New Methods Based on the Projection to Latent Structures for Monitoring, Prediction and Optimization of Batch Processes

D.L. Massart Award

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Outline

- Introduction to Batch Processing
- Modelling of a Batch Process
- Multi-phase Framework
- Applications
- Conclusions
- Acknowledgements

Introduction to Batch Processing

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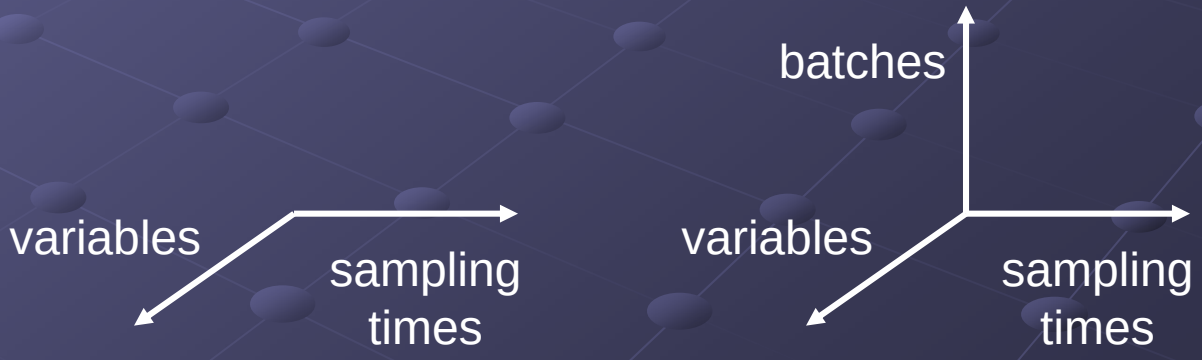
- **REPETITION OF THREE STEPS**: i) charge, ii) processing and iii) discharge.



Introduction to Batch Processing

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- **REPETITION OF THREE STEPS**: i) charge, ii) processing and iii) discharge.
- Principal advantages: Adjustable processing time, repetitive nature, flexibility, …
- Industries: pharmaceutical, chemical, biochemical, metal, etch or food industries, …
- Objective: to manufacture high value, specialty products.

Modelling of a Batch Process

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1. Introduction to Batch Processing
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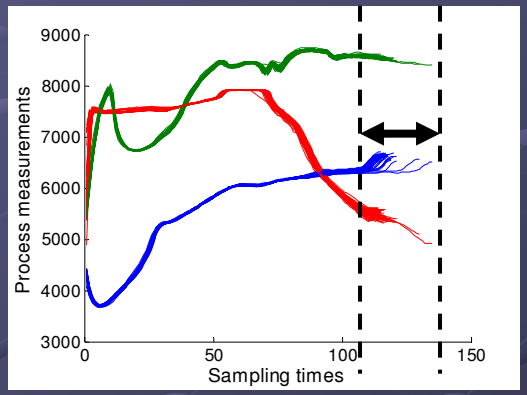
- Modelling paradigms:
  - Knowledge-based
  - Data-based
  - Hybrid



- Difficulties:
  - Nonlinear dynamics and uncertainty
  - Trajectories instead operation points ➔ Time-varying dynamics
  - Presence of noise, collinear data and outliers
  - Uneven batch length

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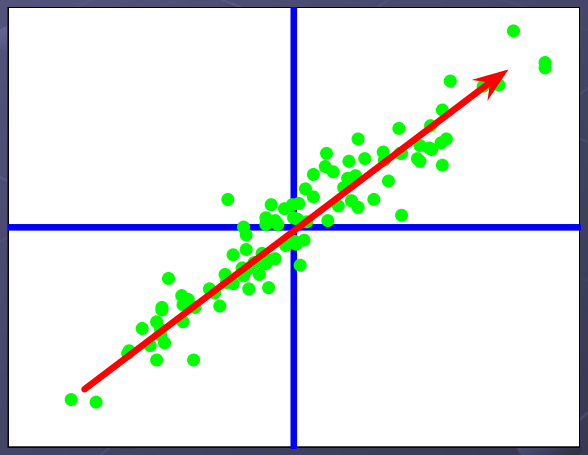
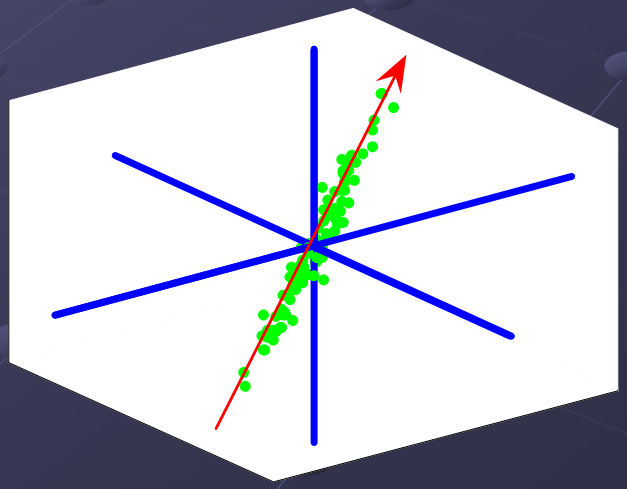
- Projection to Latent Structures-Based (PLS-Based) Methods.
  - Principal Component Analysis (PCA) and Partial Least Squares (PLS).
  - In a *n*-dimensional space, the dimension of the sub-space in which data mostly vary is much lower than *n*.





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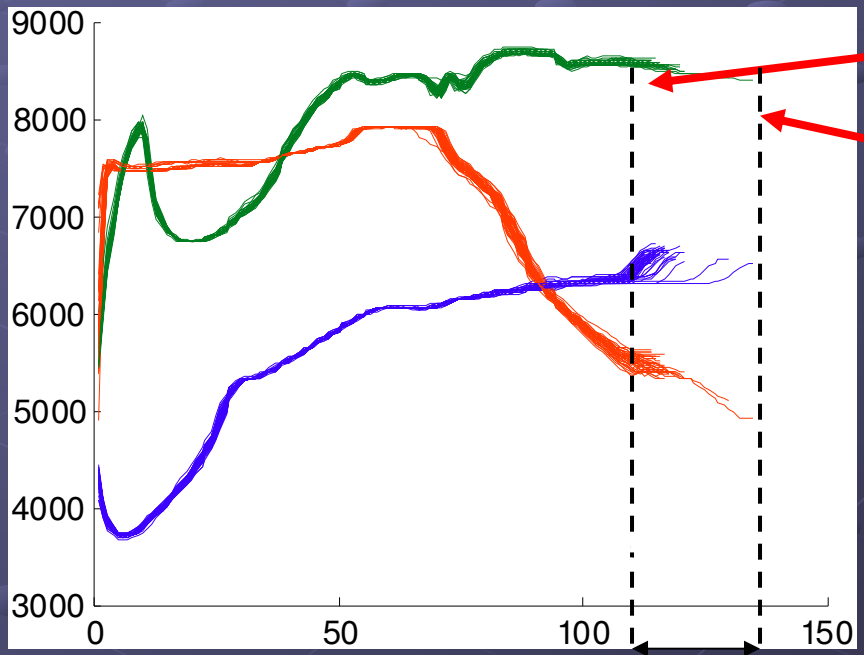
- Pre-treatement:



IV,
DTW,
COW,
PARAFAC2,
…

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- Pre-treatement:

Aligned!!!

I batches
J variables
K sampling times

- The average trajectory is subtracted

Model Structures

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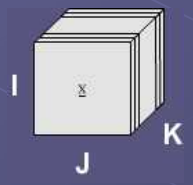

- Convert into two-way data and apply PCA, PLS, …
- Apply three-way methods: PARAFAC, Tucker-3,…

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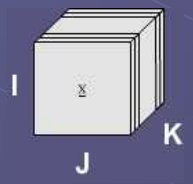

- Convert into two-way data and apply PCA, PLS, …
  - Unfold the three-way matrix.
  - Divide in K local matrices.
  - Use an adaptive approach.
- Apply three-way methods: PARAFAC, Tucker-3,…

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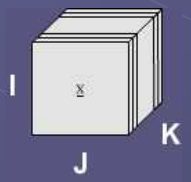
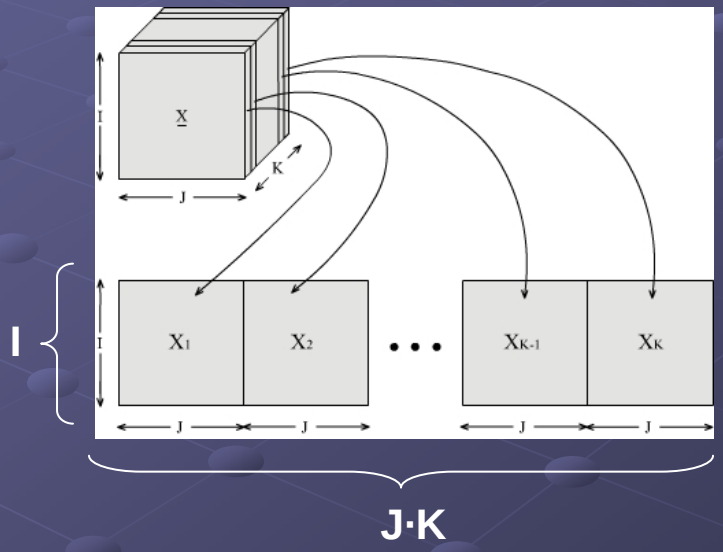


- Unfold the three-way matrix.
  - Batch-wise unfolding



Thousands of variables!!!

(X'·X) → PCA
(X'·Y·Y'·X) → PLS

$$\#Par. = \frac{(JK+1)JK}{2}$$

J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part I: Theoretical discussion*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1113

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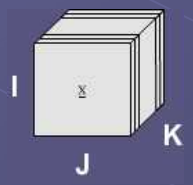

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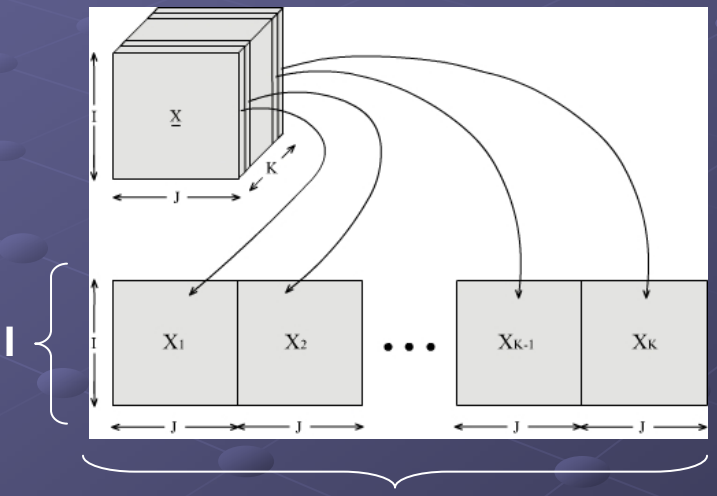
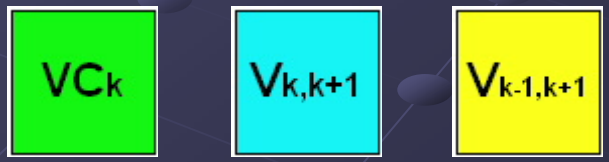


Thousands of variables!!!



Order 0 **Order 1** **Order 2**

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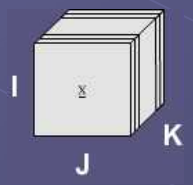

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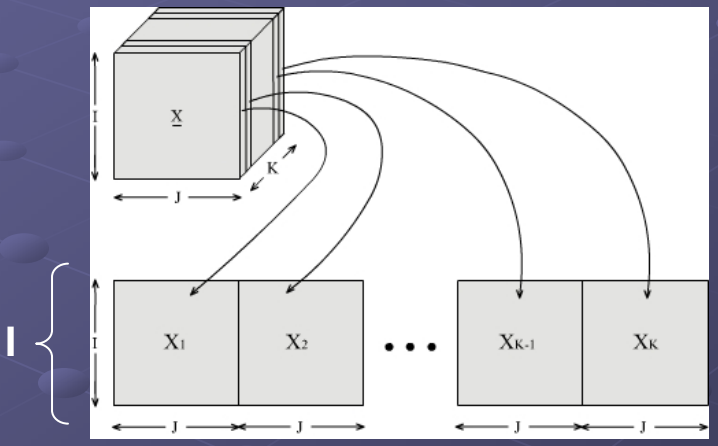

Thousands of variables!!!

Dynamics are captured in the model

Time-varying dynamics are captured

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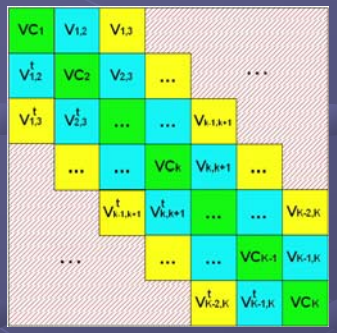
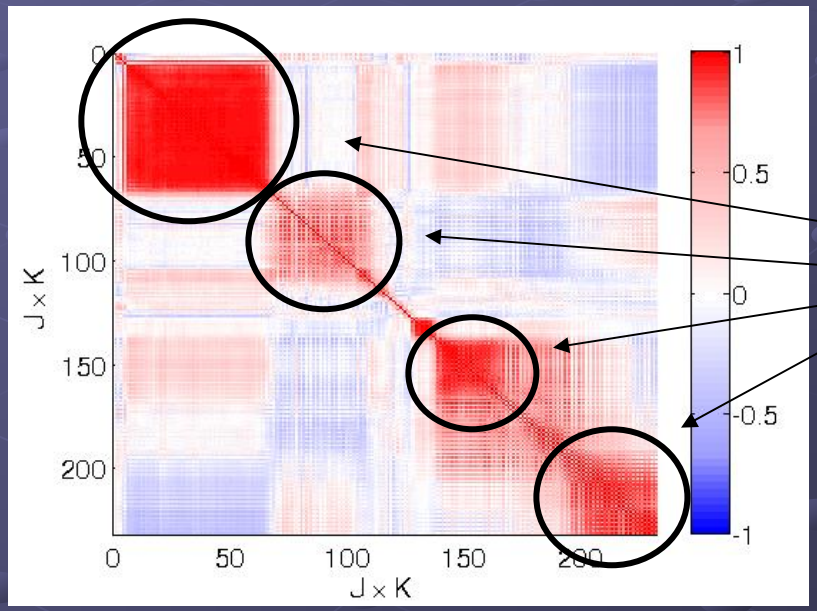


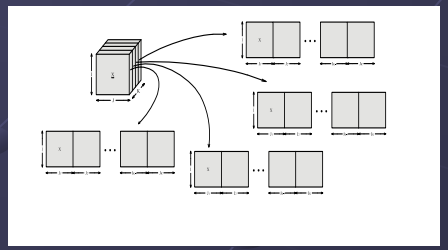
- Unfold the three-way matrix.
  - Batch-wise unfolding



(X'·X) for 2 variables x 116 sampling times

More than a half is noise!!!

Focus on important areas



Solution: Piece-wise modelling

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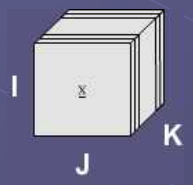
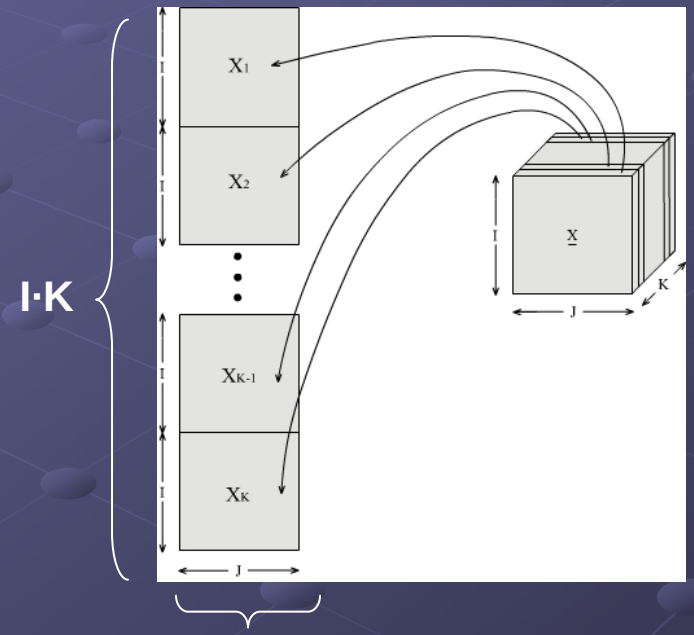


- Unfold the three-way matrix.
  - Variable-wise unfolding



(X'·X) → PCA
(X'·Y·Y'·X) → PLS

$$1/K \cdot \left(VC_1 + \ldots + VC_k + \ldots + VC_K \right)$$

$$\#Par. = \frac{(J+1)J}{2}$$

Low number of parameters

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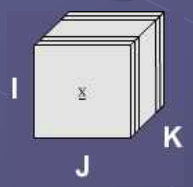


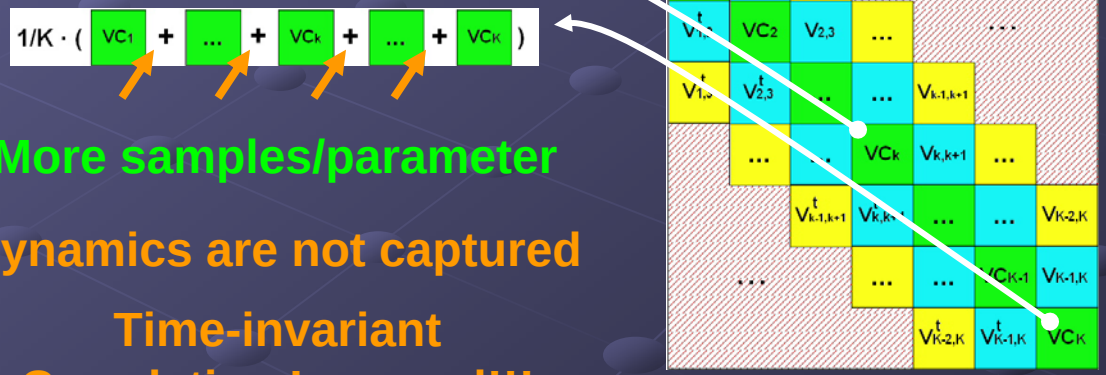
- Unfold the three-way matrix.
  - Variable-wise unfolding

Variable-wise

$$\#Par. = \frac{(J+1)J}{2}$$

Batch-wise

$$\#Par. = \frac{(JK+1)JK}{2}$$



More samples/parameter

Dynamics are not captured

Time-invariant
Correlation Imposed!!!

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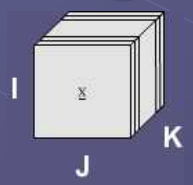
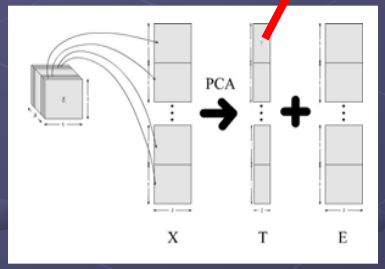
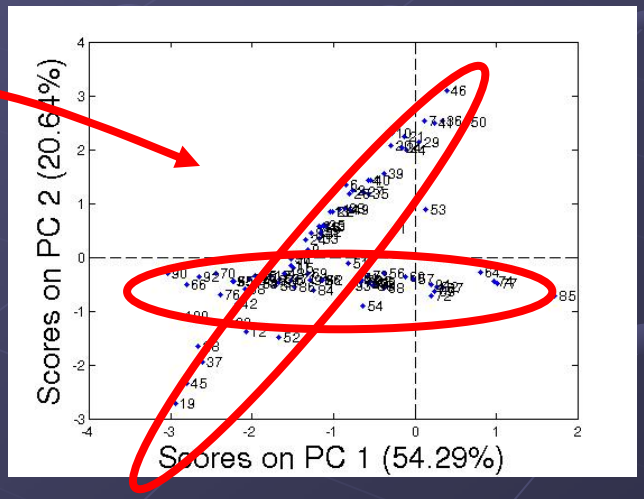


- Unfold the three-way matrix.
  - Variable-wise unfolding

Time-invariant Correlation Imposed!!!

Saccharomyces cerevisiae cultivation





V-W scores

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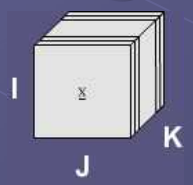

- Unfold the three-way matrix.
  - Variable-wise unfolding

Time-invariant Correlation Imposed!!!

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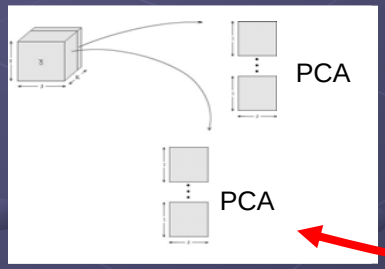

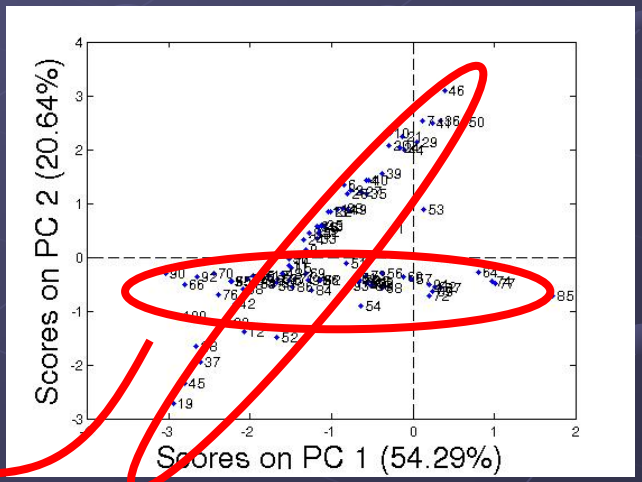

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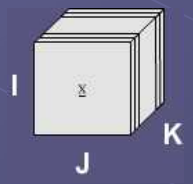
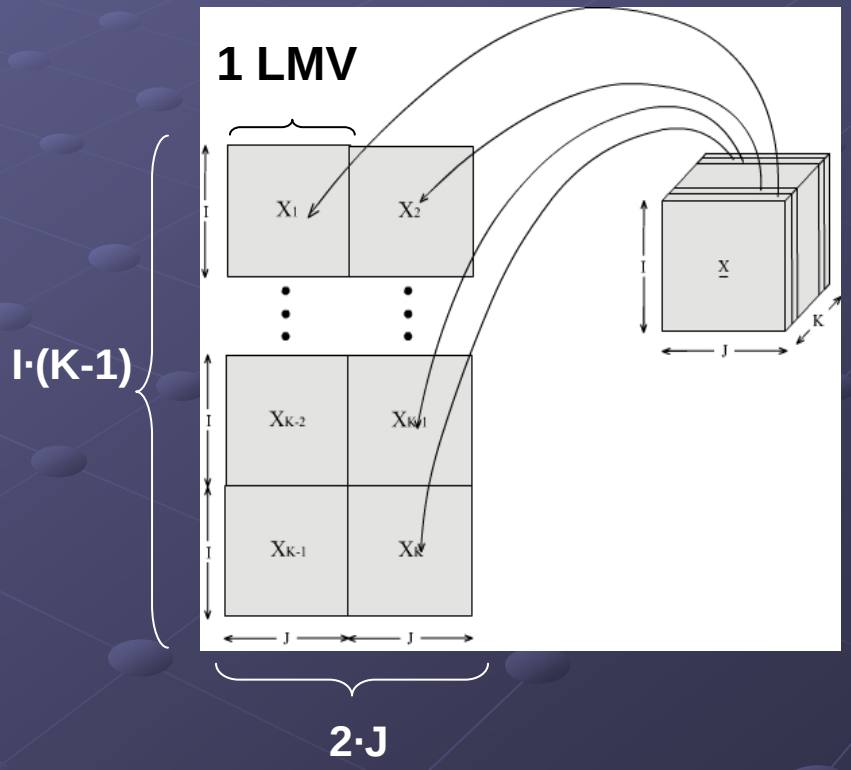


- Unfold the three-way matrix.
  - Batch dynamic unfolding = VW + LMVs



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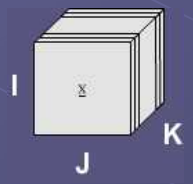

- Unfold the three-way matrix.
  - Batch dynamic unfolding

Batch dynamic (1 LMV)

$$1/(K-1)\cdot\left(\begin{bmatrix} VC_1 & V_{1,2} \\ V_{1,2}^t & VC_2 \end{bmatrix} + \begin{bmatrix} \dots & \dots \\ \dots & \dots \end{bmatrix} + \begin{bmatrix} VC_k & V_{k,k+1} \\ V_{k,k+1}^t & VC_{k+1} \end{bmatrix} + \begin{bmatrix} \dots & \dots \\ \dots & \dots \end{bmatrix} + \begin{bmatrix} VC_{K-1} & V_{K-1,K} \\ V_{K-1,K}^t & VC_K \end{bmatrix}\right)$$

Order 0

Order 1

 # LMVs = Order of dynamics

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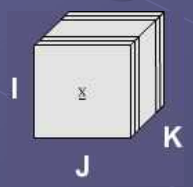

- Unfold the three-way matrix.
  - Batch dynamic unfolding

Batch dynamic (1 LMV)

Batch-wise (K-1 LMVs)

Variable-wise (0 LMVs)

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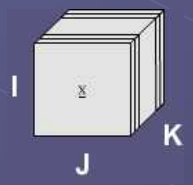

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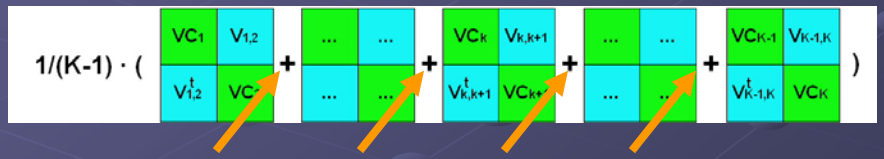
Batch dynamic (1 LMV)



Adjust the amount of dynamic information

Time-invariant Dynamics Imposed!!!

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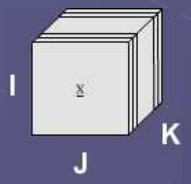
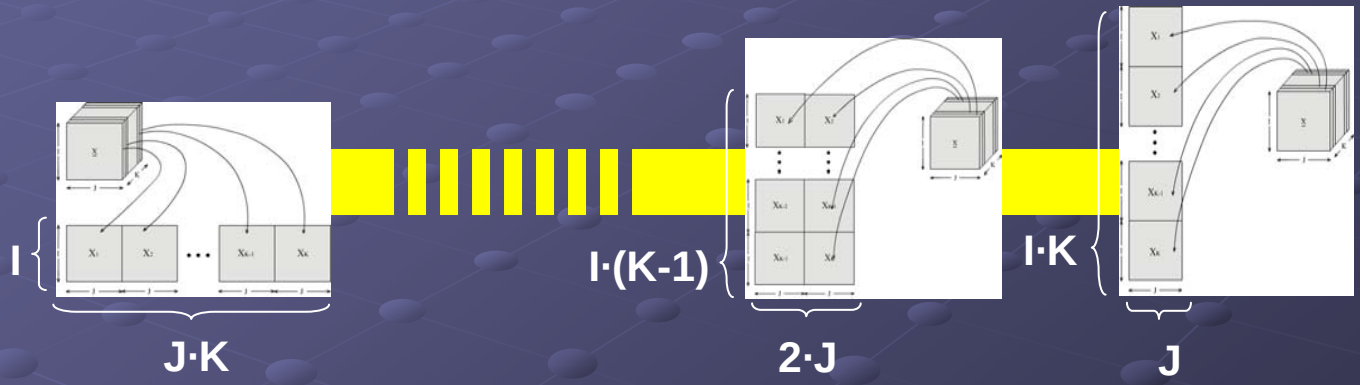


- Unfold the three-way matrix.



K-1 LMVs ⟷ **1 LMV** ⟷ **0 LMVs**

+ LMVs
- Parsimonious
+ Dynamics captured
- Constrained Dynamics

- LMVs
+ Parsimonious
- Dynamics captured
+ Constrained Dynamics

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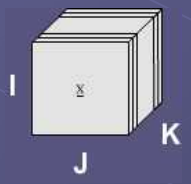
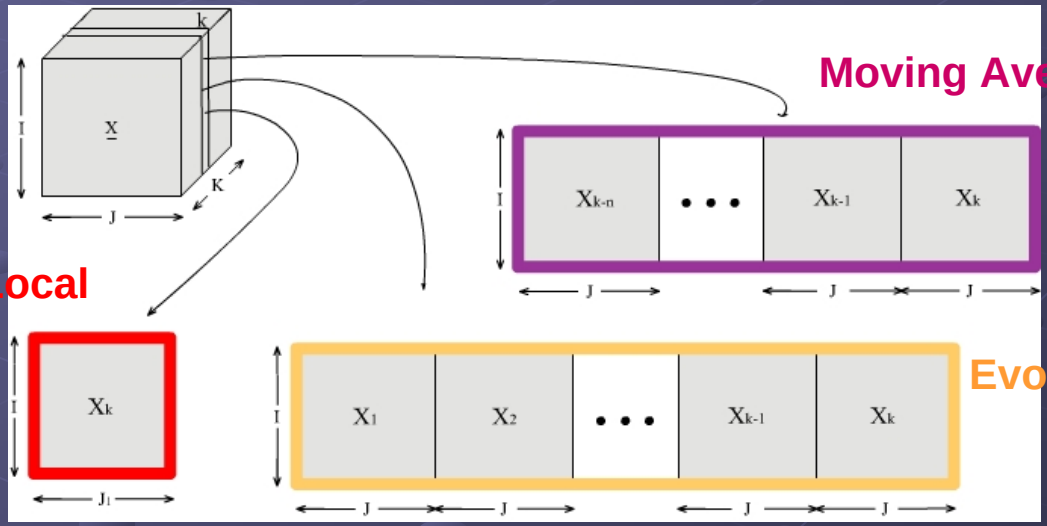


- Divide in K matrices



LMVs locally adjustable

High number of models

J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part I: Theoretical discussion*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1113

Model Structures

Outline

1. Introduction to Batch Processing
2. **Modelling of a Batch Process**
   - **a - Model Structures**
3. Multi-phase Framework
4. Applications
5. Conclusions
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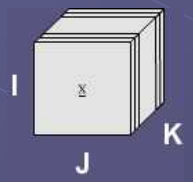

- **Context:**

  a) A large number of possible Model Structures

  b) Very different batch processes, (constant or varying dynamics, dynamics of different order, etc…)

- **NO MODELLING STRUCTURE IS THE BEST ALWAYS!!!**

- WHY DON'T WE IDENTIFY THE MODEL STRUCTURE FOR THE CURRENT CASE STUDY???

J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1151

Outline

- Introduction to Batch Processing
- Modelling of a Batch Process
- **Multi-phase Framework**
- Applications
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Multi-phase Framework

Outline

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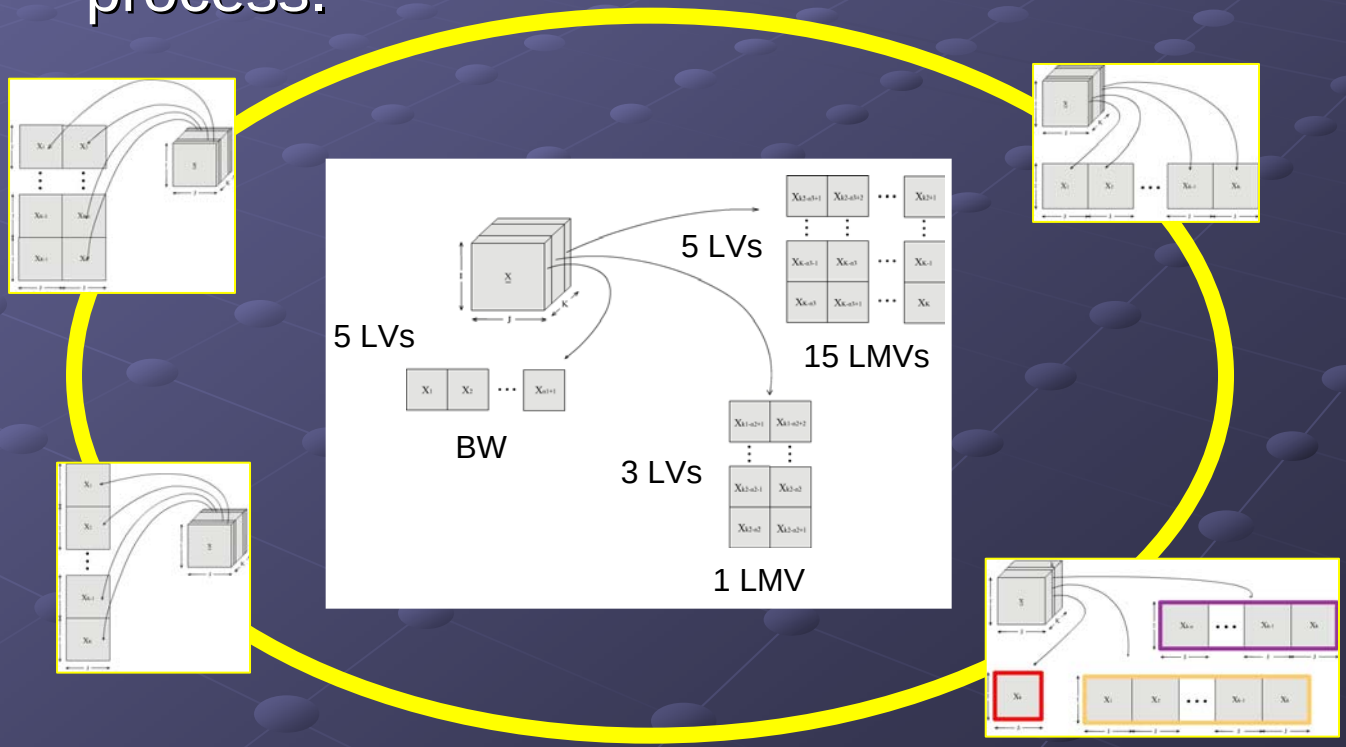
- Aim: The identification of the convenient structure of a PCA/PLS model of a batch process.



The Multi-phase modelling structure.

Multi-phase Framework

Outline

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3. **Multi-phase Framework**
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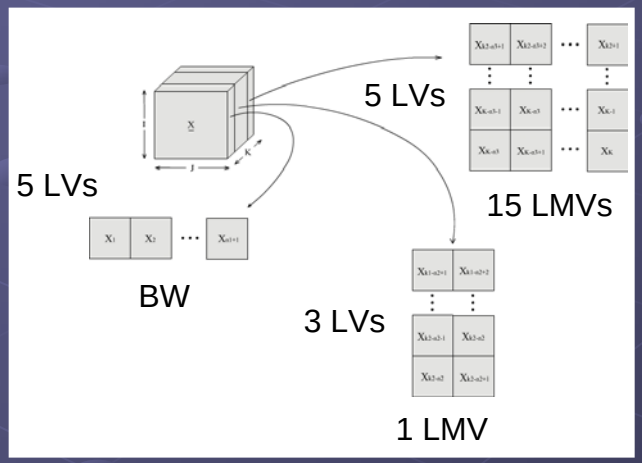
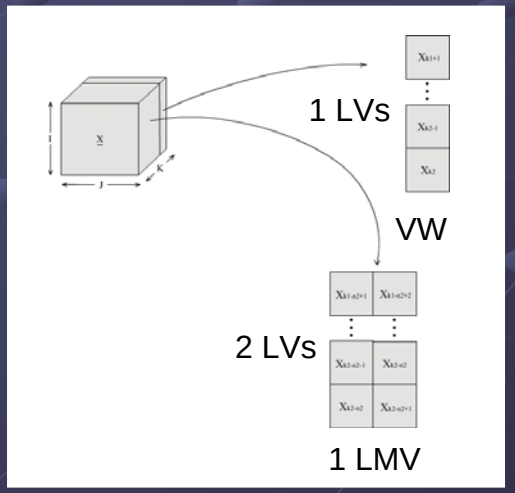
- To develop Multi-phase models we need:
  - A loss function





Which one is better?

Outline

1. Introduction to Batch Processing
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Multi-phase Framework

- To develop Multi-phase models we need:
  - A loss function
  - A calibration algorithm
    1) Greedy Optimization
    2) Merging Algorithm
    3) Tools for Visual Inspection and Decision

Outline

1. Introduction to Batch Processing
2. Modelling of a Batch Process
3. **Multi-phase Framework**
   a - Loss Function
4. Applications
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Loss Function

- Cross-validation: Prediction error
  - Challenges:
    - Easy for PLS, not easy at all for PCA.

PLS

$$Y = X \cdot B_{pls} + F$$

PCA

$$X = T \cdot P_{pca}^{\ T} + E$$

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   - **a - Loss Function**
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Loss Function

- Cross-validation: Prediction error
  - Challenges:

    - Easy for PLS, not easy at all for PCA.

1) Different data for calibration and validation.
2) Predict a variable from the rest following the PCA structure.

LnSO approach

What happens with independent variables???

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Loss Function

- Cross-validation: Prediction error
  - Challenges:

- Easy for PLS, not easy at all for PCA.

1) Different data for calibration and validation.
2) Predict a variable from the rest following the PCA structure.

LnSO approach

What happens with independent variables???

Solution: Augment X with redundant information

[X X] ➔ Not robust to noise

[X T] ➔ Robust to noise ➞ CLnSO

$$X = T \cdot P_{pca}^{\ T} + E$$

J. Camacho, J. Picó and A. Ferrer. *New Cross-Validation Methods in Principal Component Analysis*, 10th Scandinavian Symposium on Chemometrics (2007).

Loss Function

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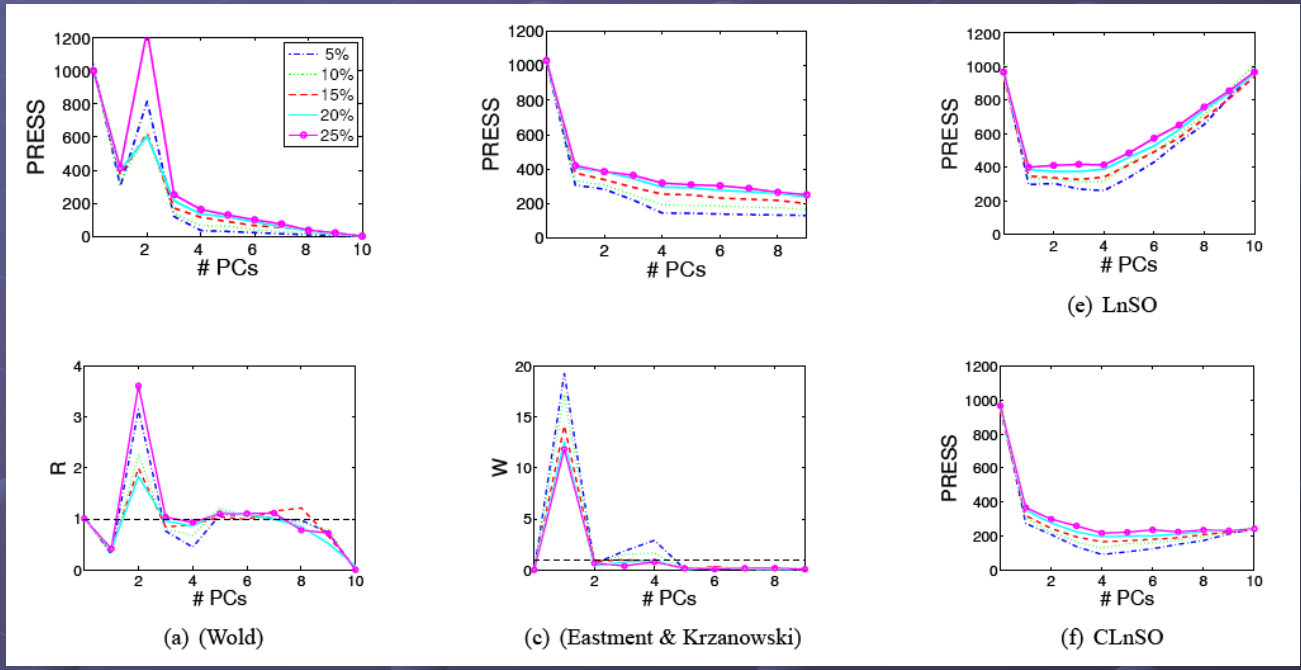
- Simulated example: **4 LV ➔ 10 OV**



The CLnSO method outperforms the other approaches in all the simulated examples to date

J. Camacho, J. Picó and A. Ferrer. *New Cross-Validation Methods in Principal Component Analysis*, 10th Scandinavian Symposium on Chemometrics (2007).

Loss Function

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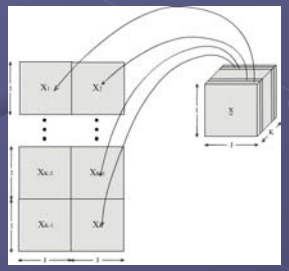
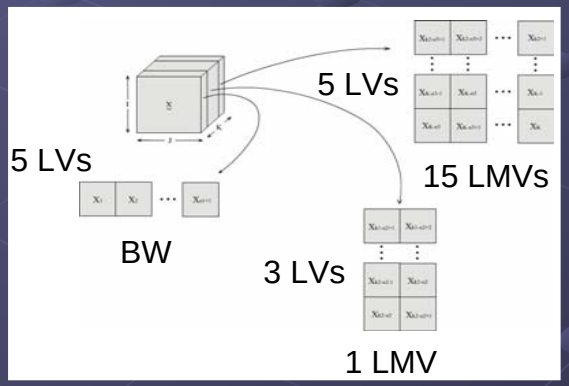
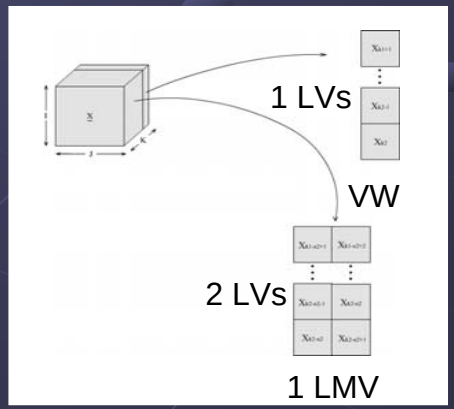


- Cross-validation: Prediction error
  - Challenges:
    - Easy for PLS, not easy at all for PCA.
    - Used to determine the number of LVs, but not for the number of sub-models and of LMVs.





J. Camacho, J. Picó and A. Ferrer. *A new algorithm for selecting the unfolding method and the number of sub-models in batch process modelling with PCA*, 10th Scandinavian Symposium on Chemometrics (2007).

Algorithms

Outline

1. Introduction to Batch Processing
2. Modelling of a Batch Process
3. **Multi-phase Framework**
   - b - Algorithms
4. Applications
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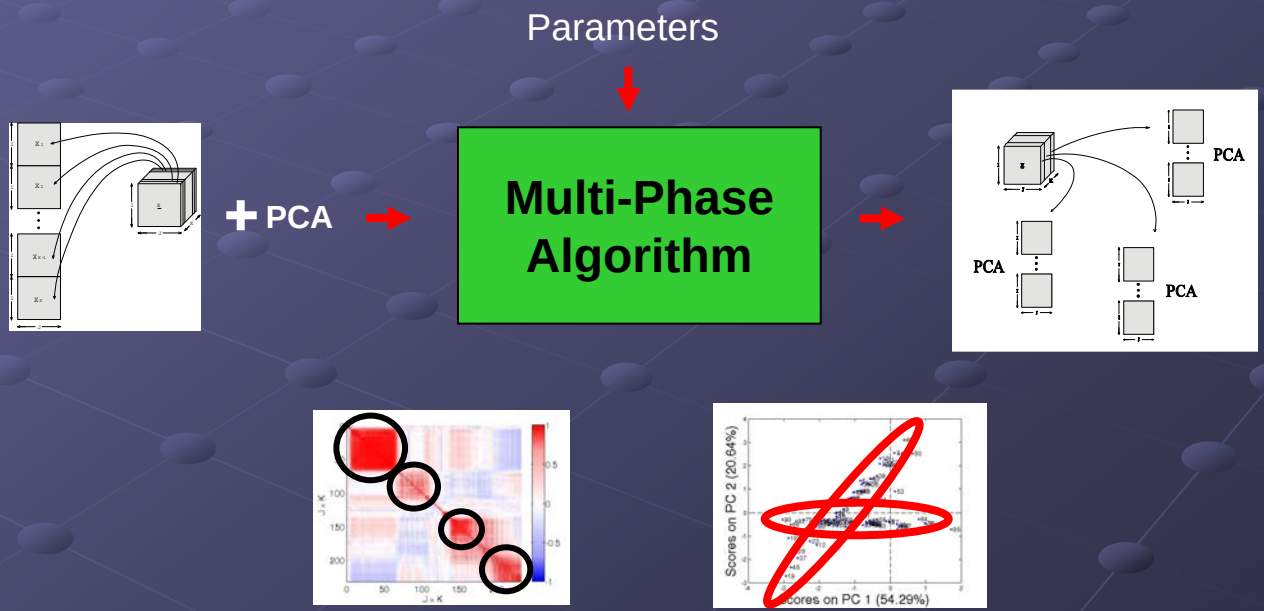
6. Acknowledgements

- Calibration: Three-step Analysis:

a) Multi-phase Algorithm



J. Camacho and J. Picó. *Multi-Phase Principal Component Analysis for Batch Processes Modelling*, Chemometrics and Intelligent Laboratory Systems, 81(2):127-136 (2006).

J. Camacho and J. Picó. *Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis*, Journal of Process Control, 10(16):1021-1035 (2006).

Algorithms

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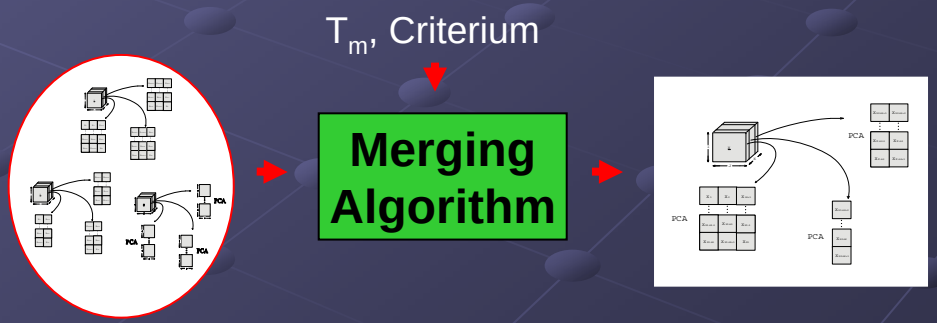
- Calibration: Three-step Analysis:

a) Multi-phase Algorithm

b) Merging Algorithm ★



★ J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1151

Algorithms

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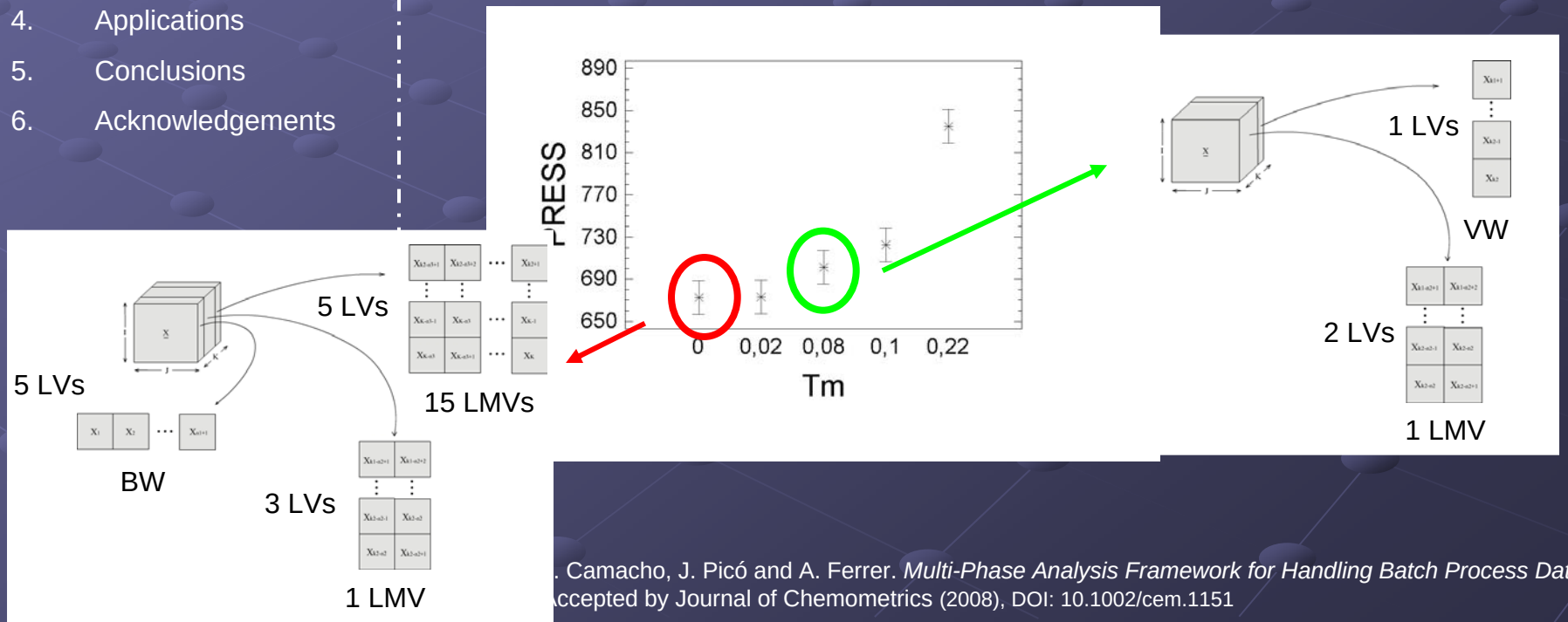
- Three-step Analysis:

c) Compromise Performance - Complexity

Anova + LSD



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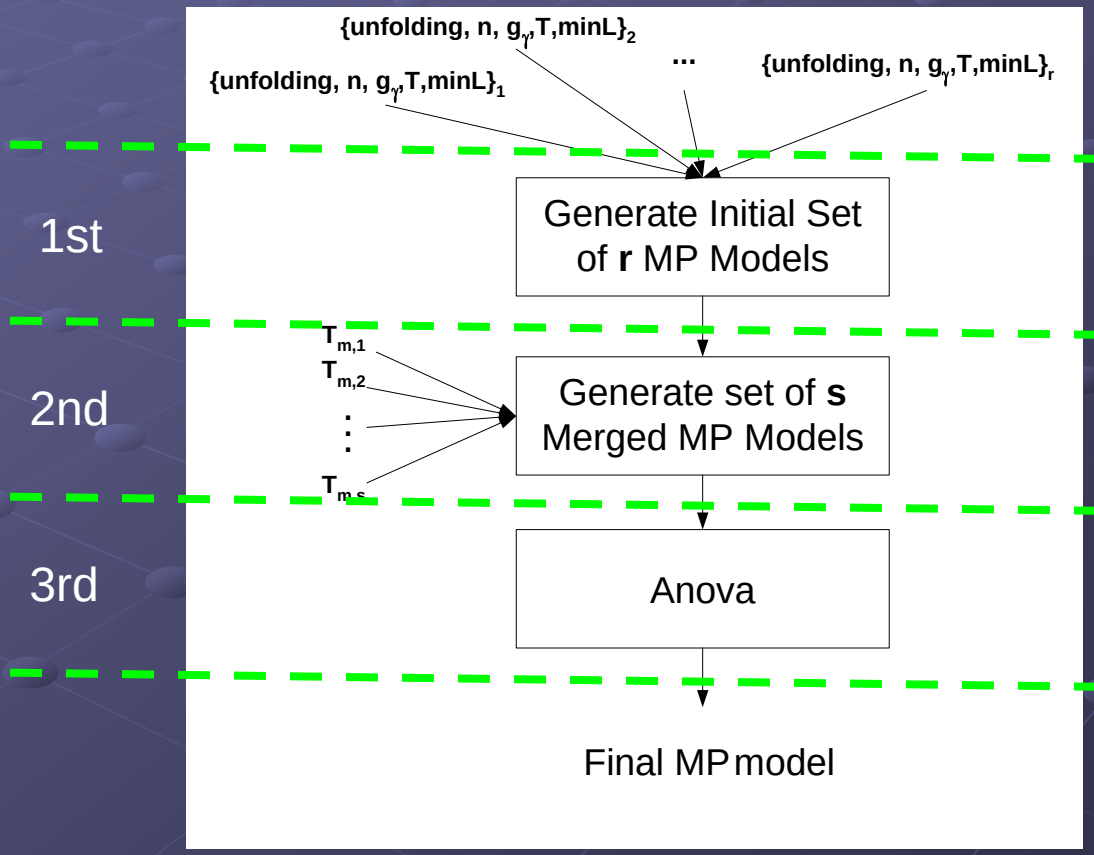
- Calibration: Multi-Phase Framework



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Outline

1. Introduction to Batch Processing
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4. **Applications**

   a - On-line monitoring
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On-line Monitoring

- Determine on-line if the product of a batch is produced under NOC.
- Quality measurements: off-line, slow, destructive and selective

The O-MS saves lots of money!!!

Outline

1. Introduction to Batch Processing
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On-line Monitoring

- Determine on-line if the product of a batch is produced under NOC.
- Quality measurements: off-line, slow, destructive and selective
- Steps
  - Align the data.
  - Convert three-way data into two-way data.
  - Fit the PCA (or PLS, etc.) model/models.
  - Construct a pair of monitoring charts based on:
    - The D-statistic (from the scores ***T***)
    - The SPE (from the residuals ***E***)

$$X = T \cdot P^T + E$$

Outline

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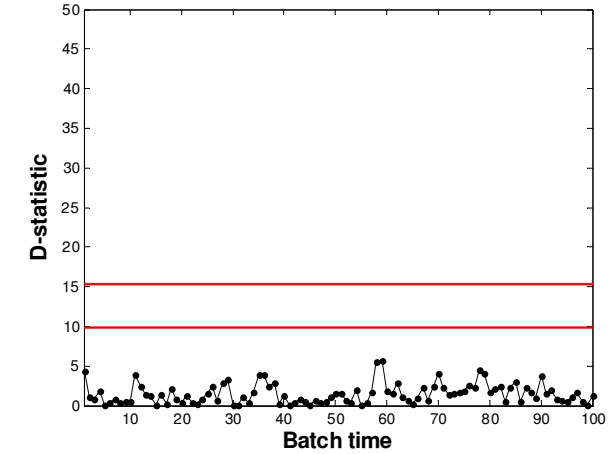
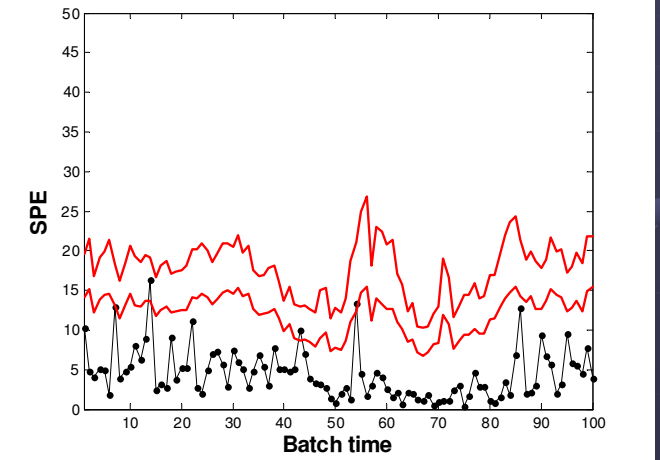
On-line Monitoring

- Monitoring Charts: D-statistic and SPE

Batch under **NOC**





- Saccharomyces cerevisiae cultivation

On-line Monitoring

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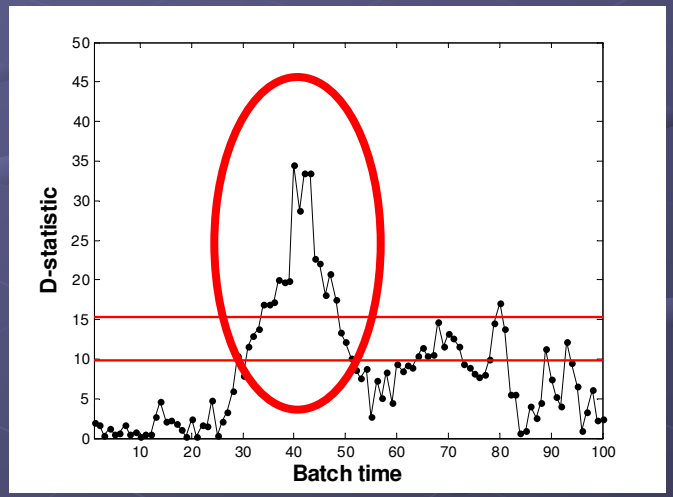
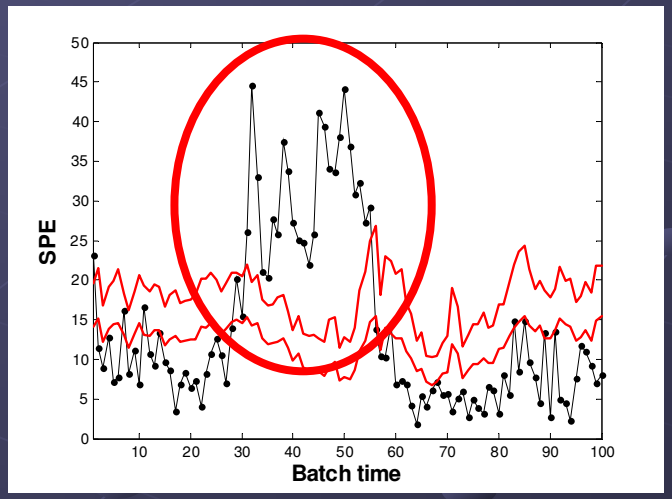
- Monitoring Charts: D-statistic and SPE

Abnormal Batch





- Saccharomyces cerevisiae cultivation

On-line Monitoring

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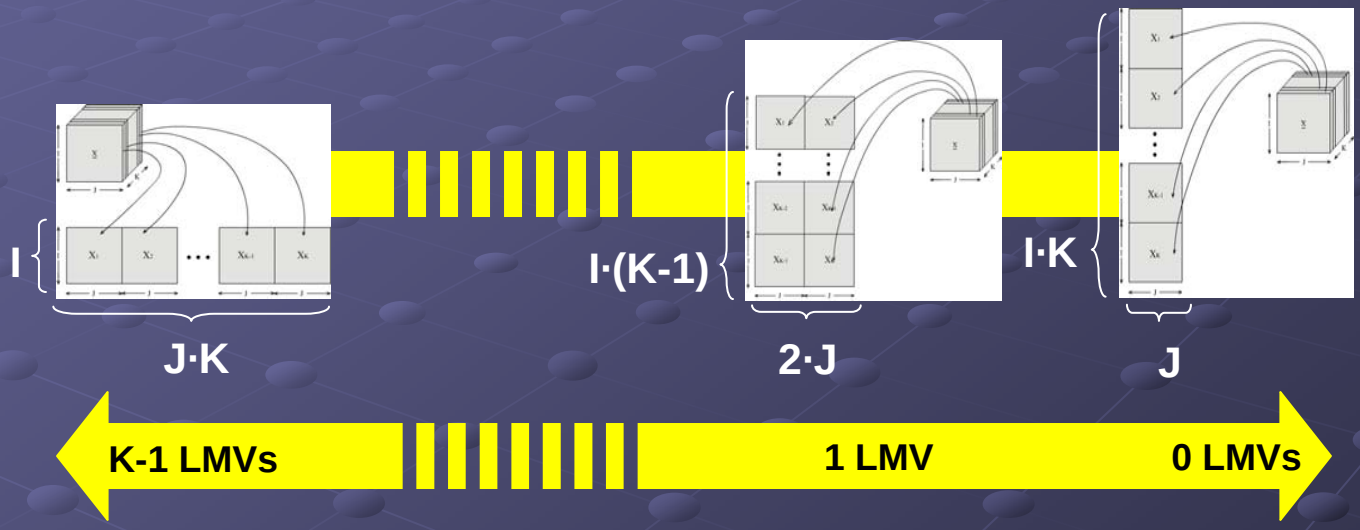
- Unfold the three-way matrix.



+ LMVs
- Parsimonious
+ Dynamics captured
- Constrained Dynamics
+ Auto-corr Stats.

- LMVs
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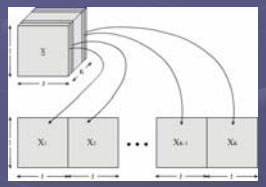
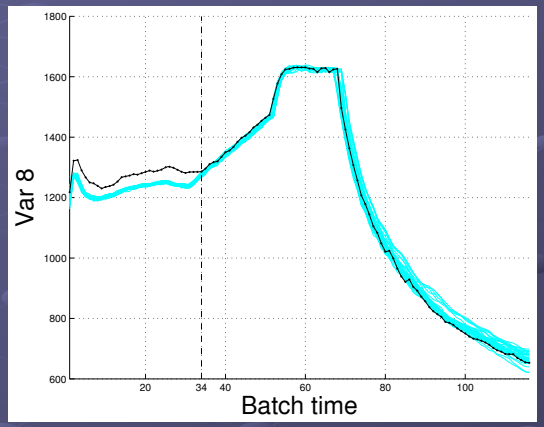
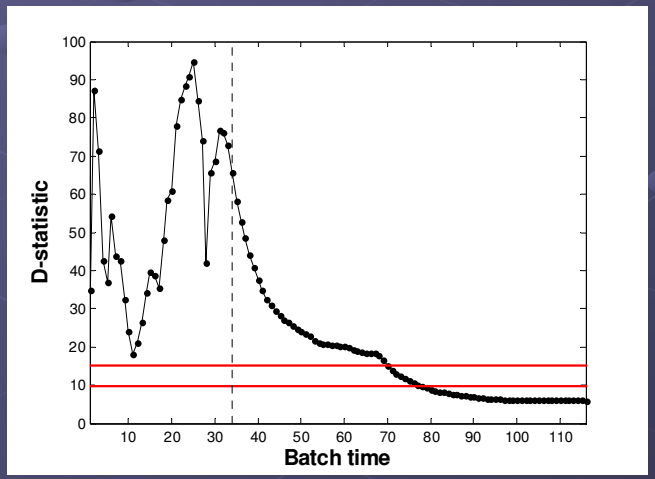
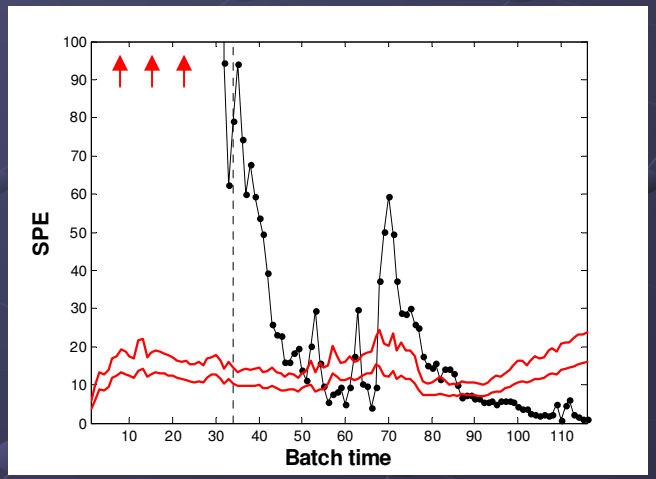
- Nylon 6'6 Polymerization









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On-line Monitoring

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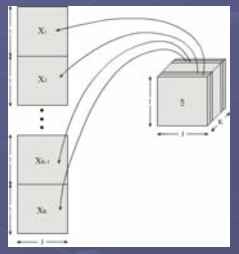

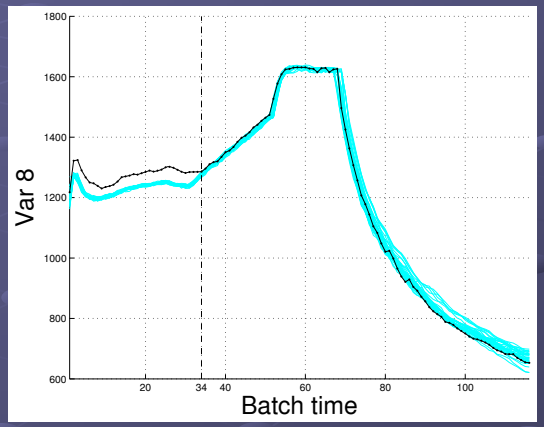

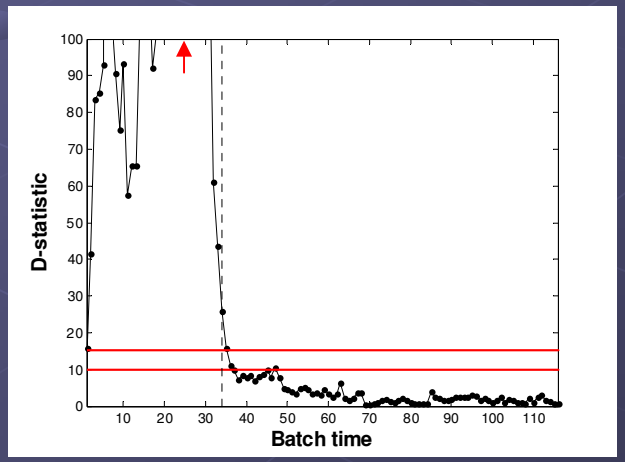

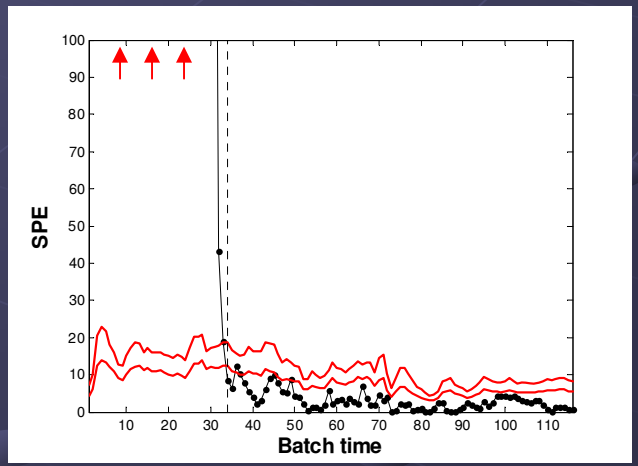

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On-line Monitoring

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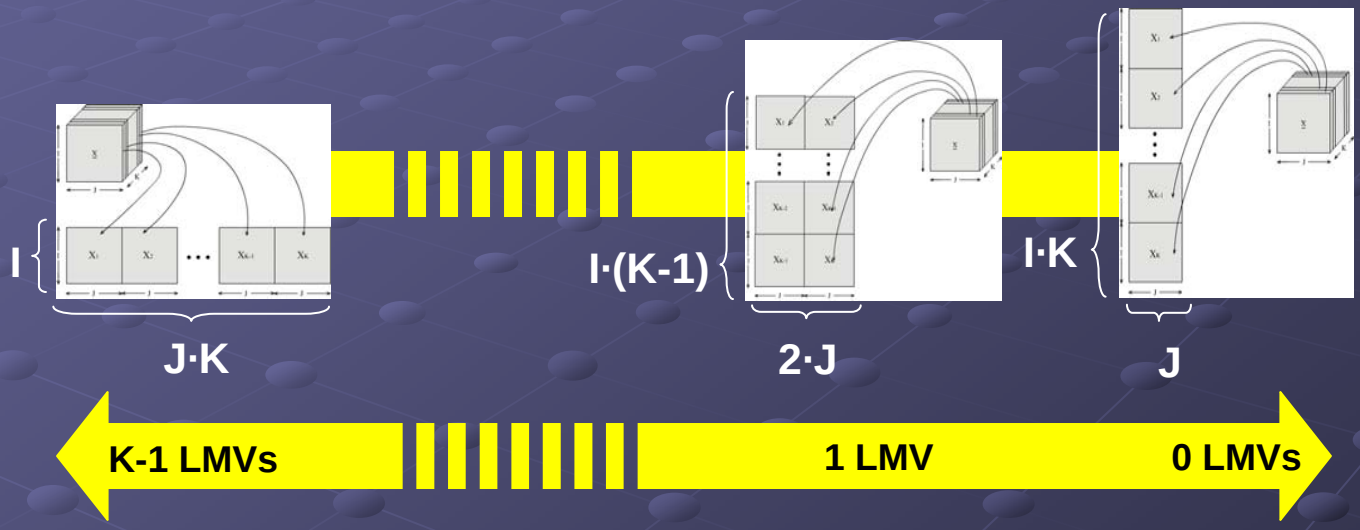
- Unfold the three-way matrix.



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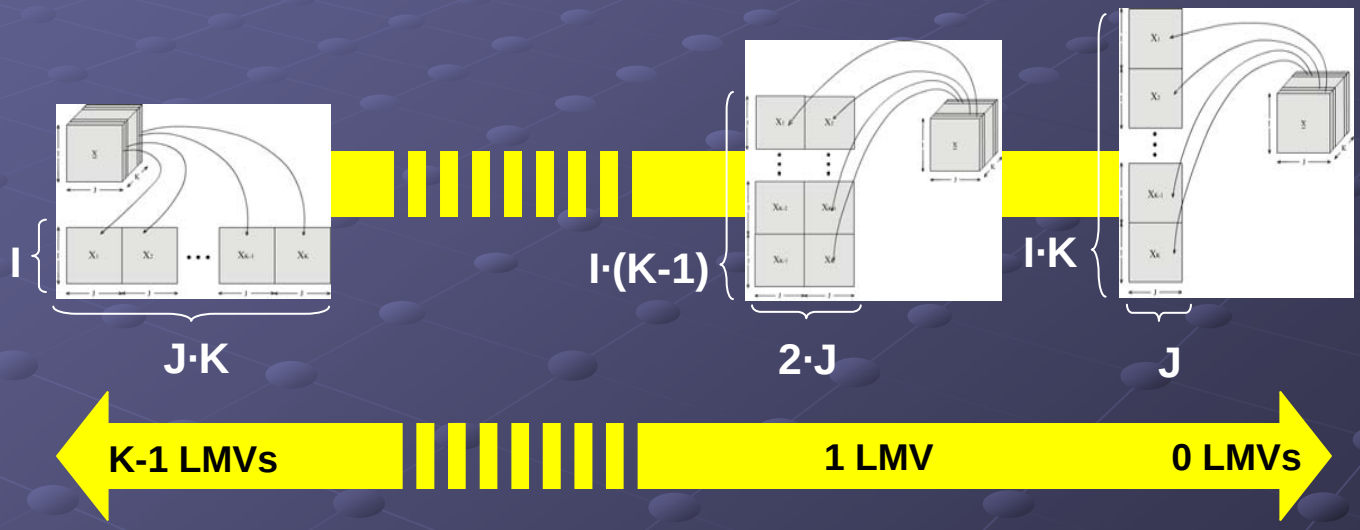
- Convert into two-way data ➔ Unfolding



Objective: **To use the minimum number of LMVs while capturing the time-varying process dynamics.**

- Constrained Dynamics	+ Constrained Dynamics
+ Auto-corr Stats.	– Auto-corr. Stats.

J. Camacho, and J. Picó. *On-line Monitoring of Batch Processes using Multi-Phase Principal Component Analysis*. Journal of Process Control, 16(10):1021-1035 (2006).

Accepted, Journal of Chemometrics (2008)

On-line Monitoring

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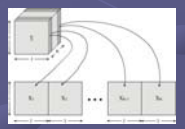
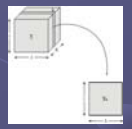
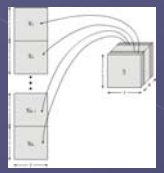
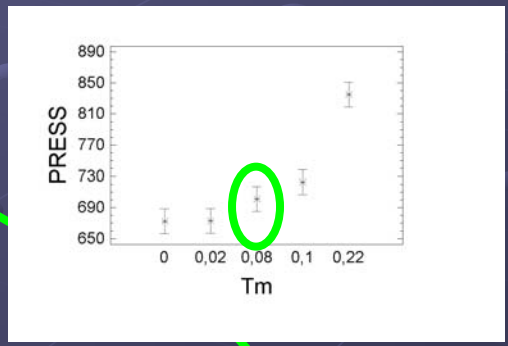
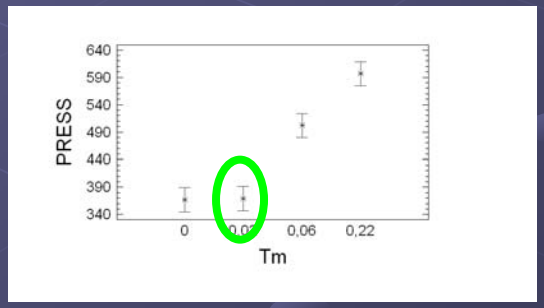




Model	Structure	AST
MP_0	11 phases, 0.8 $\overline{LMV}$, 2.1 $\overline{PC}$	**28.6**
$MP_{0.08}$	11 phases, 0.5 $\overline{LMV}$, 2 $\overline{PC}$	**28.7**
$MP_{0.22}$	7 phases, 0 $\overline{LMV}$, 1.7 $\overline{PC}$	**34.4**∗
BW	2 PCs	**26.8**
Local	2 PCs	**36.2**∗
VW	2 PCs	**34.2**∗

Saccharomyces cerevisiae cultivation



Waste-water treatment



Selected by MPF

Model	Structure	AST
MP_0	4 phases, 5 $\overline{LMV}$, 3.5 $\overline{PC}$	**28.8**
$MP_{0.02}$	5 phases, 2.5 $\overline{LMV}$, 4.5 $\overline{PC}$	**29.1**
$MP_{0.06}$	4 phases, 0.25 $\overline{LMV}$, 4 $\overline{PC}$	**36.3**∗
BW	3 PCs	**43.3**∗
Local	2 PCs	**40.6**∗
VW	2 PCs	**41.3**∗

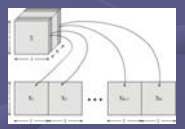
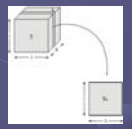
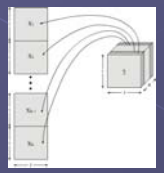
J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1151

On-line Monitoring

Outline

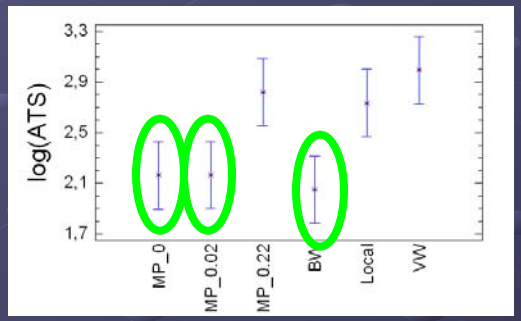
1. Introduction to Batch Processing
2. Modelling of a Batch Process
3. Multi-phase Framework
4. **Applications**

   a - On-line monitoring
5. Conclusions
6. Acknowledgements

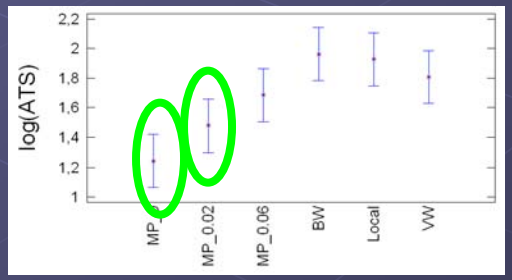




Model	Structure	AST
MP_0	11 phases, 0.8 $\overline{LMV}$, 2.1 $\overline{PC}$	**28.6**
$MP_{0.08}$	11 phases, 0.5 $\overline{LMV}$, 2 $\overline{PC}$	**28.7**
$MP_{0.22}$	7 phases, 0 $\overline{LMV}$, 1.7 $\overline{PC}$	**34.4**∗
BW	2 PCs	**26.8**
Local	2 PCs	**36.2**∗
VW	2 PCs	**34.2**∗

Saccharomyces cerevisiae cultivation



Waste-water treatment



Model	Structure	AST
MP_0	4 phases, 5 $\overline{LMV}$, 3.5 $\overline{PC}$	**28.8**
$MP_{0.02}$	5 phases, 2.5 $\overline{LMV}$, 4.5 $\overline{PC}$	**29.1**
$MP_{0.06}$	4 phases, 0.25 $\overline{LMV}$, 4 $\overline{PC}$	**36.3**∗
BW	3 PCs	**43.3**∗
Local	2 PCs	**40.6**∗
VW	2 PCs	**41.3**∗

Selected by MPF

J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Accepted by Journal of Chemometrics (2008), DOI: 10.1002/cem.1151

On-line Prediction

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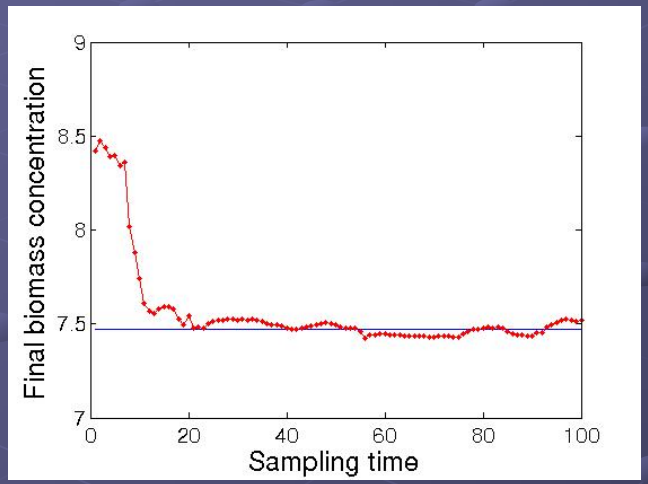
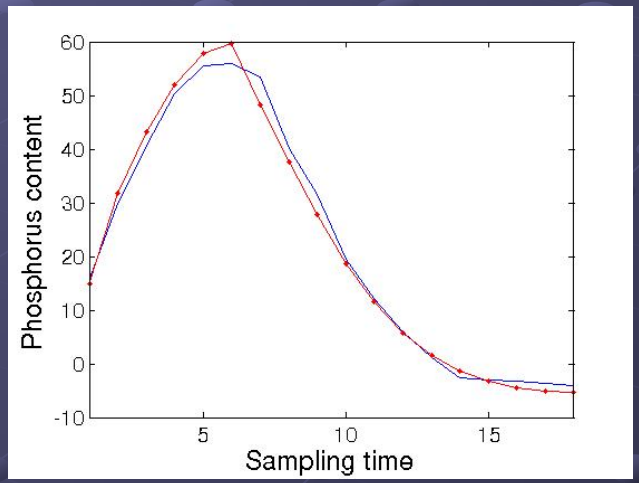
End-quality prediction



Variables estimation



- High economical component

Slight improvements are important!!!!

On-line Prediction

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1. Introduction to Batch Processing
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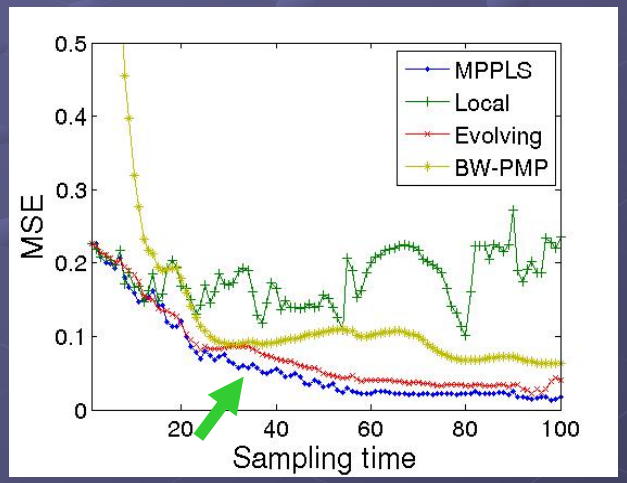
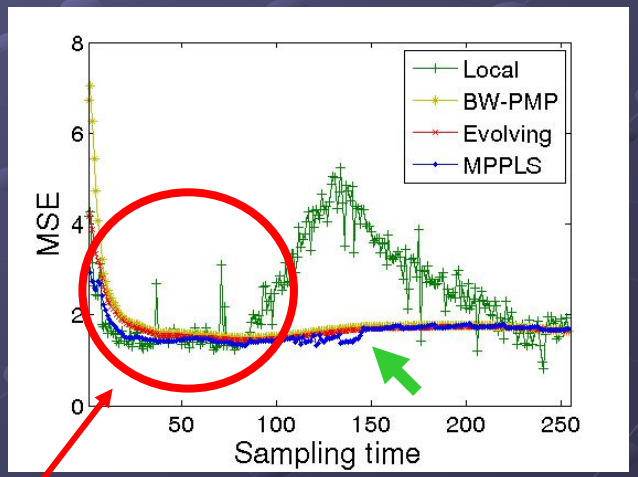
- End-quality prediction performance:

Saccha. cerev.



Waste-water treat.



Anaerobic stage

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On-line Prediction

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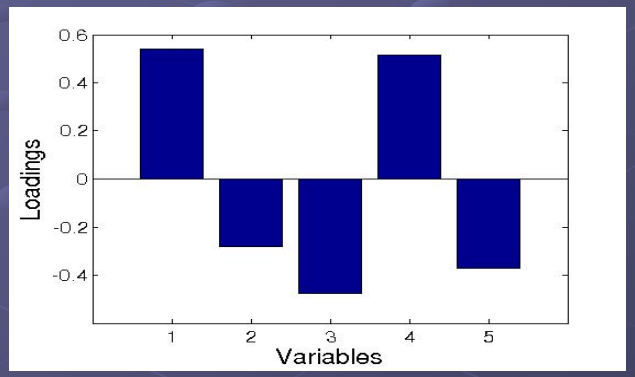
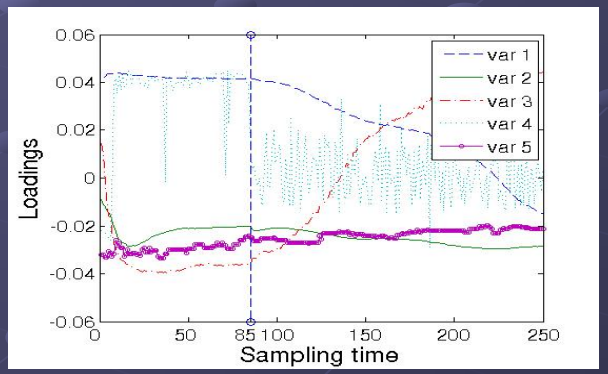
- Model simplification and Process understanding:

MPPLS = VW-PLS
(Anaerobic Stage)



1 PC = 5 parameters
(5 variables)

BW-PLS ó
Local



1 PC = 1250 parameters
(5 var x 250 sam. tim.)

99.6 % of reduction in the number parameters and better performance (MSE) !!!

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Outline

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   c - Optimization
5. Conclusions
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Optimization

- Objectives: maximize production, improve quality, improve safety conditions, reduce costs, etc.
- Extremely hard task
  - Lack of measurements
  - Uncertainties and Non-linear nature
  - Non-convexity
  - Slow response
- fundamental knowledge ➔ quality of the model or the assumptions assumed.

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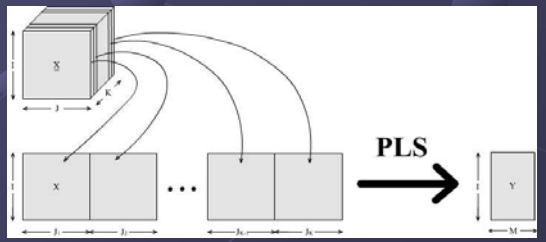
Optimization

- Run-to-run (R2R) optimization
  - Learn from the past batches to improve the performance of the current one
- Three ideas:

a) The batch-wise unfolding : X(I, J, K) ➔ X(I, JK)

b) A PLS model ➔ gradient of a function

c) Non-linearities and Non-convexity ➔ adaptive PLS model + heuristic rules (CV).



J. Camacho, J. Picó and A. Ferrer. *Self-tuning run to run optimization of fed-batch processes using unfold-PLS*, AIChE Journal, 53(7):1789-1804 (2007).

Optimization

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- Self-tuning algorithm:
  - Step 1: Process a new batch *i* with control law u_i.
  - Step 2: Rebuild the BW-PLS model with the data of batch i.
  - Step 3: Compute the gradient and the next control law.
  - Step 4: Increment the counter $i = i+1$ and loop back to Step 1.

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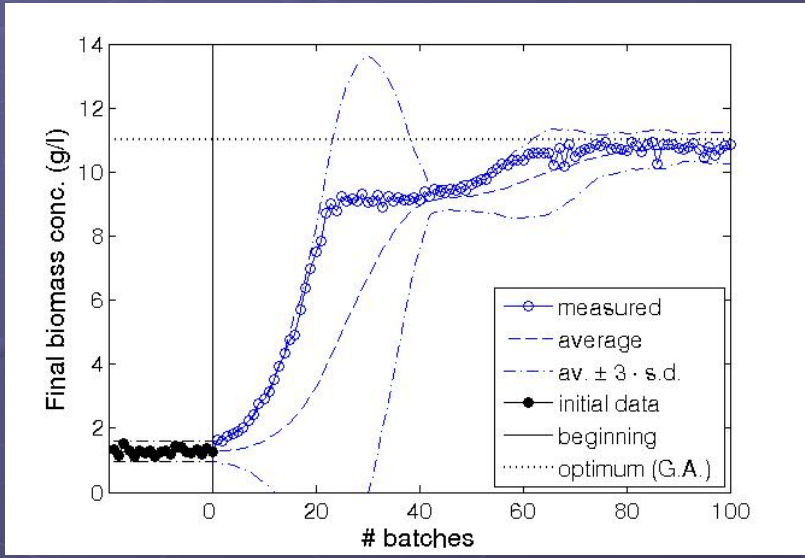
Optimization

- Saccharomyces cerevisiae fed-batch cultivation



Input: Feeding profile of substrate

Ouput: Biomass concentration

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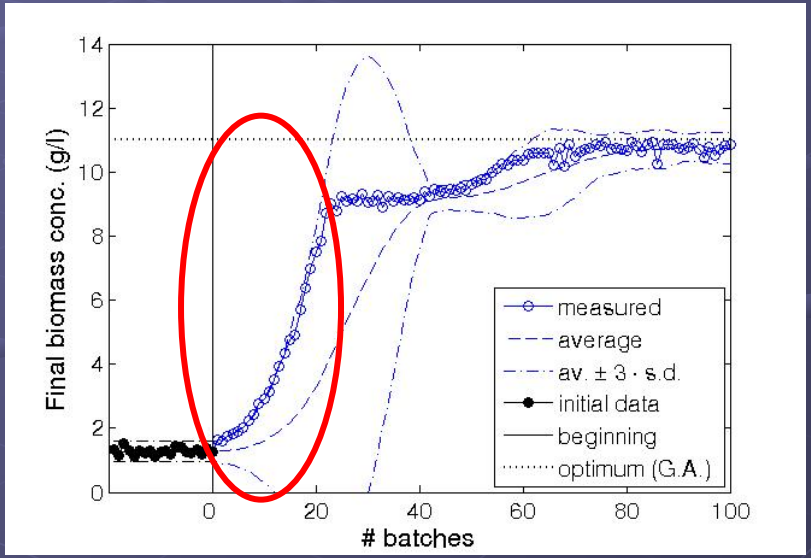

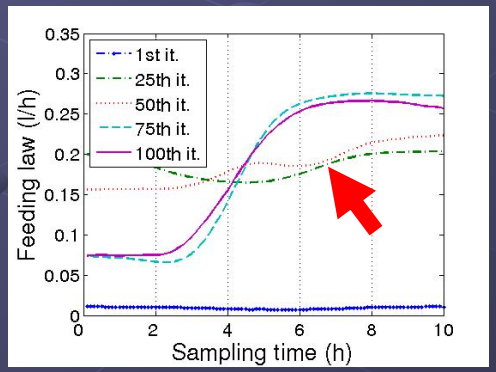

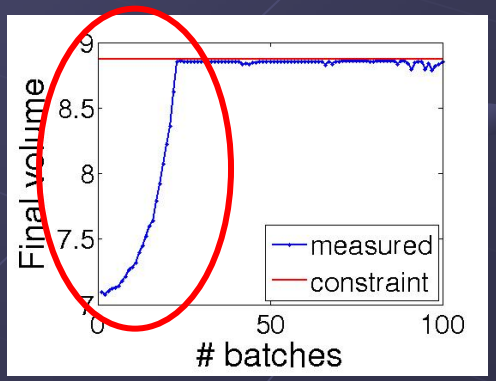

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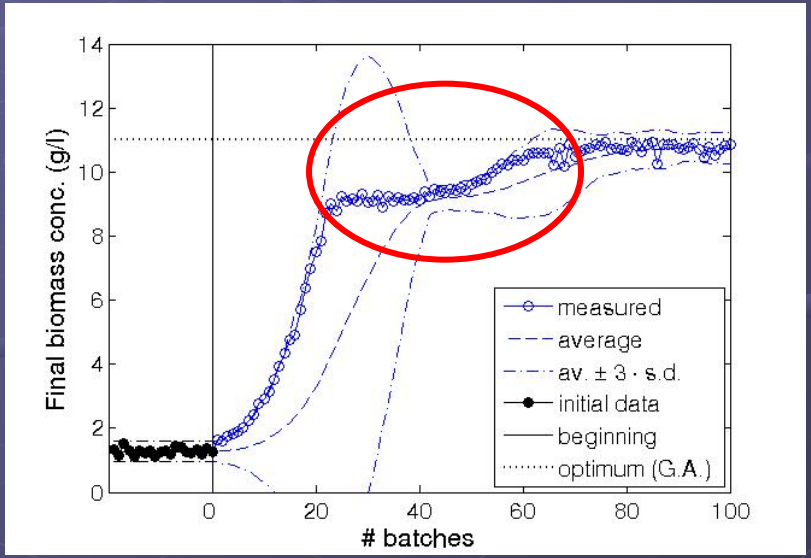

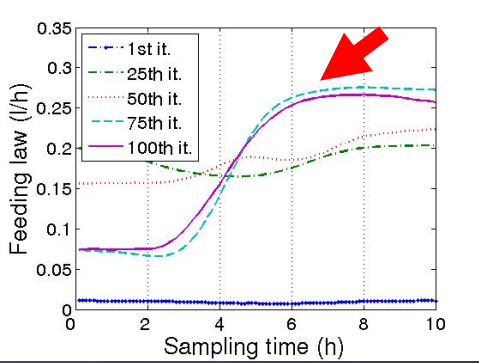

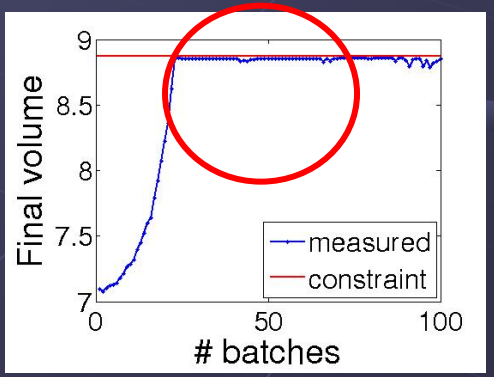

J. Camacho, J. Picó and A. Ferrer. *Self-tuning run to run optimization of fed-batch processes using unfold-PLS*, AIChE Journal, 53(7):1789-1804 (2007).

Outline

- Introduction to Batch Processing
- Modelling of a Batch Process
- Multi-phase Framework
- Applications
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- **Acknowledgements**

Outline

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Conclusions

- Contributions:
  - Theoretical study of the principal modelling structures.
  - Contributions on the cross-validation of PCA and PLS.
  - Definition of a new modelling framework for batch processes.
  - Contributions to the off-line and on-line monitoring of batch processes with PCA.
  - Contributions to the on-line prediction in batch processes with PLS.
  - Development of a new optimization algorithm for batch processes.

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Conclusions

- Refereed Journal Papers

[1] J. Camacho and J. Picó. *Monitorización de Procesos por Lotes mediante PCA Multifase*, **Revista Iberoamericana de Automática e Informática Industrial**, 3(3):78-91 (2006).

[2] J. Camacho and J. Picó. *Multi-Phase Principal Component Analysis for Batch Processes Modelling*, **Chemometrics and Intelligent Laboratory Systems**, 81(2):127-136 (2006).

[3] J. Camacho and J. Picó. *Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis*, **Journal of Process Control**, 10(16):1021-1035 (2006).

[4] J. Camacho, J. Picó and A. Ferrer. *Self-tuning run to run optimization of fed-batch processes using unfold-PLS*, **AIChE Journal**, 53(7):1789-1804 (2007).

[5] J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part I: Theoretical discussion*, Accepted by **Journal of Chemometrics** (2008), DOI: 10.1002/cem.1113

[6] J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part II: PLS comparative*, Submitted to **Journal of Chemometrics** (2008).

[7] J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Accepted by **Journal of Chemometrics** (2008), DOI: 10.1002/cem.1151

[8] J. Camacho, J. Picó and A. Ferrer. *Leave-n-Samples-Out Cross-validation in PCA for Missing Data Imputation and Measurement Noise Reduction*, In elaboration for **Chemometrics and Intelligent Laboratory Systems** (2008).

[9] J. Camacho, J. Picó and A. Ferrer. *Assessment of Cross-validation for determining the number of Principal Componets in PCA*, In elaboration for **Technometrics** (2008).

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Conclusions

- Conference contributions

[10] J. Camacho, J. Picó and A. Ferrer. *A new look at the dynamic covariance structure of various approaches for batch process modelling*, 10th Scandinavian Symposium on Chemometrics (2007).

[11] J. Camacho, J. Picó and A. Ferrer. *New Cross-Validation Methods in Principal Component Analysis*, 10th Scandinavian Symposium on Chemometrics (2007).

[12] J. Camacho, J. Picó and A. Ferrer. *A new algorithm for selecting the unfolding method and the number of sub-models in batch process modelling with PCA*, 10th Scandinavian Symposium on Chemometrics (2007).

[13] J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, 10th Scandinavian Symposium on Chemometrics (2007).

[14] J. Camacho, J. Picó and A. Ferrer. On-line monitoring of batch processes: Does the modelling structure matter?. CAC, 2008.

[15] J. Camacho, J. Picó and A. Ferrer. Leave-n-Samples-Out Cross-validation in PCA for Missing Data Recovery and Robustness in front of Measurement Noise. CAC, 2008.

[16] J. Camacho, J. Picó and A. Ferrer. New advances in the on-line monitoring of batch processes. IFPAC. 2008.

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New Methods Based on the Projection to Latent Structures for Monitoring, Prediction and Optimization of Batch Processes

D.L. Massart Award

Author: José Camacho Páez

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