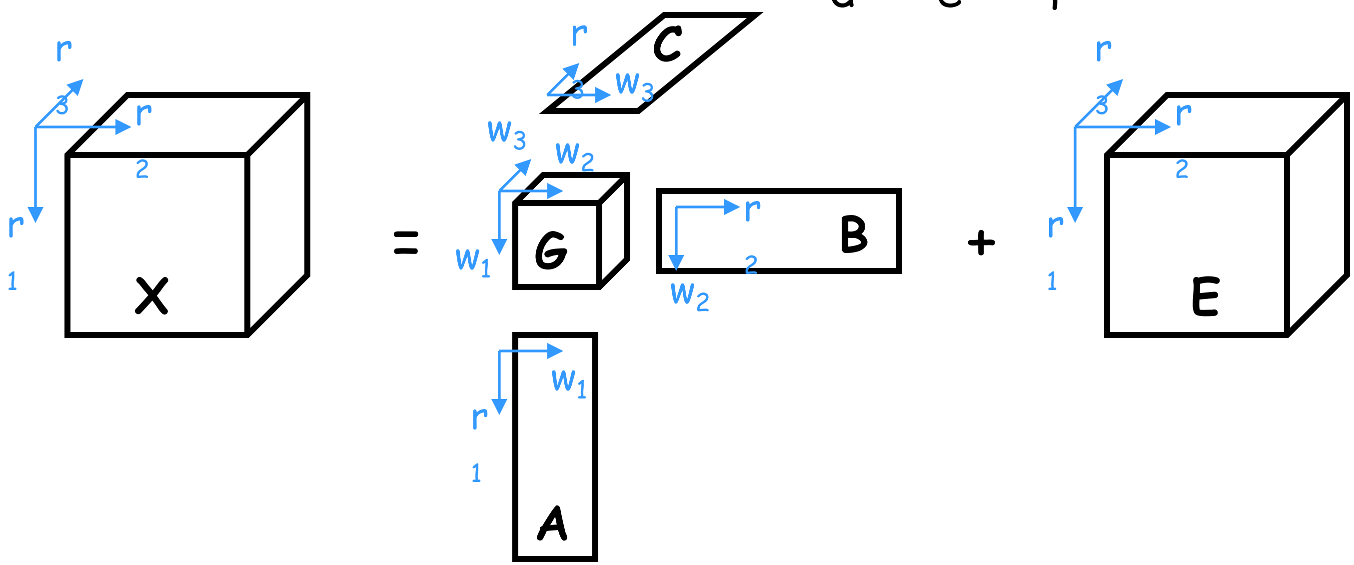


Nway exploratory methods

Nway models: extensions of PCA for Nway data

Tucker3 model:

$$x_{ijk} = \sum_{d} \sum_{e} \sum_{f} a_{id} b_{je} c_{kf} g_{def} + e_{ijk}$$



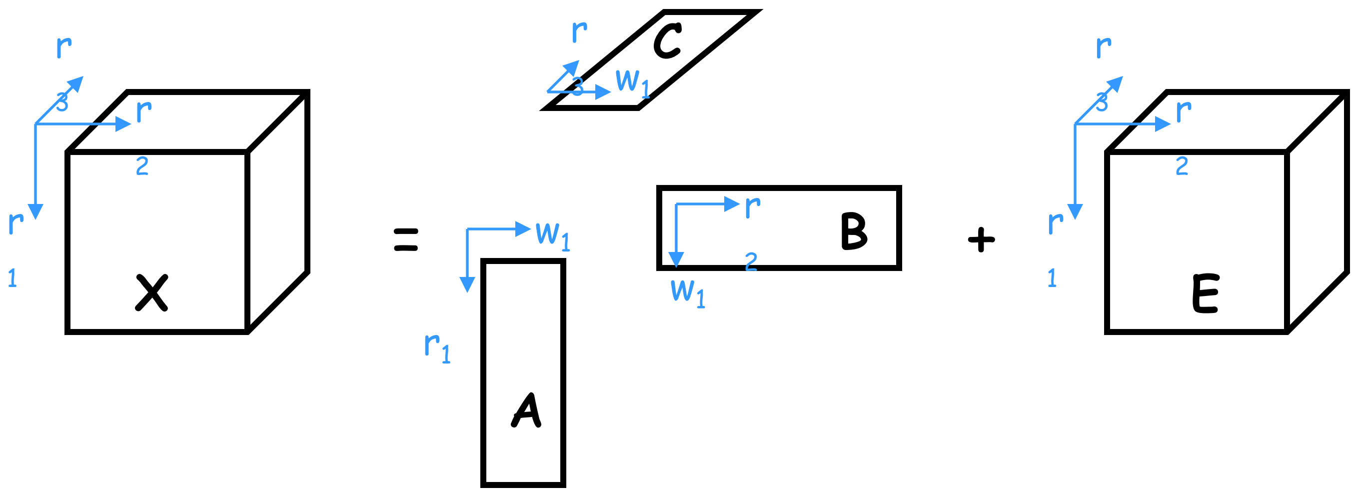
Tucker criterion $\Phi^{i} = \underset{\Phi^{i} \in E^{i}}{\arg\min} \| \underline{Y} - P_{\otimes_{i=1}^{N} \Phi^{i}}(\underline{Y}) \|_F^2 .$

Algorithm: ALS (iterative)

Nway exploratory methods

Nway models: extensions of PCA for Nway data

PARAFAC model: $x_{ijk} = \sum_{f=1} a_{if} b_{jf} c_{kf} + e_{ijk}$



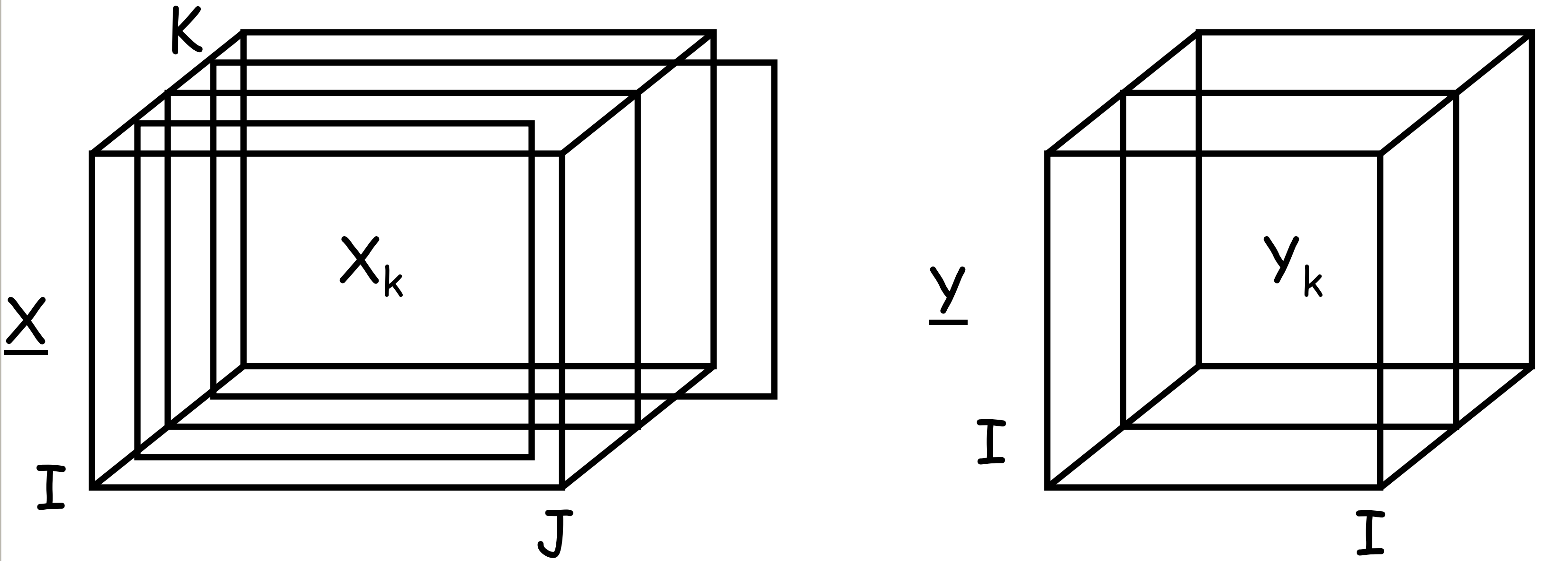
PARAFAC criterion:

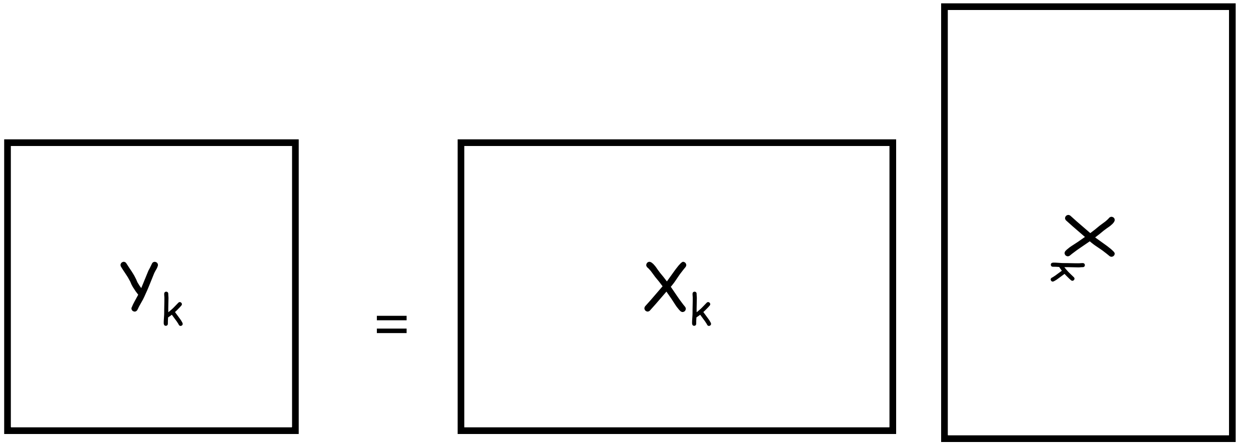
$$(a_i, b_i, c_i) = \underset{a_i \in E^1, b_i \in E^2, c_i \in E^3}{\operatorname{argmin}} \| \underline{Y} - \sum_{f=1}^{F} \lambda_f \, a_f \otimes b_f \otimes c_f \|_F^2$$

Algorithm: ALS (iterative)

Nway exploratory methods

PARAFAC2 model:





N-Way exploratory methods

PARAFAC2 model:

$$Y = (C^T|\otimes|C^T)^T \,\mathrm{diag}(\mathrm{vec}H)(A \otimes A)^T$$

Kiers et al. (1998)

$$X = AD_k(B_k)^T = AD_k(P_kB)^T$$

Y: each frontal slice in $\underline{Y}$ is the cross product of the corresponding slice in $\underline{X}$

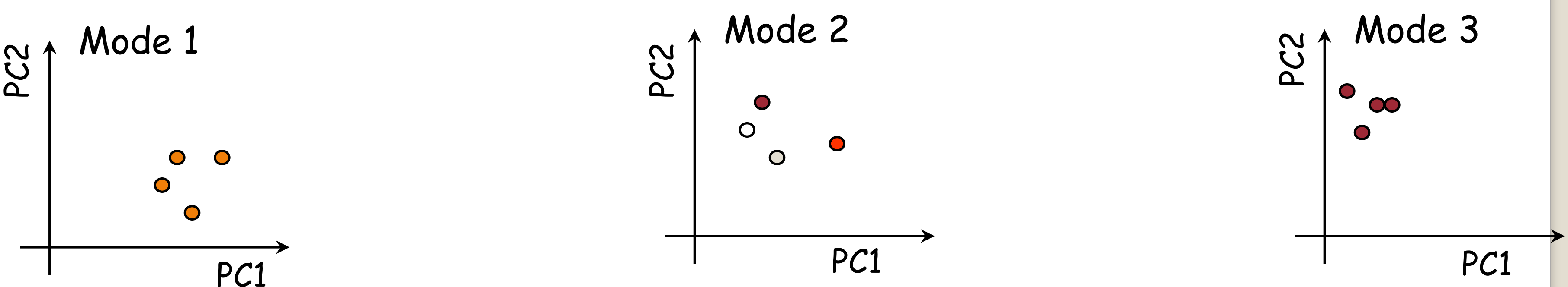
$H = B^TB$

Only the cross product of B is estimated (not B itself)

Nway exploratory methods

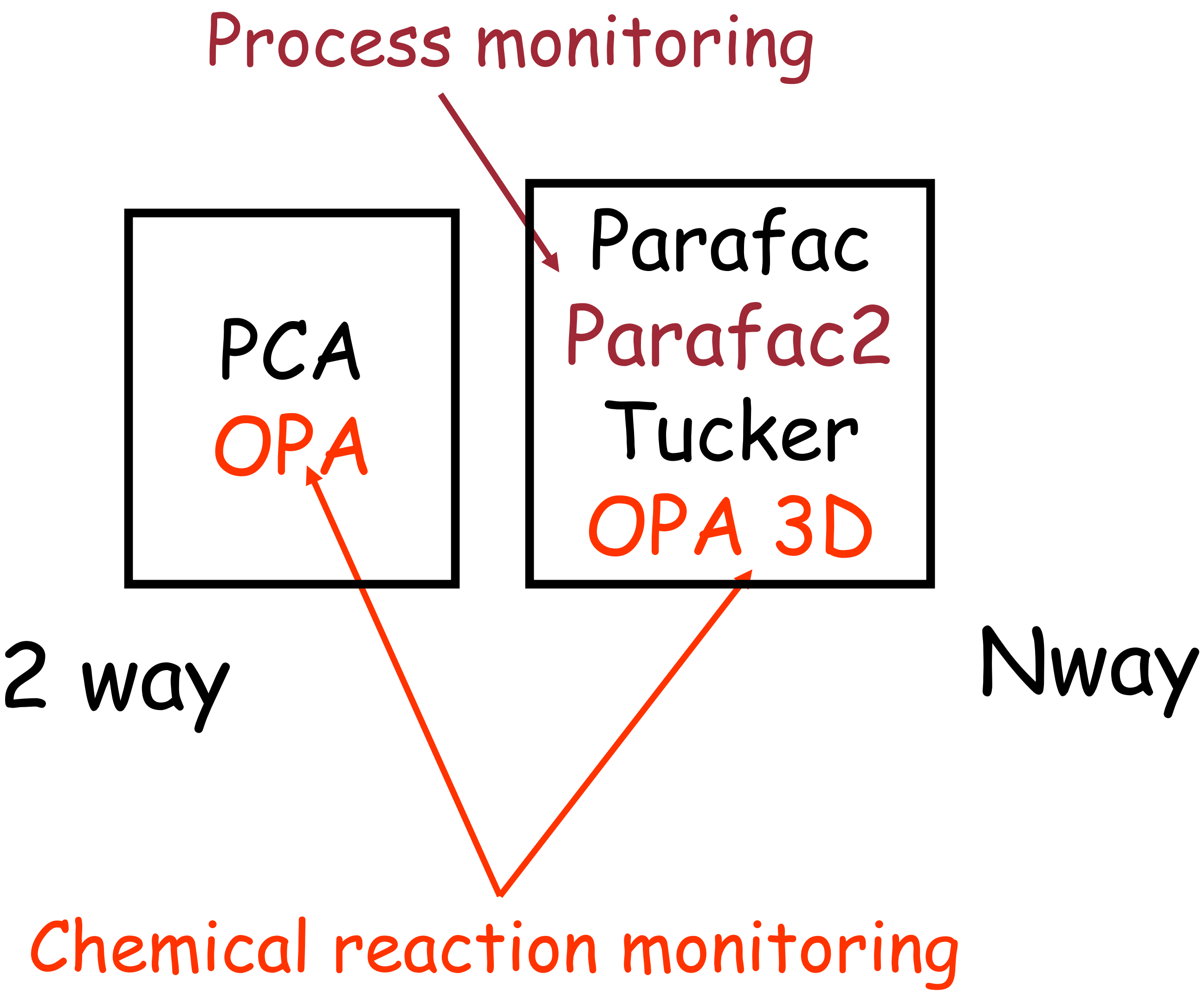
Why Nway methods? Advantages:

- can be considered as an optimisation method with regards to PCA
- fit to the structure. Nway models respect the Nway the data structure (≠ unfolding).
- Nway methods most Robust as regards with noise
- allows simultaneous analysis



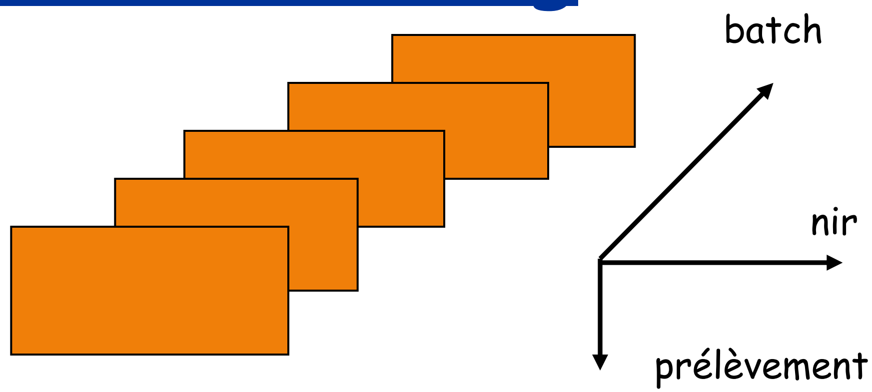
- Can be extended to 4D, 5D...
- Number of parameters much less numerous than ACP
    - eg: cube 10x700x35: $r_{NWAY}(I+J+K)=735$, $r_{PCA}(I+JK)= 1750$
    - eg: cube 10x700x35x20: $r_{NWAY}(I+J+K+L)=755$, $r_{PCA}(I+JKL)= 490.010$

Batch monitoring (only one X matrix)



Process monitoring

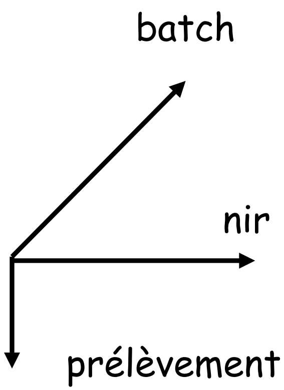
Method: PARAFAC 2

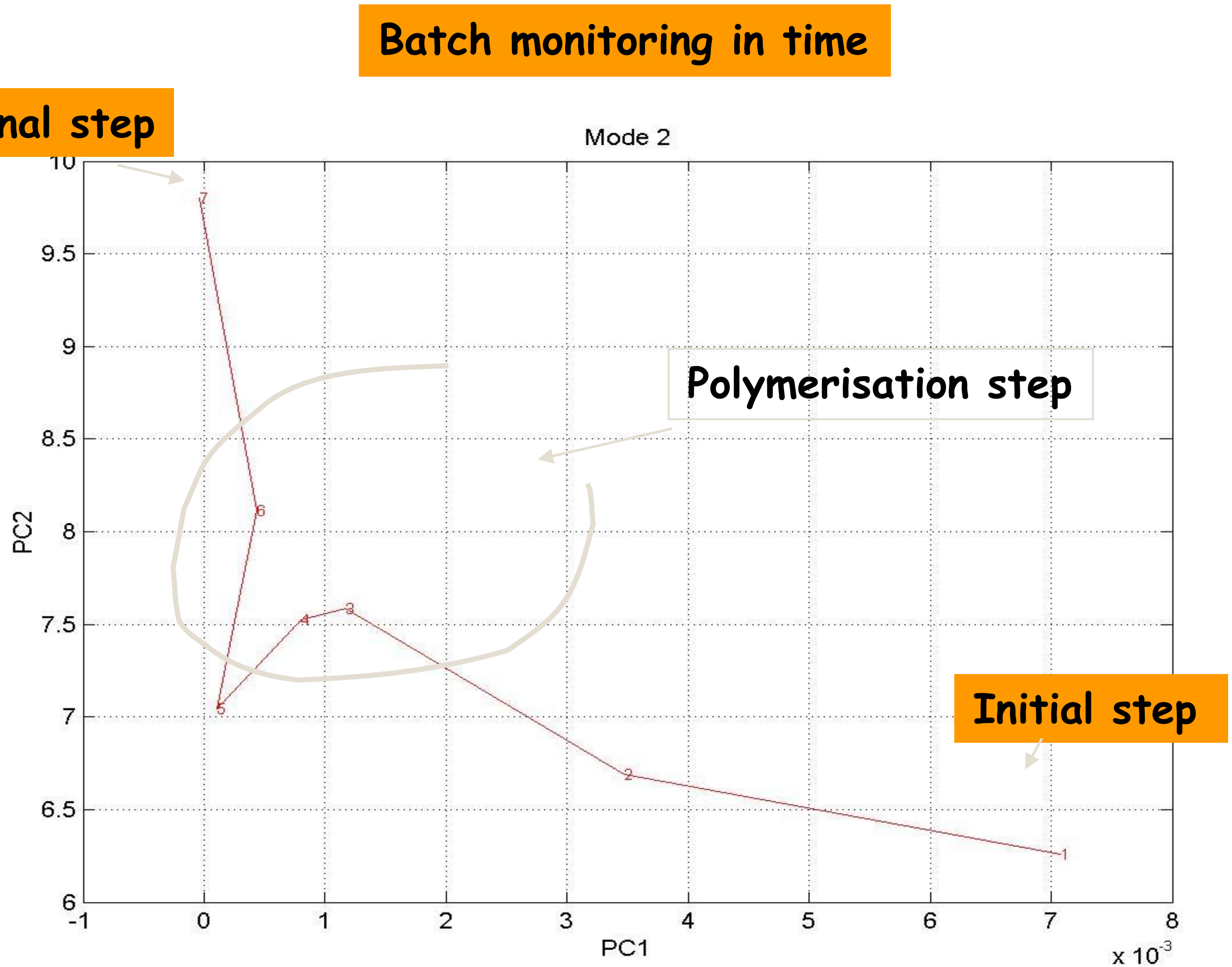


10 batches
Each batch has between 5 and 8 NIR spectra
Each spectrum has 699 wavelenghts

Process monitoring

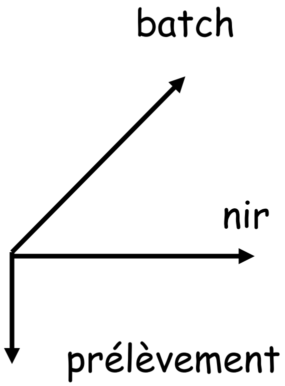
Method: PARAFAC 2

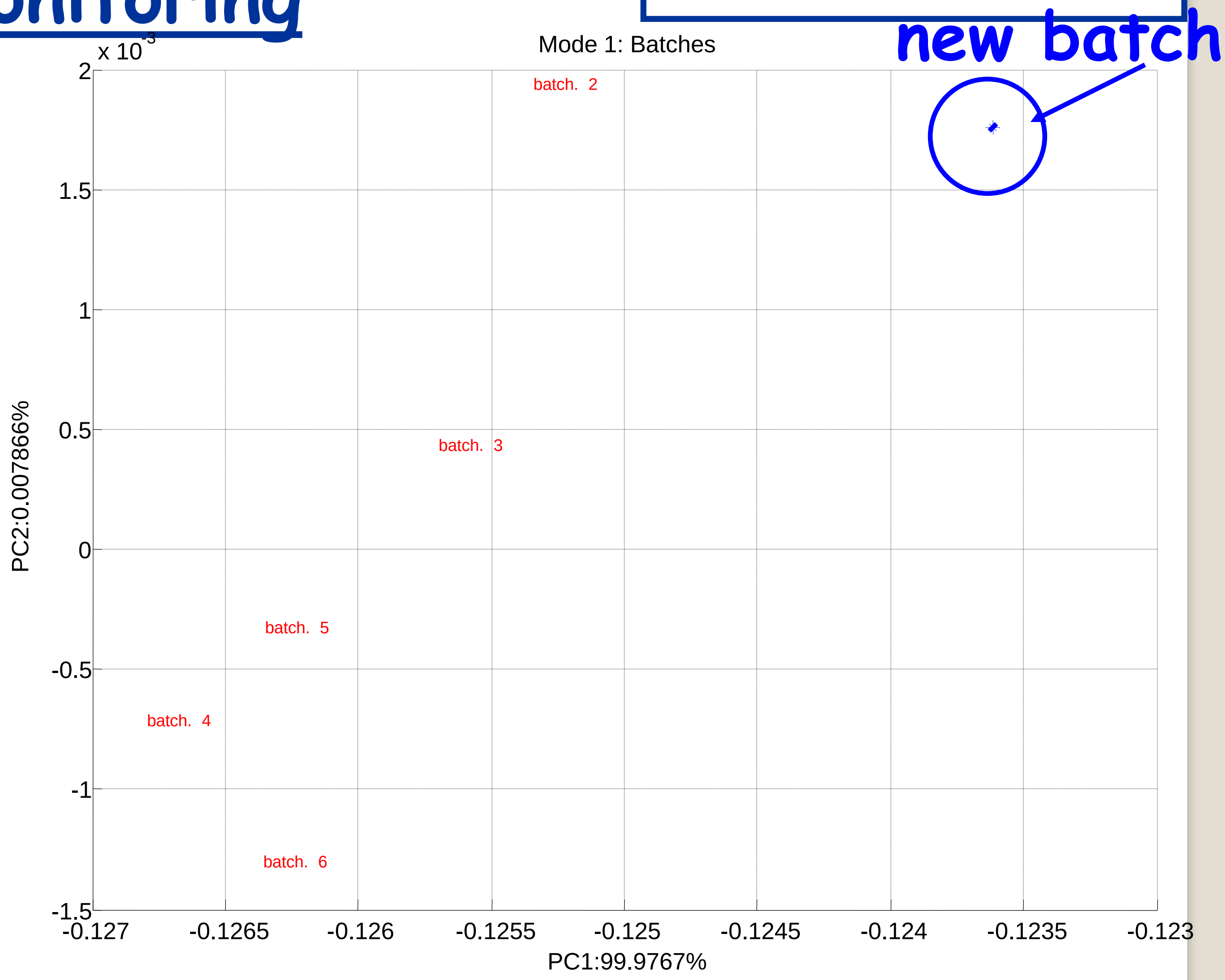




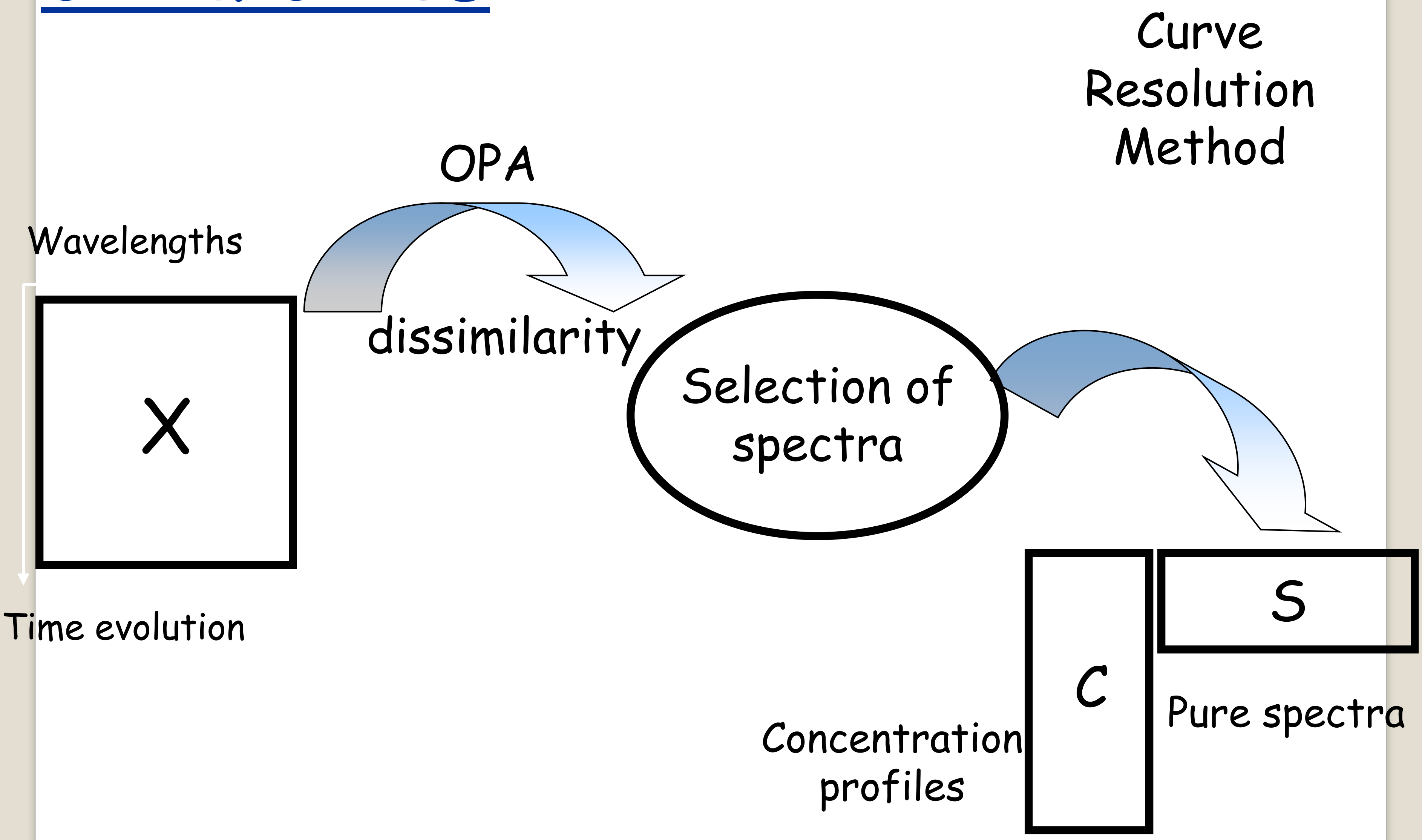
Process monitoring

Method: PARAFAC 2

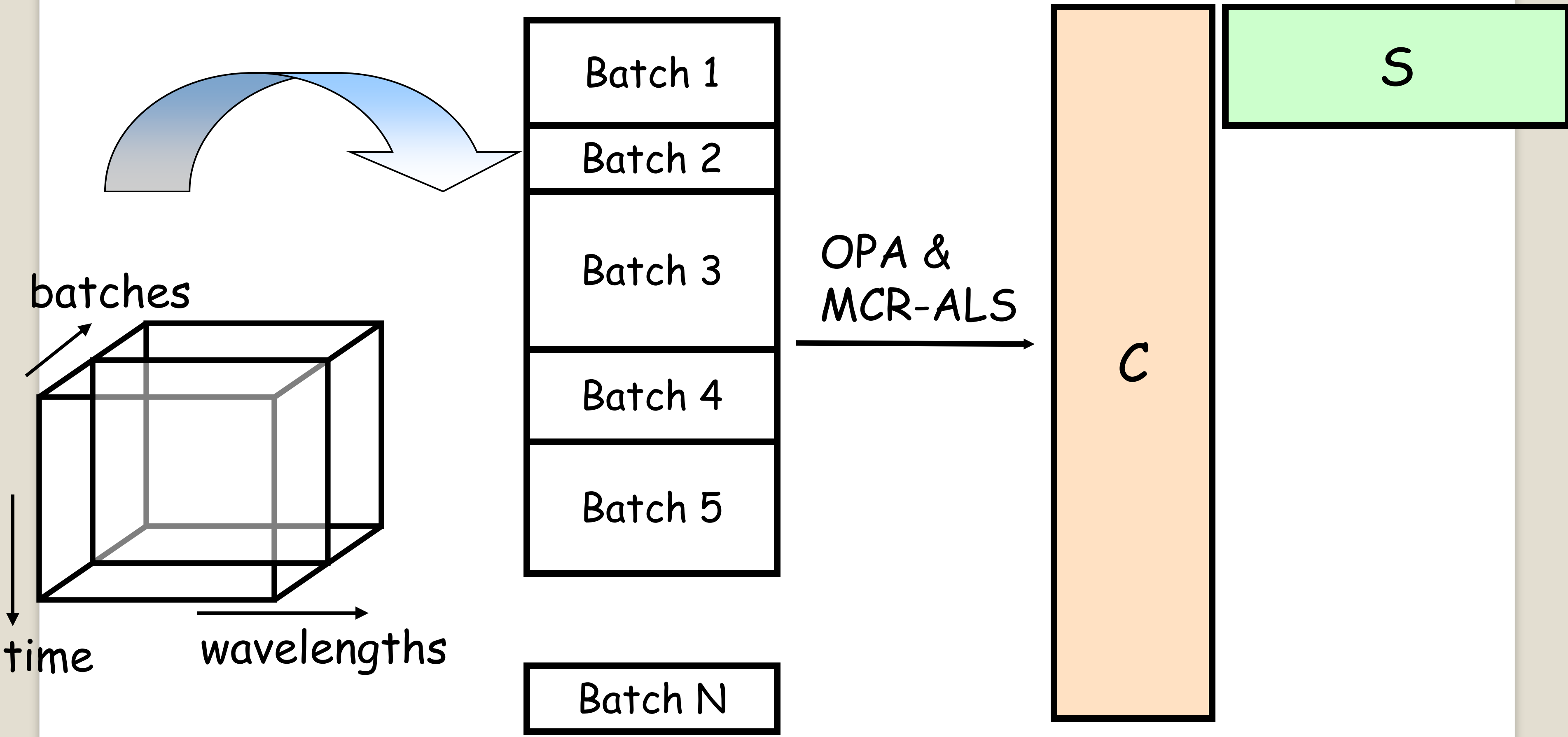




OPA & OPA3D


Curve
Resolution
Method
OPA
Wavelengths
dissimilarity
X
Selection of
spectra
Time evolution
S
C
Pure spectra
Concentration
profiles

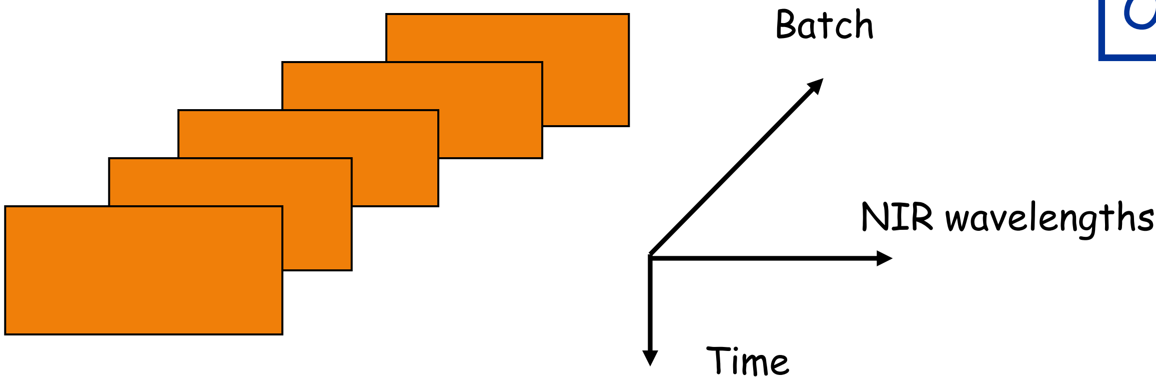
OPA & OPA3D



batches
time
wavelengths
Batch 1
Batch 2
Batch 3
Batch 4
Batch 5
Batch N
OPA &
MCR-ALS
C
S

Chemical reaction monitoring

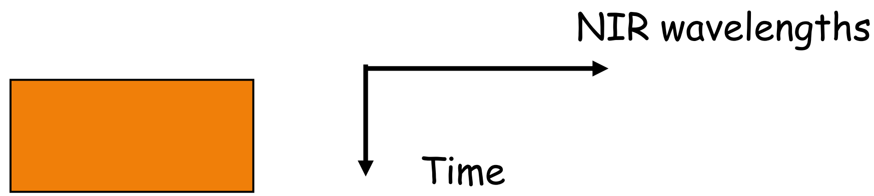
Method:
OPA & OPA3D



The curve resolution methods such as OPA are used during process monitoring to obtain concentration profiles and/or pure spectra of a mixture.

Chemical reaction monitoring

Only 1 batch
Method: OPA



Hypothesis:
At time t, spectrum:

$$X(w) = a_{1t} f_1(w) + a_{2t} f_2(w) \;.....+ a_{kt} f_k(w) + E$$

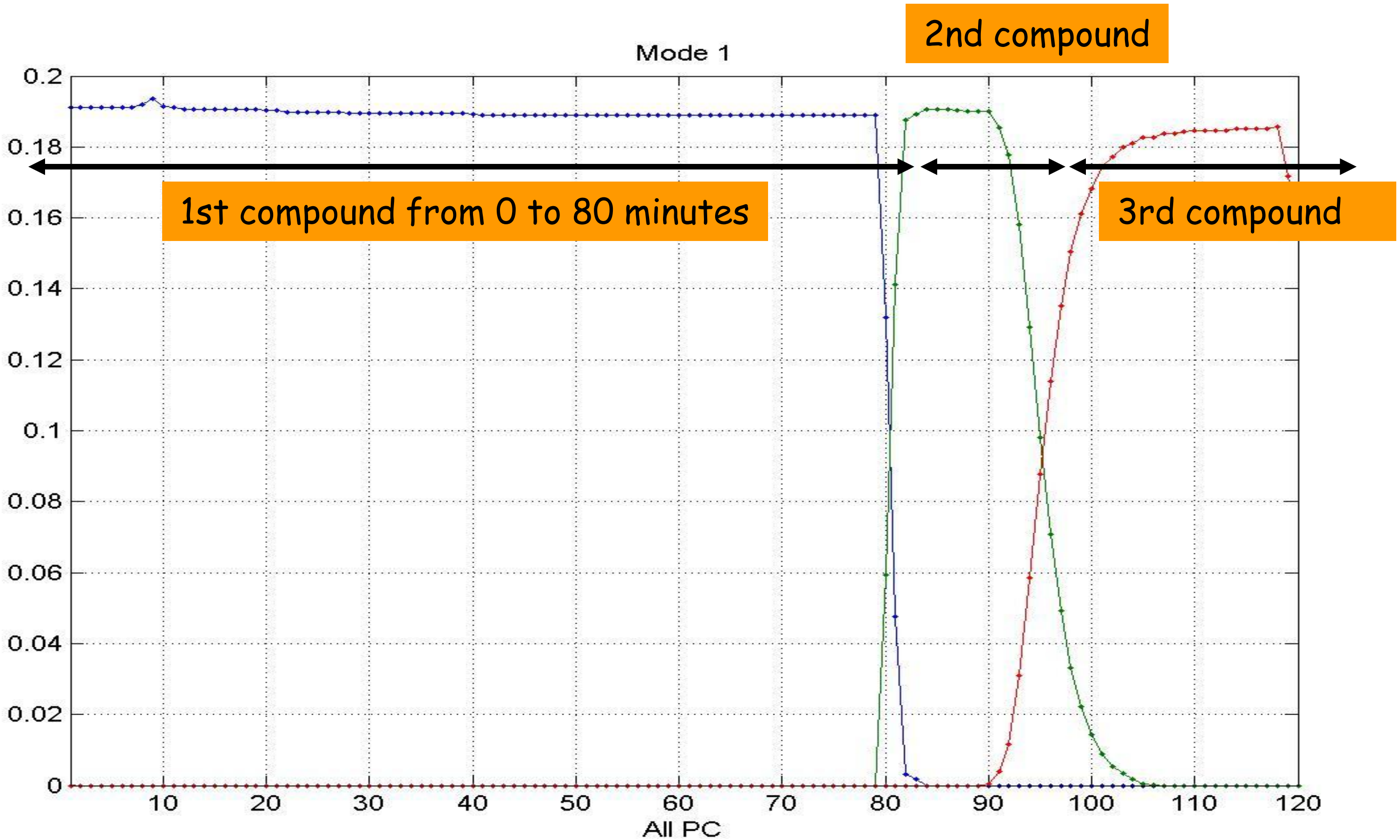
Resolution algorithm: ***ALS***

Initialisation: knowledge about dissimilarity method.
But basis component spectra could also be input or several other methods exist

Chemical reaction monitoring

Method:OPA

120 spectra (measured every minutes) with 201 wavelengths.
Goal:chemical reaction monitoring

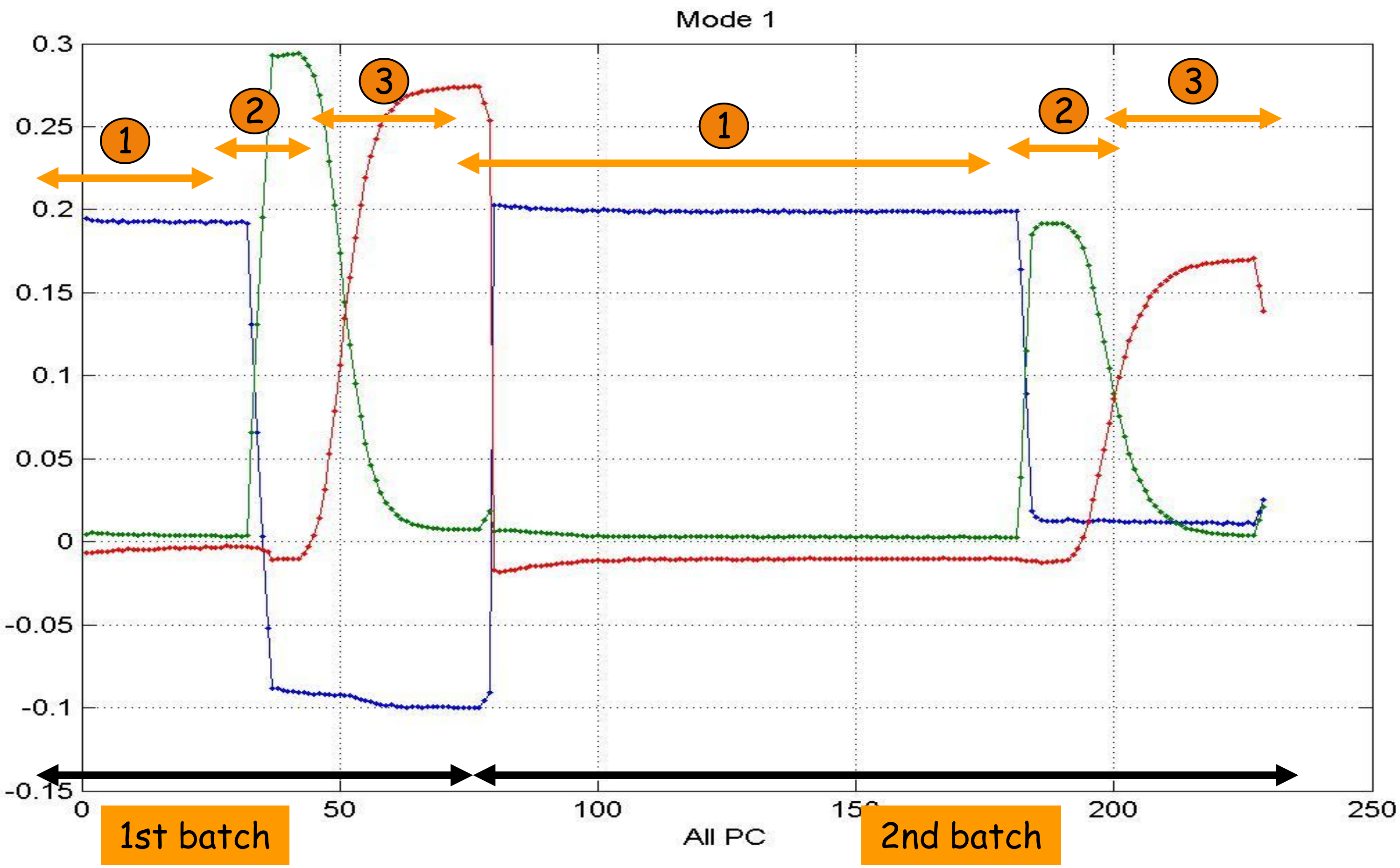


Concentration profil of the different compounds

Chemical reaction monitoring

Several batches
Method: OPA 3D

Two batches with 79 and 150 spectra (229)
Goal: follow the apparition of the 3 components of the reference batches



Batch monitoring (explore or regress 2 matrices)

PLS
IV-PCA

n-PLS
IV-Tucker

2 way

N way

Regression for process monitoring

Nway exploratory methods

Nway models: extensions of PCA for Nway data

IV Tucker model:

Tucker's criterion

$$F^i = \underset{F^i \in E^i}{\operatorname{argmin}} \| \underline{Y} - P_{\otimes_{i=1}^{N} F^i}(\underline{Y}) \|_F^2$$

IV-Tucker's criterion: linear constraints

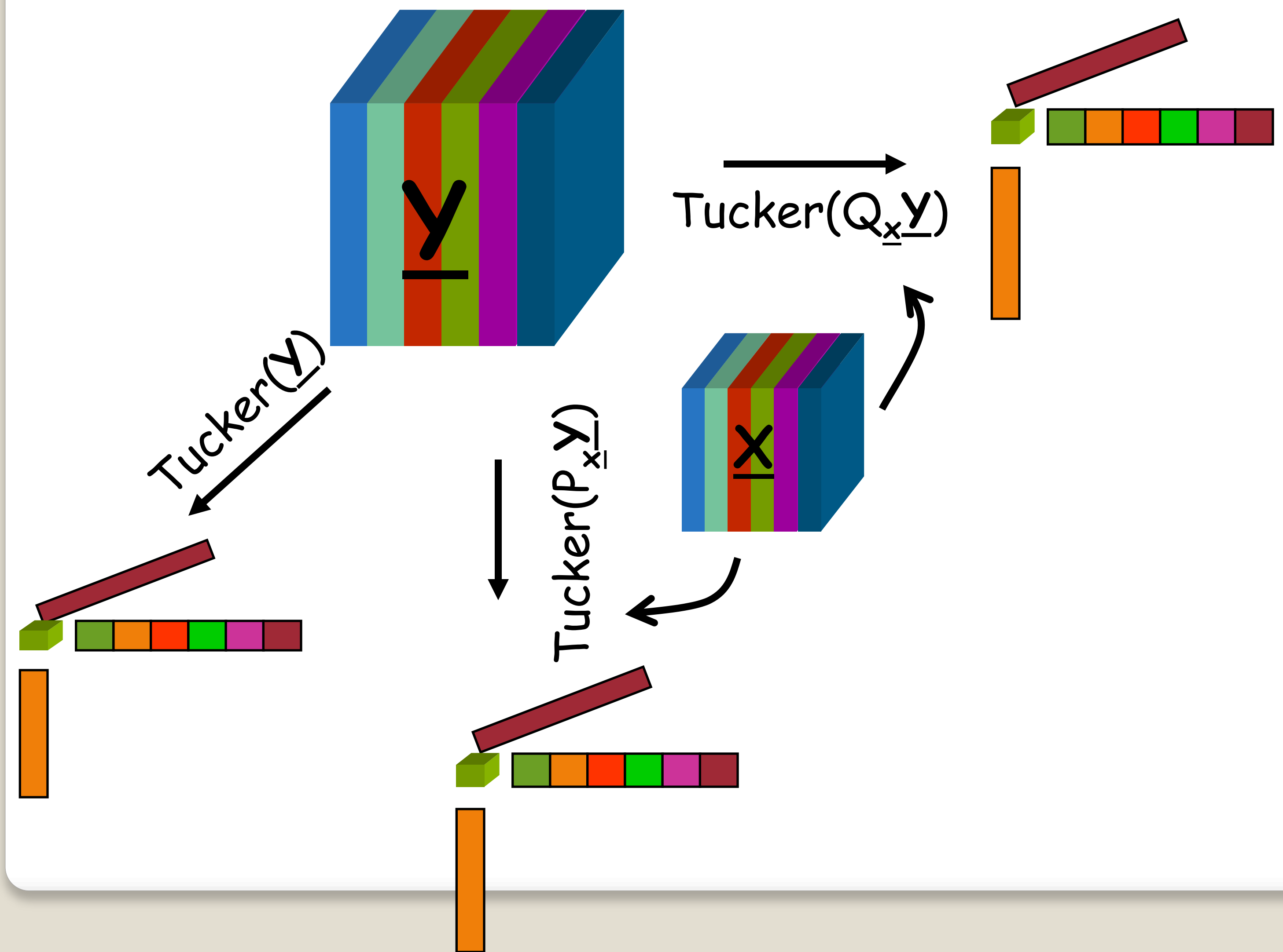
$$F^i = \underset{F^i \in G^i \in E^i}{\operatorname{argmin}} \| \underline{Y} - P_{\otimes_{i=1}^{N} F^i}(\underline{Y}) \|_F^2$$

Several modes can be constrained

Nway exploratory methods

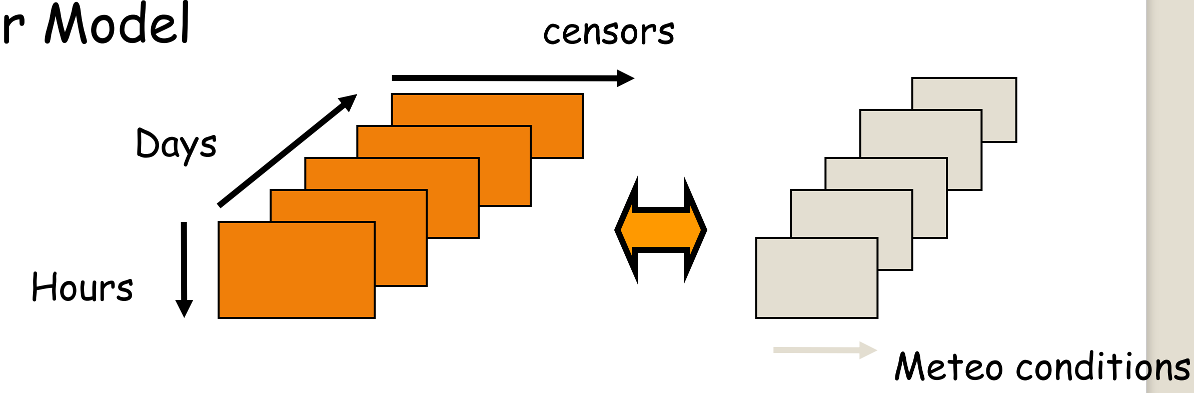
Nway models: extensions of PCA for Nway data

IV Tucker model:



Nway exploratory methods

Application of IV Tucker Model



1- To predict ozone concentrations in Paris, according to climate information.

Predictive model

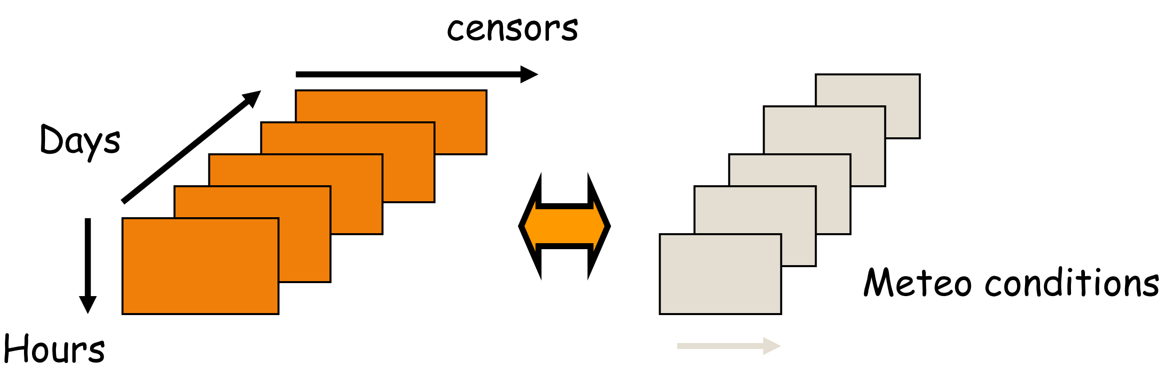
2- To detect variations of ozone

in relation with the climate

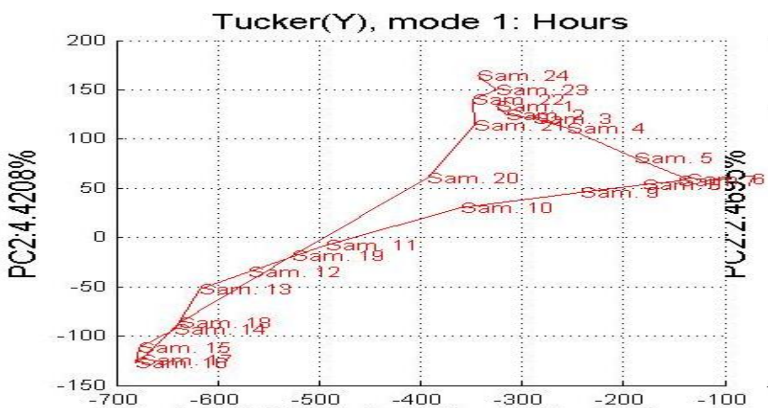
independant from the climate

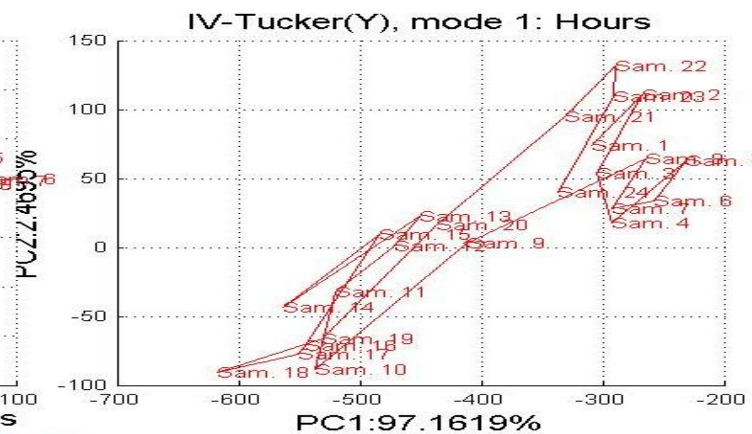
Causal model

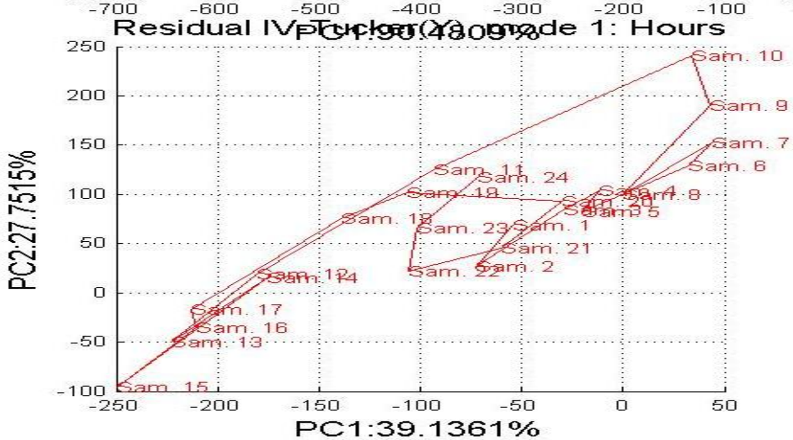
Method:IV Tucker



Application on O3 pollution data
pollution 24x13x2
météo 24x13x2

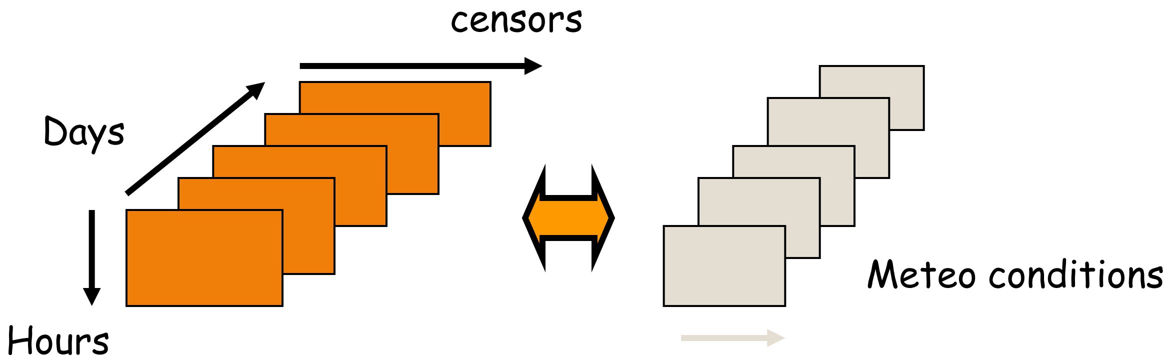






Aim: constraints analysis

Method:IV Tucker



Application on O3 pollution data
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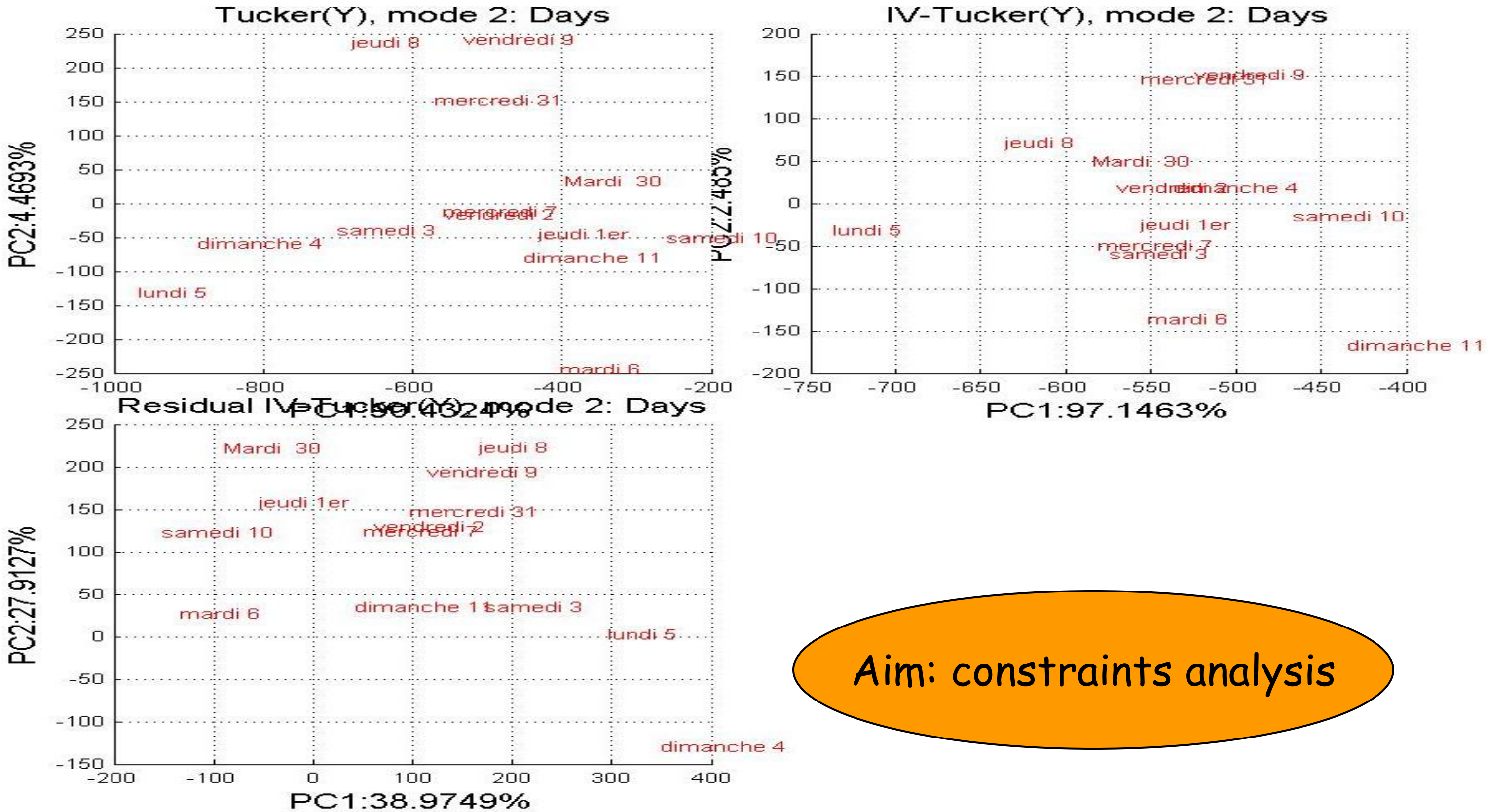
météo 24x13x2



Aim: constraints analysis

Method: IV Tucker Prediction

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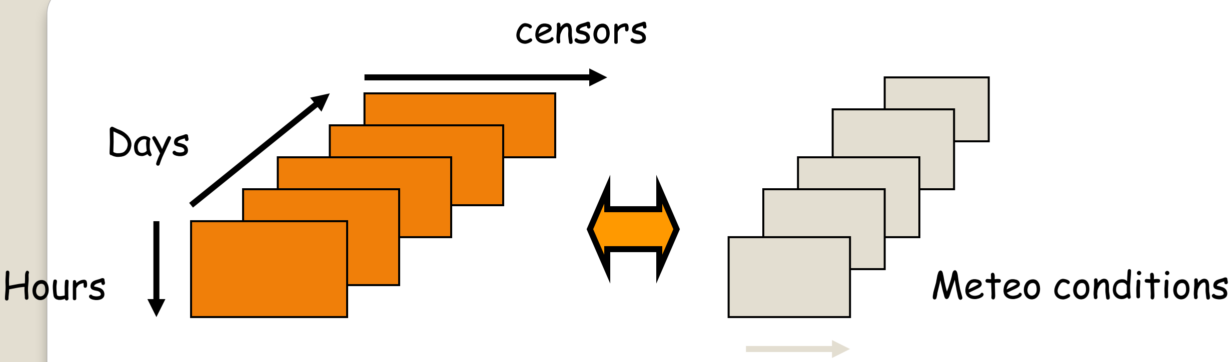
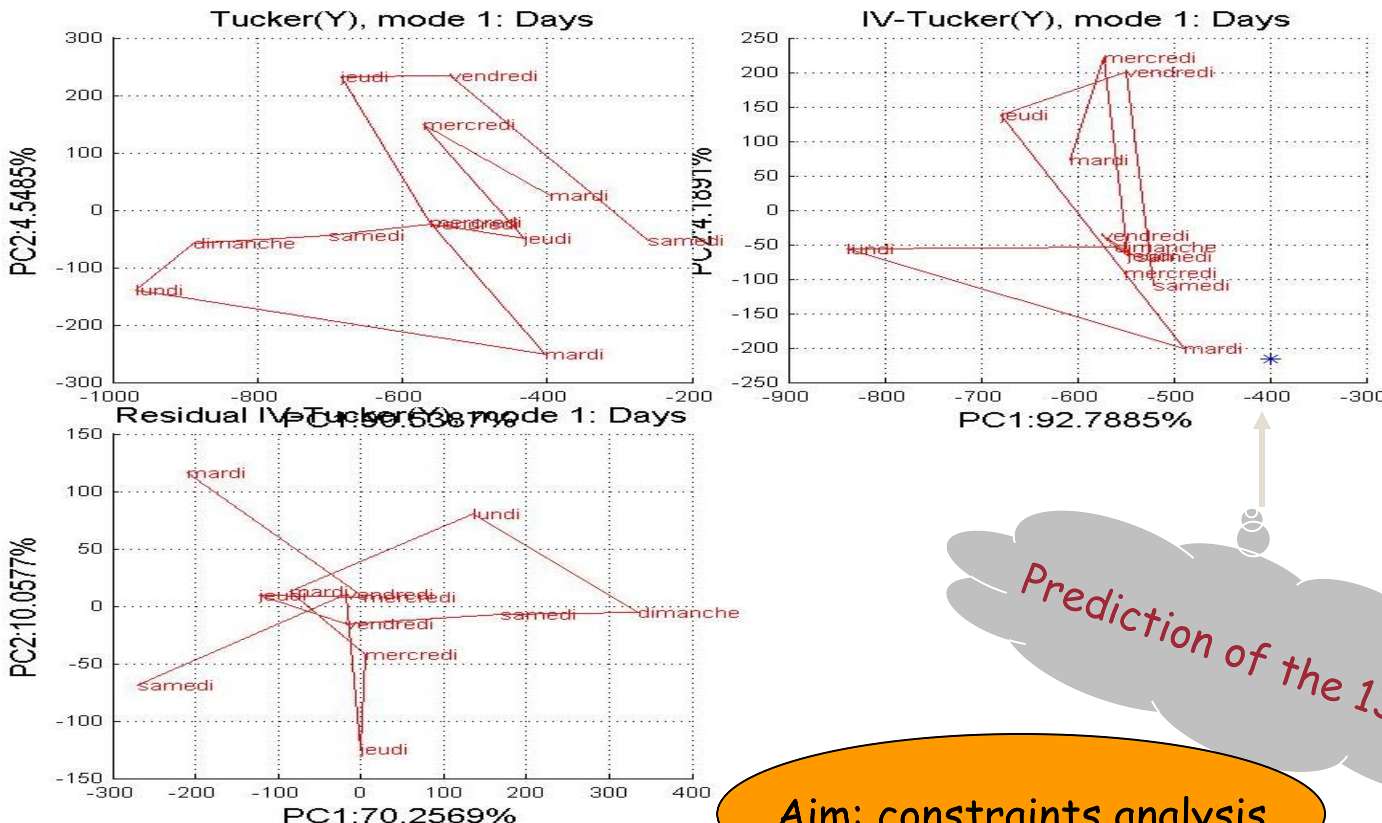
météo 24x13x2





Prediction of the 13th day

Aim: constraints analysis

Nway methods in process control

ChemoAC / VICIM symposium - S.Gourvénec, C-A.Saby