Multi-Phase Analysis Framework for Handling Batch Process Data

J. Camacho, J. Picó
Department of Systems Engineering and Control.

A. Ferrer
Department of Applied Statistics, Operations Research and Quality.

Technical University of Valencia
Cno. de Vera s/n, 46022, Valencia, Spain

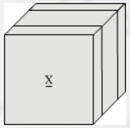
Index

- **Introduction to Batch Processing**
- **Model Structures**
- **Aim of the work**
- Multi-Phase Framework
- End-quality Prediction
- Other Applications
- Conclusions

Index

Introduction to Batch Processing

- **Repetitive nature:** charge, processing and discharge.
- **Three-way data:** a set of variables are measured at different sampling times during the processing of a batch, and this is repeated for a number of batches.
- The duration of the processing of a batch may be variable in some processes ➔ Aligment methods.
- After the alignment, data matrix $\underline{\mathbf{X}}$ $(I \times J \times K)$ contains the values of J variables at K sampling times in I batches.

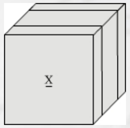


Index

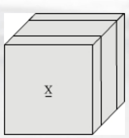
Model Structures

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

Trilinear Nature???



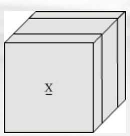
Index



Model Structures

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

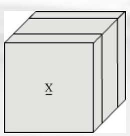
Index



Model Structures

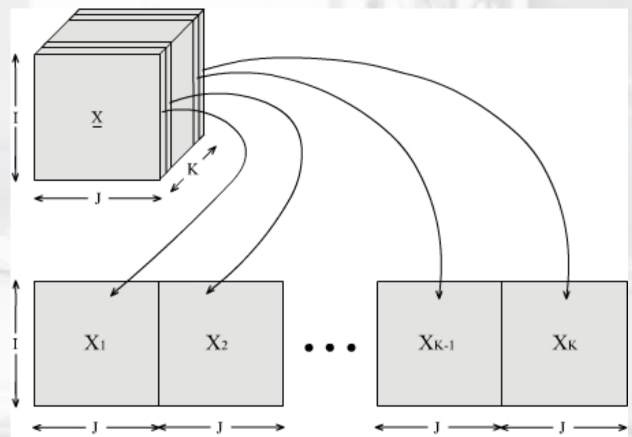
- Convert into two-way data and apply PCA, PLS, …
  - Unfold the three-way matrix.
  - Divide in K local matrices.
  - Use an adaptive approach.
- Apply three-way methods: PARAFAC, Tucker-3,…

Index



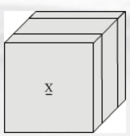
Model Structures

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



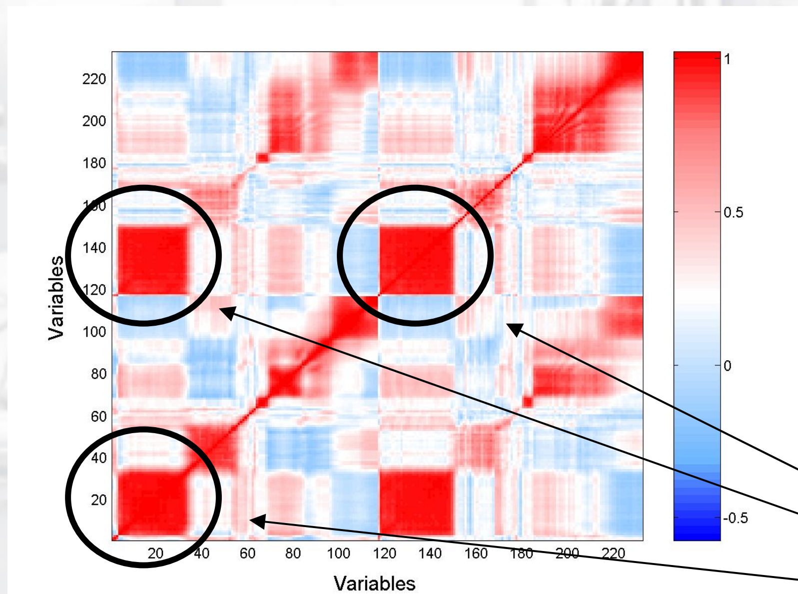
Thousands of variables!!!

Index



Model Structures

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



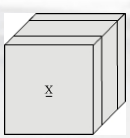
Dynamics are built in the model

More than a half is noise!!!

Variables close in time are more related

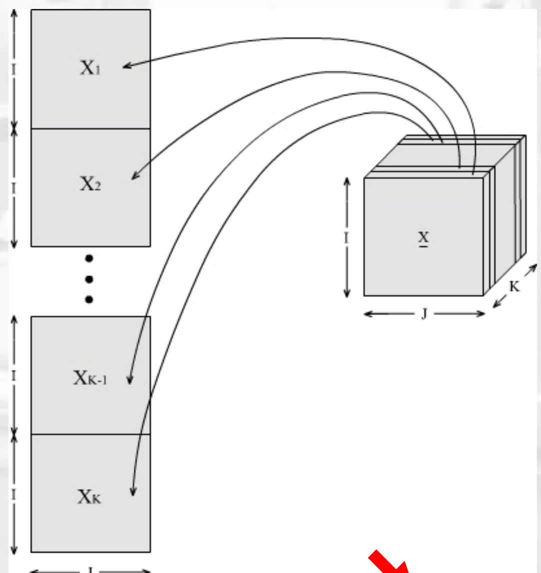
2 variables x 116 sampling times

Index



Model Structures

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



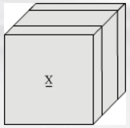
Low number of parameters

More samples/parameter

dynamics are not built in the model

Constant Correlation Imposed!!!

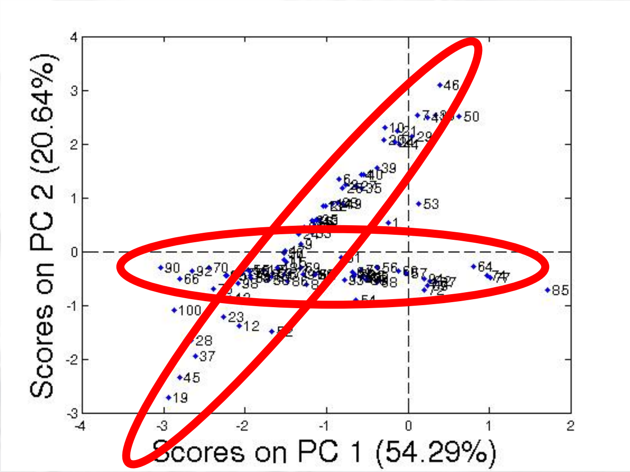
Index



Model Structures

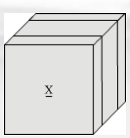
- Unfold the three-way matrix.
  - Variable-wise unfolding

Constant Correlation Imposed!!!



V-W scores

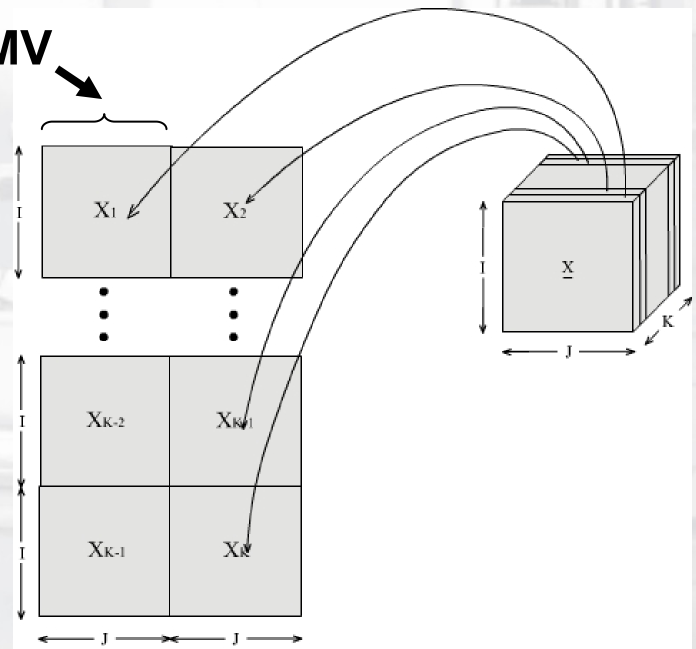
Index



Model Structures

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

1 LMV



↓LMVs ≈ VW

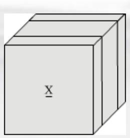
↑LMVs ≈ BW

Adjust the amount of dynamic information

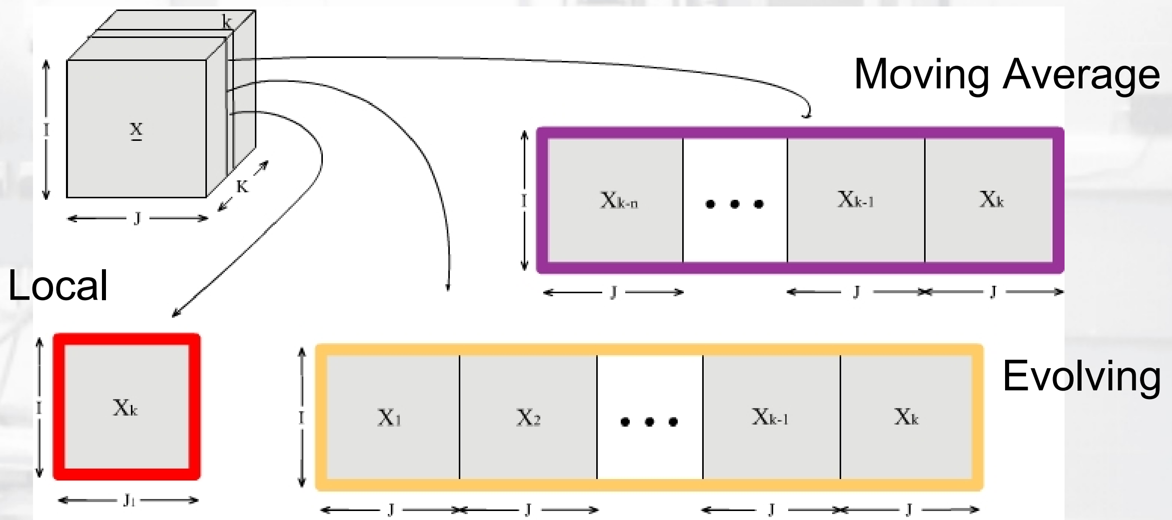
Dynamics are imposed to be constant

Model Structures

Index



- Divide in K matrices



LMVs locally Adjustable

High number of models

Index

Aim of the work

- **Context:**
  a) A large number of possible Model Strutures, each of them with advantages and drawbacks.
  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???

Index

- Introduction to Batch Processing
- Model Structures
- Aim of the work
- **Multi-Phase Framework**
- End-quality Prediction
- Other Applications
- Conclusions

Index

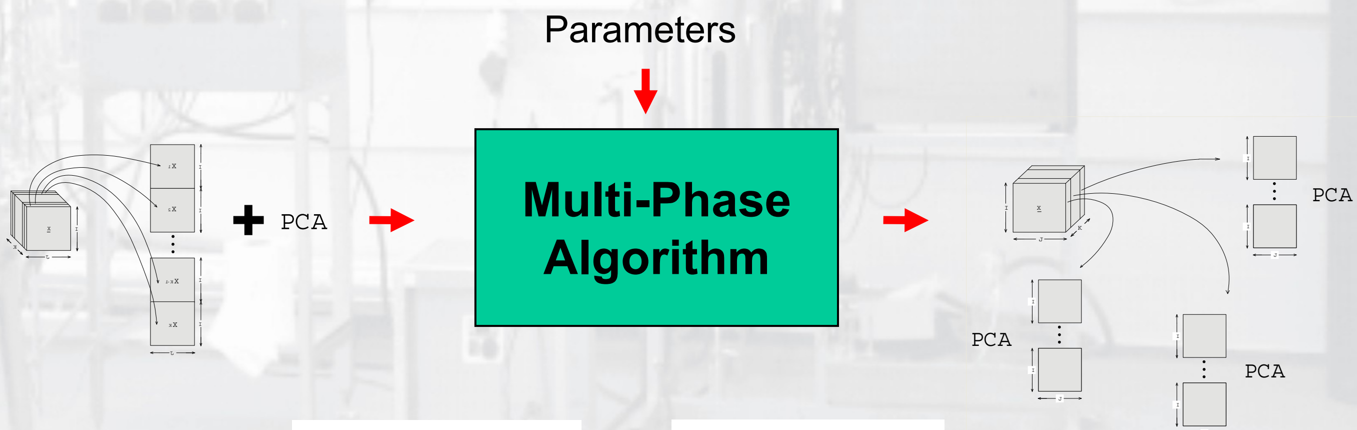
Multi-Phase Framework

- Three-steps Analysis:

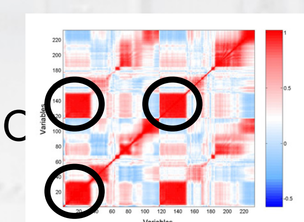
a) Multi-phase Algorithm.

Camacho J, Picó J , Multi-phase principal component analysis for batch processes modelling. *Chemometrics and Intelligent Laboratory Systems.* 2006; 81:127-136.

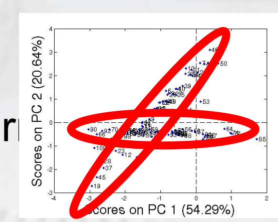
Camacho J, Picó J. Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis. *Journal of Process Control.* 2006;10:1021-1035.



Greedy C



atter



Index

Multi-Phase Framework

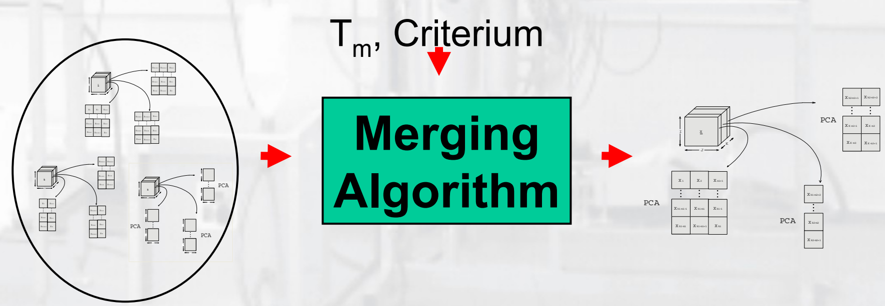
- Three-steps Analysis:

a) Multi-phase Algorithm.

Camacho J, Picó J , Multi-phase principal component analysis for batch processes modelling. *Chemometrics and Intelligent Laboratory Systems.* 2006; 81:127-136.

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

b) Merging Algorithm:



Index

Multi-Phase Framework

- Three-steps Analysis:

a) Multi-phase Algorithm.

Camacho J, Picó J , Multi-phase principal component analysis for batch processes modelling. *Chemometrics and Intelligent Laboratory Systems.* 2006; 81:127-136.

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

b) Merging Algorithm:

Why merge?

Greedy Optimization ➔ Sub-optimal solution

To allow obtaining sub-models with different unfolding methods

c) Compromise Performance - Complexity

Anova + LSD

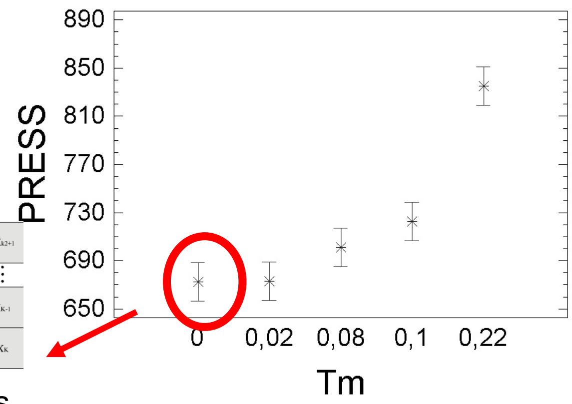
Multi-Phase Framework

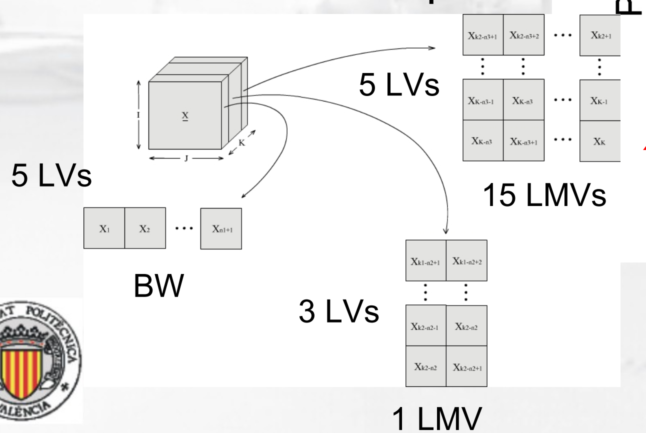
Index

- Three-steps Analysis:

c) Compromise Performance - Complexity

Anova + LSD





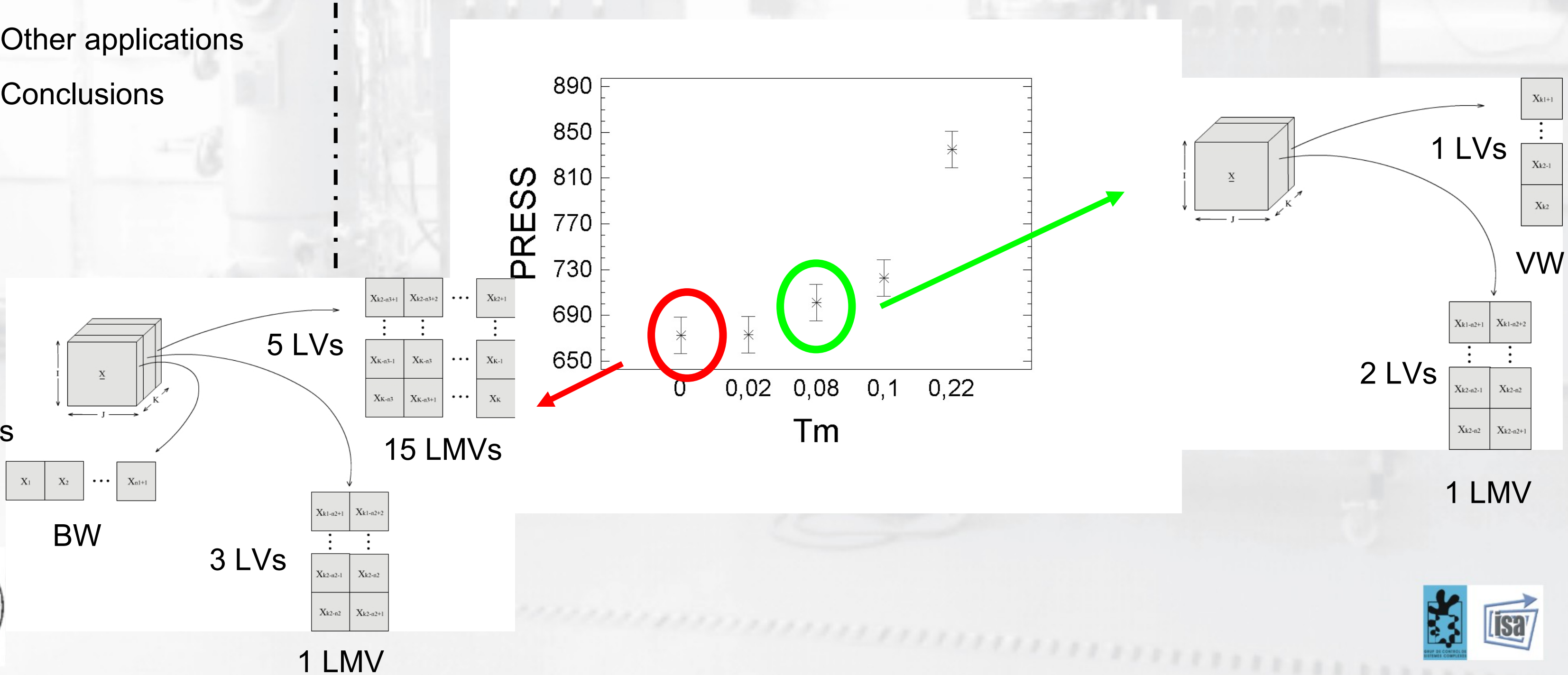
Index

Multi-Phase Framework

- Three-steps Analysis:

c) Compromise Performance - Complexity

Anova + LSD

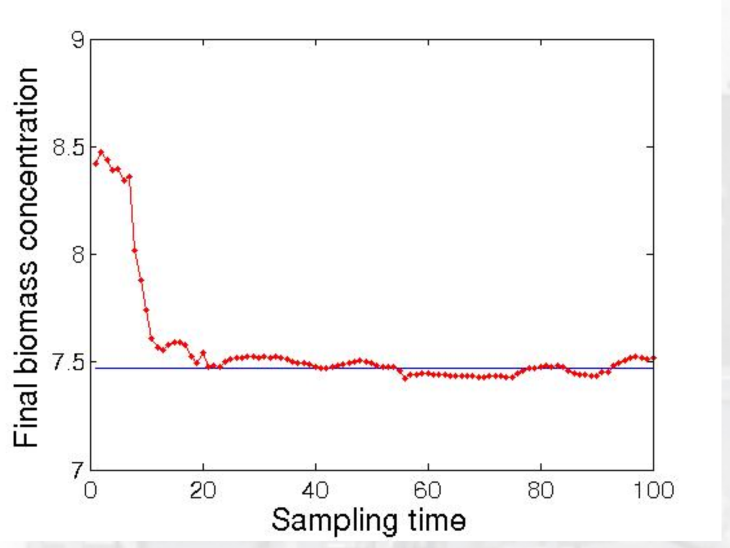


Index

End-Quality Prediction

Index

- On-line prediction



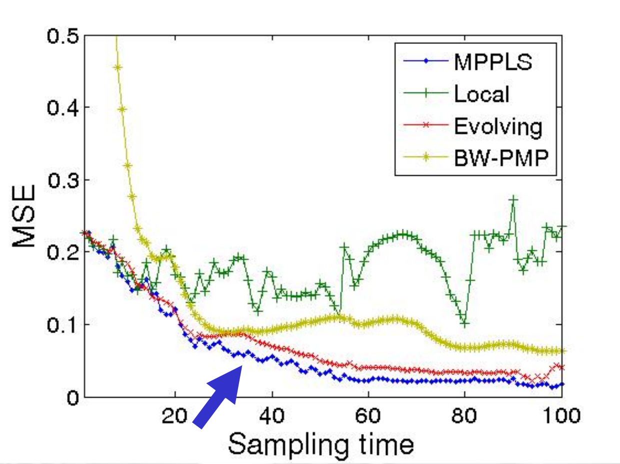
Index

1. Introduction to Batch Processing.
2. Model Structures
3. Aim of the work
4. Multi-Phase Framework
5. **End-quality Prediction**
6. Other applications
7. Conclusions

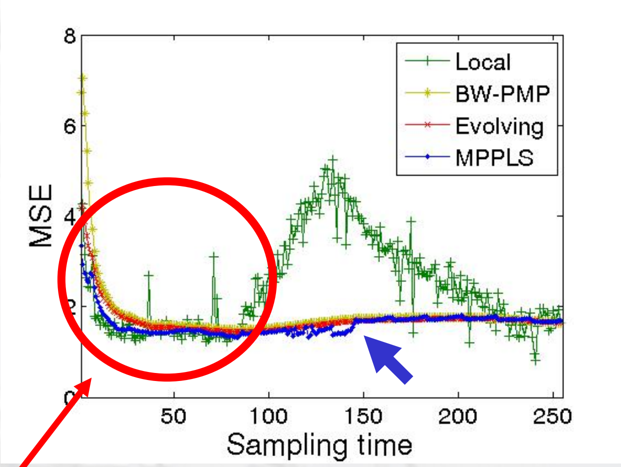
End-Quality Prediction

- Prediction performance:

Saccha. Cerev.



Waste-water treat.

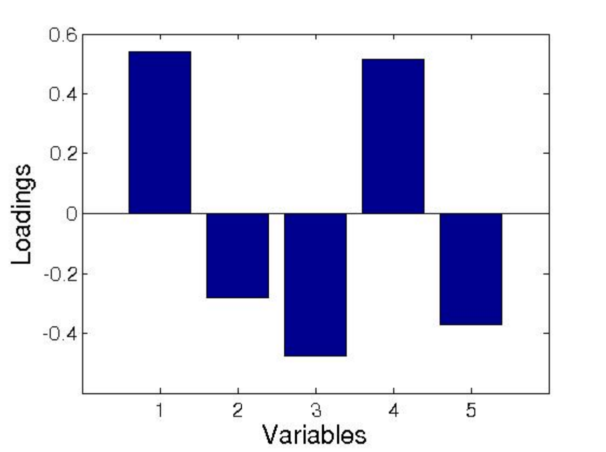


Anaerobic stage

End-Quality Prediction

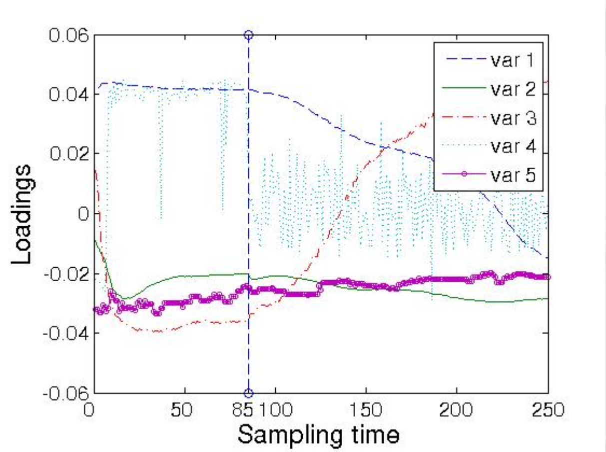
- Process understanding:

MPPLS = VW-PLS
(Anaerobic Stage)



1 PC = 5 parameters
(5 variables)

BW-PLS



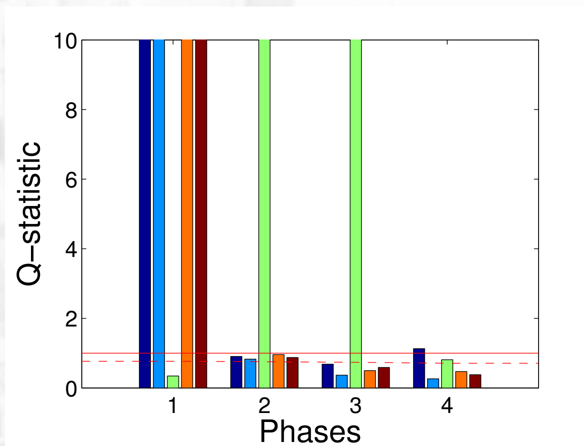
1 PC = 1250 parameters
(5 var x 250 sam. tim.)

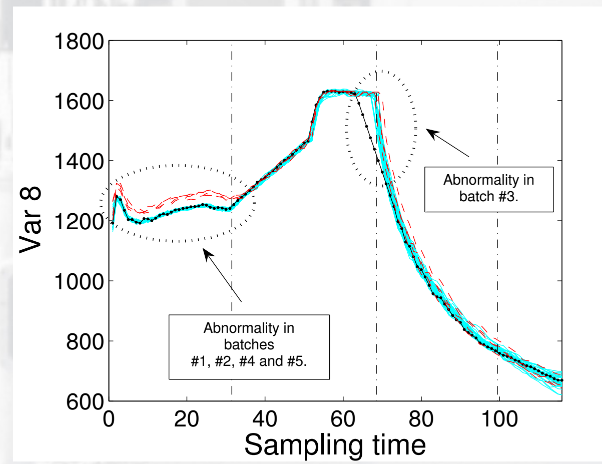
Index

Other Applications

- **Off-line Monitoring: Batch-Wise PCA**

  a) The Charts of MP are more informative.





Index

Other Applications

- **Off-line Monitoring: Batch-Wise PCA**

  a) The Charts of MP are more informative.

- **On-line Monitoring: PCA**

  a) MP avoids problems found in some modelling structures:
  - BW models have low detection capabilities in the D-statistic and high Overall Type I Risk in the SPE.
  - VW models have high OTI Risk in the D-statistic.
  - Local models have high OTI Risk in the SPE.

  b) MP yields monitoring systems of fast response to faults.

- **Estimation of trayectories (Soft-sensors): PLS**

  a) MP yields accurate estimations, outperforming BW, VW, Local, Evolving and Adaptive approaches.

Index

- Introduction to Batch Processing
- Model Structures
- Aim of the work
- Multi-Phase Framework
- End-quality Prediction
- Other Applications
- **Conclusions**

Conclusions

- The Multi-phase (MP) framework, with application to off-line and on-line monitoring, final quality prediction and estimation of trajectories of variables in batch processes, has been presented.
- The MP approach is based on the data-driven identification of the (PCA or PLS) model structure, using pattern recognition and optimization techniques. ➔ Flexibility to adjust the structure to the case: Number of sub-models, dynamics, …
- This approach has several general advantages:
  - The identification of the structure of the models and the convenient use of the tools within the MP framework helps to improve the process understanding.
  - The MP approach allows to obtain a compromise solution between complexity and performance.
  - The MP approach yields good performance in several applications.

Multi-Phase Analysis Framework for Handling Batch Process Data

J. Camacho, J. Picó
Department of Systems Engineering and Control.

A. Ferrer
Department of Applied Statistics, Operations Research and Quality.

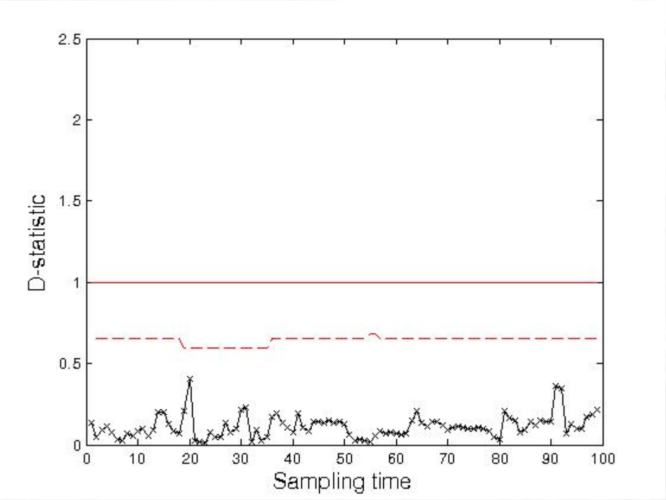
Technical University of Valencia
Cno. de Vera s/n, 46022, Valencia, Spain

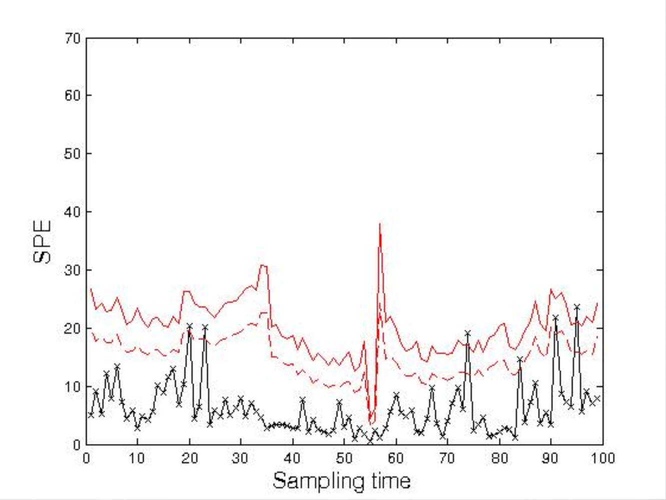
On-line Monitoring

Index

- Monitoring Charts: D-statistic and SPE

Batch under **NOC**



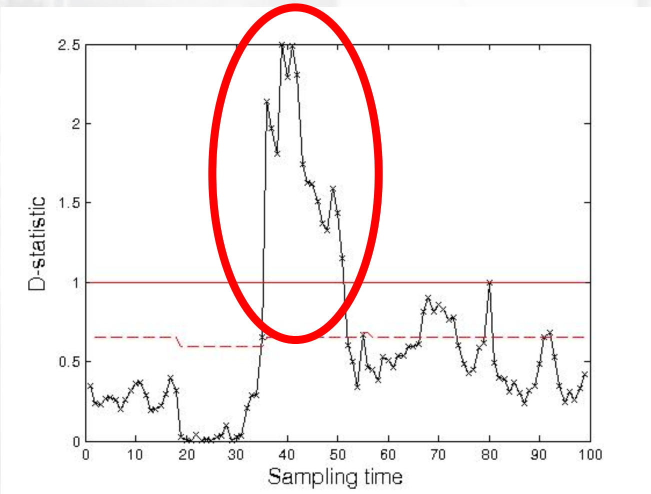


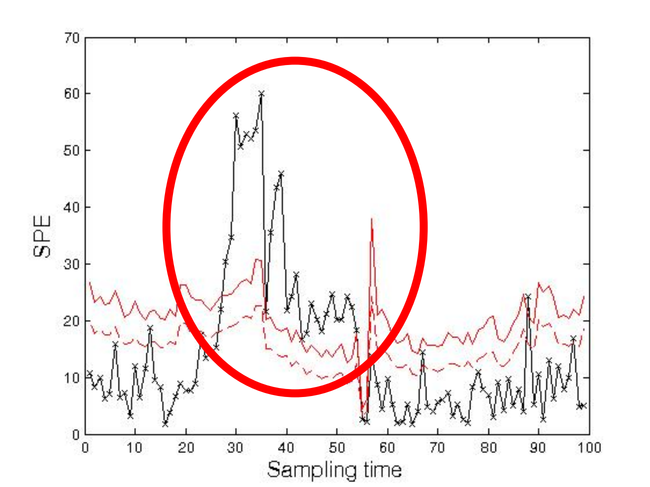
Index

On-line Monitoring

- Monitoring Charts: D-statistic and SPE

Abnormal Batch





Index

On-line Monitoring

- Case Studies:

Process	Calibration	NOC Test	Abnormalities
Nylon 6'6 Polymerization	$\underline{\mathbf{X}} = (31 \times 9 \times 116)$	$\underline{\mathbf{X}} = (5 \times 9 \times 116)$	$\underline{\mathbf{X}} = (5 \times 9 \times 116)$
Saccharomyces Cerevisiae Cultivation	$\underline{\mathbf{X}} = (30 \times 10 \times 100)$	$\underline{\mathbf{X}} = (14 \times 10 \times 100)$	$\underline{\mathbf{X}} = (20 \times 10 \times 100)$
Waste-Water Treatment	$\underline{\mathbf{X}} = (69 \times 5 \times 340)$	$\underline{\mathbf{X}} = (35 \times 5 \times 340)$	$\underline{\mathbf{X}} = (40 \times 5 \times 340)$

Index

On-line Monitoring

- Preliminary Study: Saccharomyces Cerevisiae Cultivation.

PCs	BW-ZD		Local		VW	
	D-st	SPE	D-st	SPE	D-st	SPE
1	3.71%	**7.29%**	2.64%	**7%**	4.79%	**5.5%**
2	3.71%	**6.86%**	3.43%	**8.79%**	**5.71%**	4.07%
3	0.07%	**7.5%**	2.71%	**12.36%**	**7.79%**	4%
4	0%	**8.86%**	3.36%	**13.86%**	**8.21%**	5%
5	0.29%	**9.71%**	4.5%	**16.43%**	**13.14%**	4.21%
6	0.5%	11%	**6.79%**	**20.71%**	**14.79%**	3.64%

Overall Type I Risk computed from the NOC test set,
Imposed significance level 1%

$$OTI = 100 \cdot \frac{n_f}{I \cdot K} \%$$

n_f ➔ number of faults

Conclusion: The structure of the model is important in the on-line monitoring.

Index

On-line Monitoring

Solutions:

a) To readjust the control limits of the monitoring charts using a left-one-out approach.

b) To identify the covenient model structure ➔ Multi-Phase Framework

Conclusion: The structure of the model is important in the on-line monitoring.

On-line Monitoring

- Nylon 6'6 Polymerization:

Model	Structure	Parameters	OTI (ISL=1%)		AST
			D-st	SPE	
MP	1 phase, 1 LMV, 2 PCs	**36**	0%	0.86%	**0**
BW-ZD	3 PCs	**3132**	0%	0.17%	**0**
Local	3 PCs	**3132**	0.34%	0.34%	**0**
VW	2 PCs	**18**	0%	0.86%	**0**

Index

On-line Monitoring

- Saccharomyces Cerevisiae Cultivation:

Model	Structure	Parameters	OTI (ISL=1%) D-st	OTI (ISL=1%) SPE	AST
MP	11 phases, 0.5 $\overline{LMV}$, 2 $\overline{PC}$	**340**	1.07%	1.64%	**28.7**
BW-ZD	2 PCs	**2000**	0%	2.43%	**26.8**
Local	2 PCs	**2000**	1.93%	2.43%	**36.2**
VW	2 PCs	**20**	1.5%	1.71%	**34.2**

PCs	BW-ZD D-st	BW-ZD SPE	Local D-st	Local SPE	VW D-st	VW SPE
1	3.71%	**7.29%**	2.64%	**7%**	4.79%	**5.5%**
2	3.71%	**6.86%**	3.43%	**8.79%**	**5.71%**	4.07%
3	0.07%	**7.5%**	2.71%	**12.36%**	**7.79%**	4%
4	0%	**8.86%**	3.36%	**13.86%**	**8.21%**	5%
5	0.29%	**9.71%**	4.5%	**16.43%**	**13.14%**	4.21%
6	0.5%	**11%**	**6.79%**	**20.71%**	**14.79%**	3.64%

		…meters	OTI (ISL=1%) D-st	OTI (ISL=1%) SPE	AST
		[illegible]70	0.38%	1.49%	**29.1**
BW-ZD	3 PCs	**5100**	0.4%	0.86%	**43.3**
Local	2 PCs	**3400**	0.87%	0.91%	**40.6**
VW	2 PCs	**10**	0.3%	0.89%	**41.3**