Emerging trends in Statistical Process Control of Industrial Processes

Marco S. Reis

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Chemical Process Engineering and Forest Products Research Center – CIEPQPF

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Department of Chemical Engineering
University of Coimbra

Outline

1. Introduction & Background on SPC
2. Current Trends & Examples
   - From univariate, to multivariate, to high-dimensional ("mega-variate")
   - From monitoring the mean, to dispersion, to correlation
   - From stationary, to dynamic, to non-stationary
   - From sensor data to higher-order profiles
   - From detection, to diagnosis, to prognosis
3. Conclusions

1. Introduction & Background

Statistical Process Control (SPC)

≈

(Statistical) Process Monitoring (SPM)

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Fault Detection and Diagnosis (FDD)

≈

(…)

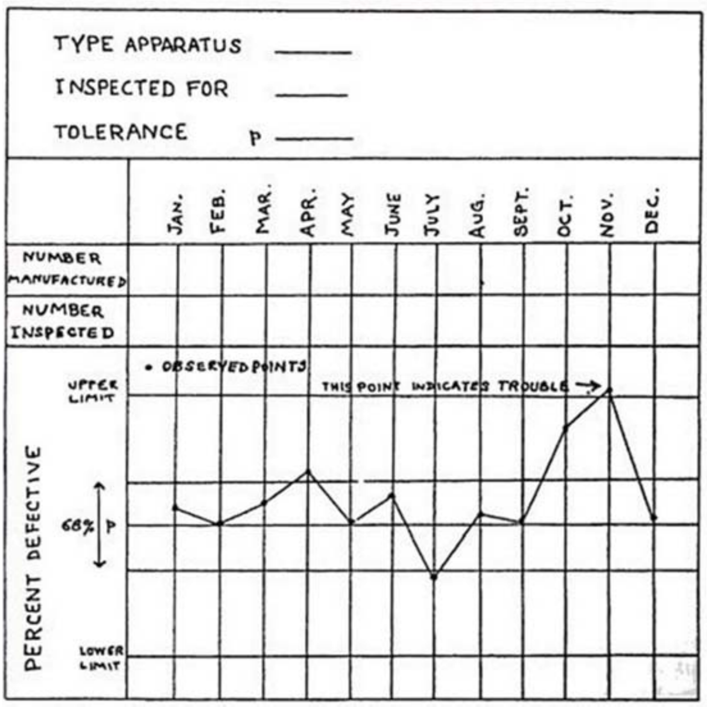
1. Introduction & Background

- Statistical Process Monitoring (SPM): Goal
  - Verify if process behaviour is consistent with normal operating conditions.
    - Detection: rapidly detect abnormalities in process operation
    - Diagnosis: look for the root cause of abnormal behaviour
    - Fault criticality assessment
    - Decision: stop the process and fix the problem or accommodate the fault and proceed

Rapidly detect and act on abnormalities in process operation.

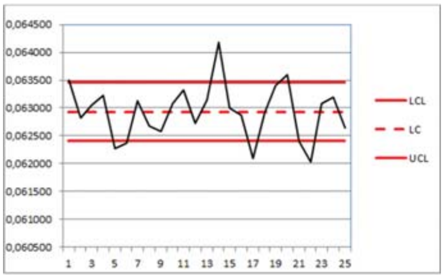
ICQEM 2016 GEPSI – PSE Group • Process Chemometrics Lab.

The beginning…



Walter Shewhart first control chart: Western Electric (Hawthorne Works, Chicago, 1924)

1. Introduction & Background



Chance / Common Causes → Process Variability

~~Assignable / Special Causes~~

Eliminate

1. Introduction & Background

- Benefits from SPM
  - Increase safety of people
  - Protect critical industrial assets
  - Increase process efficiency: ↓ out-of-spec product, ↓ scrap, …
  - Improve quality: ↑ product consistency, ↓ defects
  - Improve economic results
  - Reduce environmental impact
  - …

Goal

Present an overview of some of the main trends on SPM over the last 90+ years

- *From univariate, to multivariate, to high-dimensional*
- *From monitoring the mean, to dispersion, to correlation*
- *From stationary, to dynamic, to non-stationary*
- *From sensor data to higher-order profiles*
- *From detection, to diagnosis, to prognosis*

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Topics

- From univariate, to multivariate, to high-dimensional
- From monitoring the mean, to dispersion, to correlation
- From stationary, to dynamic, to non-stationary
- From sensor data to higher-order profiles
- From detection, to diagnosis, to prognosis

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From univariate, to multivariate, to high-dimensional (“megavariate”)

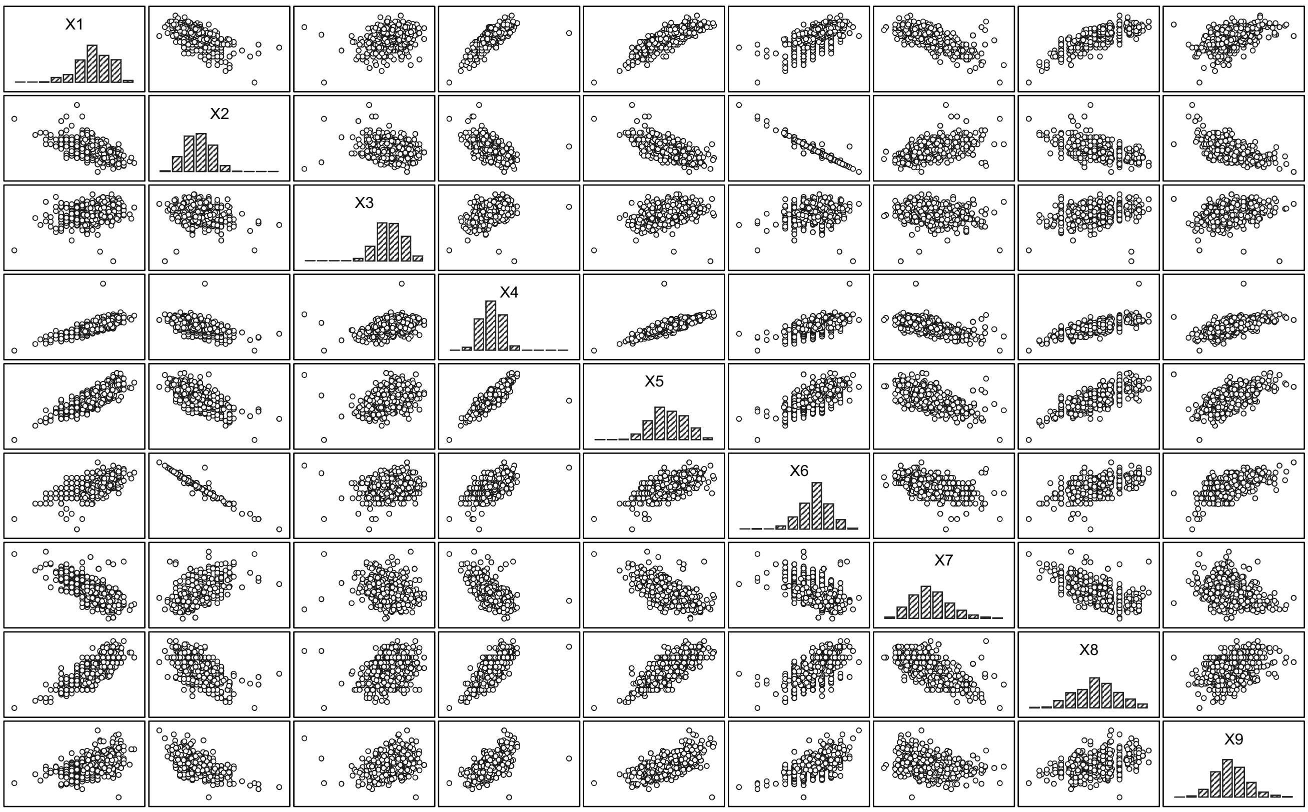
Univariate

x_1
21,43
23,97
21,48
21,68
22,87
22,14
20,80
21,97
21,16
22,55
22,30
21,42
24,84
20,69

Multivariate

x_1	x_2	x_3	x_4	(...)
21,43	1,35	22,13	214,32	
23,97	23,76	24,38	239,72	
21,48	-3,81	21,62	214,76	
21,68	-17,42	20,26	216,77	
22,87	-13,72	20,63	228,75	
22,14	18,85	23,88	221,39	
20,80	7,11	22,71	207,99	
21,97	-17,75	20,23	219,74	
21,16	-4,29	21,57	211,60	
22,55	0,42	22,04	225,51	
22,30	18,53	23,85	223,04	
21,42	5,46	22,55	214,18	
24,84	8,81	22,88	248,35	
20,69	7,84	22,78	206,94	

Megavariate



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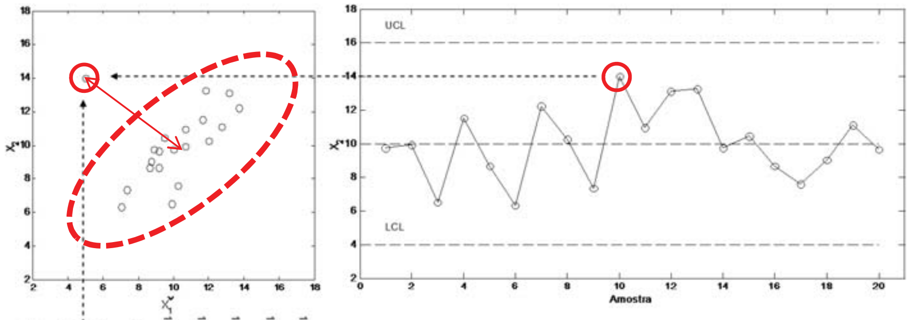
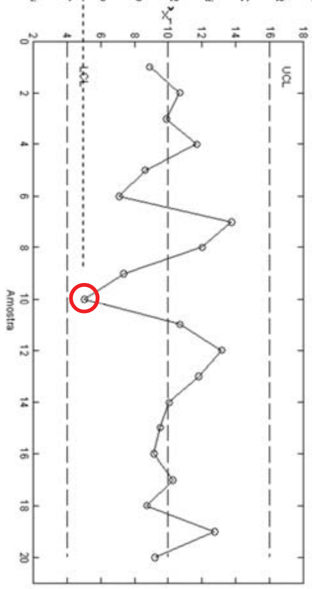

Hotelling's T² (1931)

$$T_i^2 = n\left(\overline{\mathbf{x}}_i - \overline{\overline{\mathbf{x}}}\right)^T \overline{\mathbf{S}}^{-1}\left(\overline{\mathbf{x}}_i - \overline{\overline{\mathbf{x}}}\right)$$

H. Hotelling

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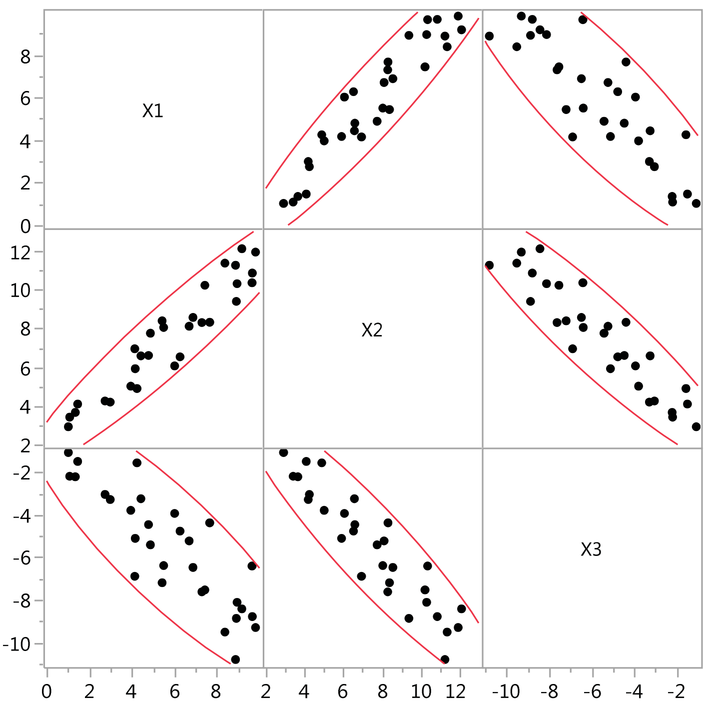
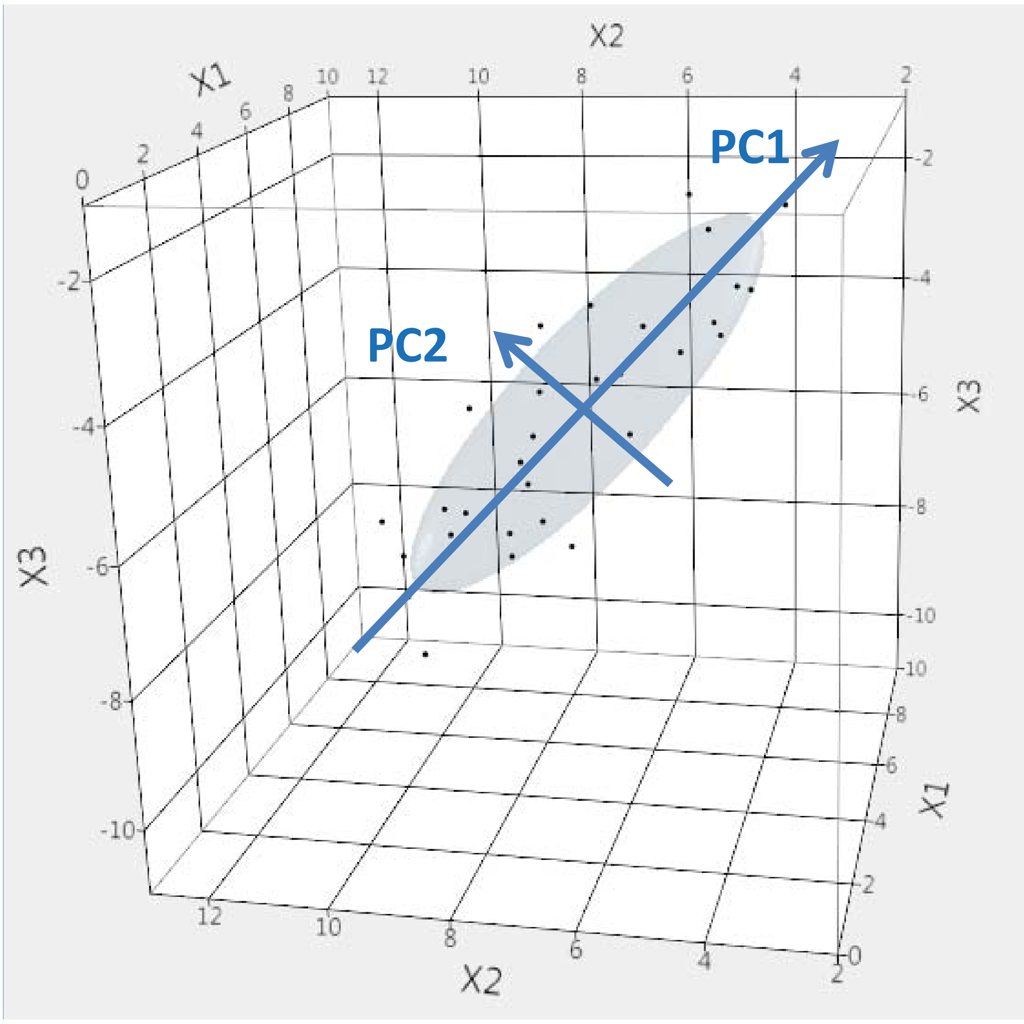
PCA



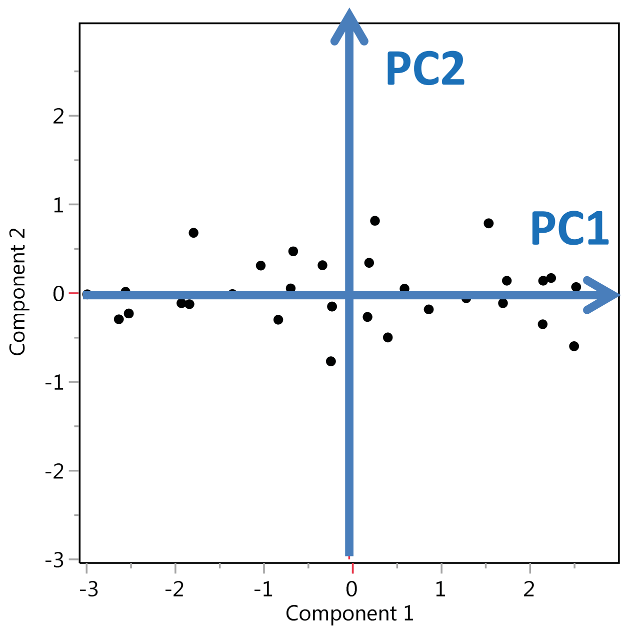


PCA

Principal Components: on Correlations

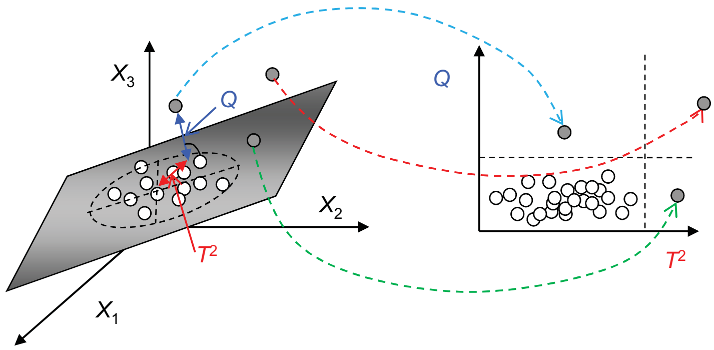
Number	Eigenvalue	Percent	20 40 60 80	Cum Percent
1	2,8235	94,115		94,115
2	0,1406	4,687		98,802
3	0,0359	1,198		100,000

X =



+ E

PCA-MSPC (1959/1991)



J. Edward Jackson

J. F. MacGregor

Example:

Megavariate statistical process control in electronic devices assembling (M. Reis; P. Delgado)

- Solder Paste Deposits (SPD's) are of critical importance, because:
  - They provide the necessary fixation for all the electronic components
  - Functionalize the operation of electronic components
- Different shapes
- Different positions
- …

Reis, M. S., & Delgado, P. (2012). A large-scale statistical process control approach for the monitoring of electronic devices assemblage. *Computers and Chemical Engineering*, 39, 163-169.

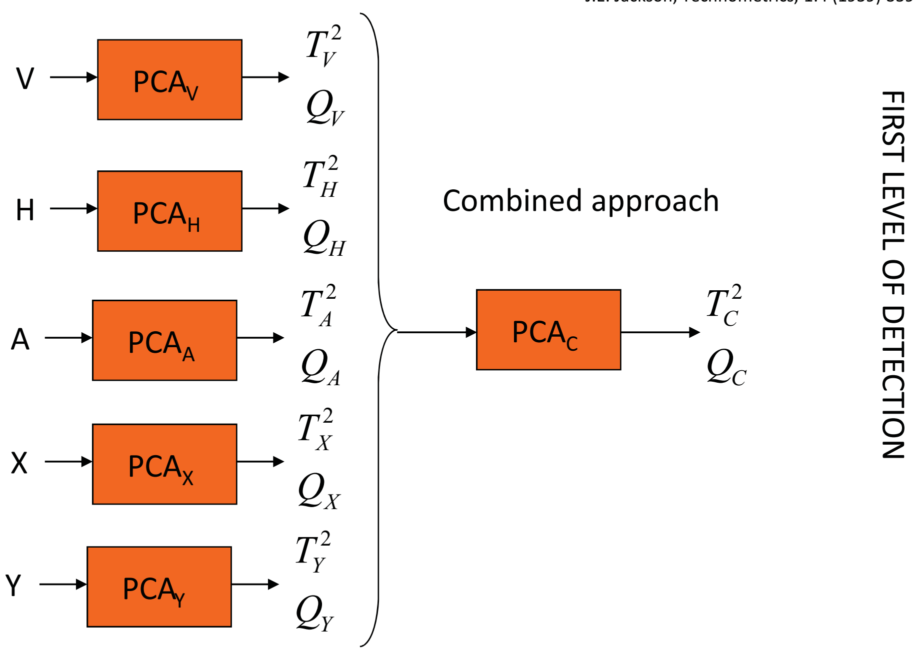
The problem

- 100% inspection of Printed Circuit Boards (PCB's).
- Each PCB has more than 3000 deposits (SPD's) of different shapes.
- Operators have less than 1 min to decide about the status of each PCB.
- Each solder deposit is evaluates according to 5 parameters obtained through Moiré interferometry
  - Volume (V)
  - Area (A)
  - Height (H)
  - Offset in the X coordinate (X)
  - Offset in the Y coordinate (Y)

> 15 000 measurements for each PCB!

- Multivariate Statistical Process Control using Principal Components Analysis (PCA-MSPC*)

* J.E. Jackson, Technometrics, 1:4 (1959) 359-377.



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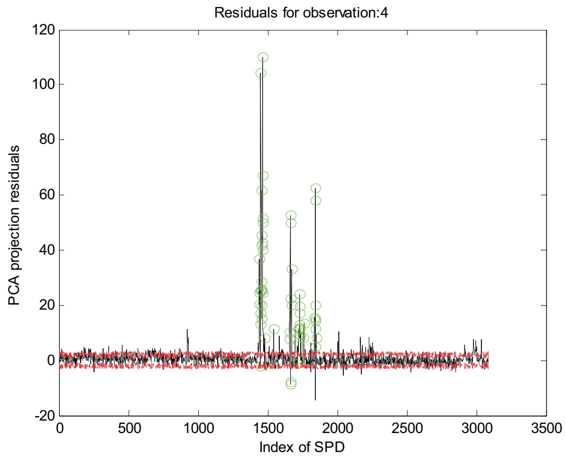
SECOND LEVEL OF DETECTION

- Analysis of the residuals from the projection of each multivariate observation to the PCA subspace.



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RESULTS FOR THE FIRST LEVEL OF DETECTION

Detection Statistics	Measurements used to compute the relative area under the **ROC curve** (values in %)					
	Height (H)	*Area (A)*	*Volume (V)*	*Offset X*	*Offset Y*	*Combined approach*
T^2	70.00	62.50	85.63	76.88	70.63	90.00
Q	93.13	93.75	91.88	85.00	83.13	90.63

10 PCB's classified as "good" were used to represent NOC data in SPC (estimate the PCA subspace, …)
16 PCB's classified as "fail" (16) and "good" (5) were used to test the procedure

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RESULTS FOR THE SECOND LEVEL OF DETECTION

Detection Statistics	Measurements used to identify abnormal SPD's (values in %)					
	Height (H)	*Area (A)*	*Volume (V)*	*Offset X*	*Offset Y*	*Combined approach*
Mean	80.33	65.82	76.04	60.23	54.38	72.47
Standard Deviation	20.07	29.97	21.02	21.23	29.93	17.31

Reis, M.S. and P. Delgado, *A large-scale statistical process control approach for the monitoring of electronic devices assemblage.* Computers and Chemical Engineering, 2012. **39**: p. 163-169.

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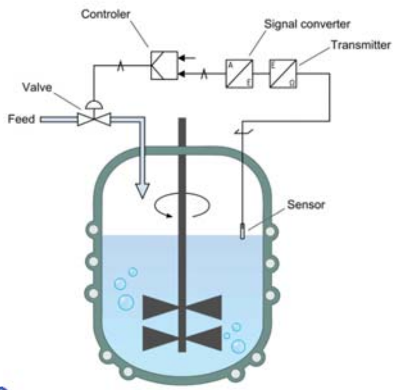
From monitoring the mean, to dispersion, to correlation

Monitoring the mean and dispersion

- Most MSPC schemes are focused on **location** (mean level);
  - Shewhart
  - EWMA
  - CUSUM
  - Hotelling's T^2
  - PCA-MSPC

Monitoring the correlation

- Most industrial processes are heavily controlled
  - Feedback control loops (PID)
  - Cascade control
  - Model predictive control
  - …

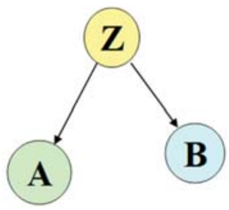


- When a fault arises, controllers fight to keep the mean levels on track:
  - **Faults are "masked"** by the controller actions!
  - But the **correlation structure** of the process variable changes!

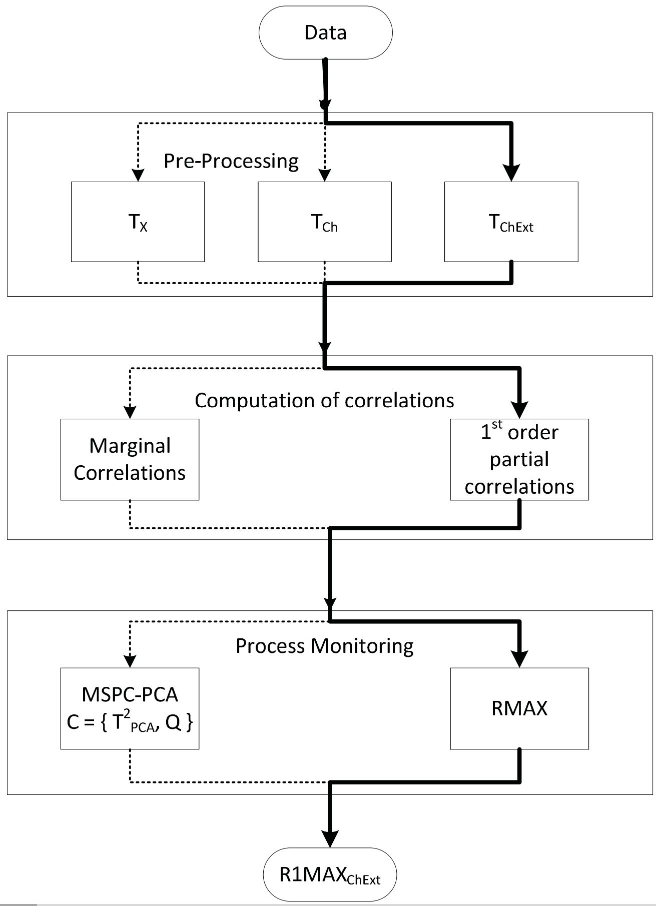
SPM based on partial correlations

- Marginal correlations are unable to discern between direct and indirect associations between variables
- Partial correlations offer a better description of the process Normal Operating Conditions (NOC) network structure

Corr(A,B) ↑↑
but
R(A,B|Z) is ↓



$$r_{AZ} = 0.8 \qquad r_{AZ \cdot B} = 0.7295$$
$$r_{BZ} = 0.6 \qquad r_{BZ \cdot A} = 0.4104$$
$$r_{AB} = 0.48 \qquad r_{AB \cdot Z} = 0$$



$$RMAX = \max\left\{\left|w(\mathbf{r})\right|\right\}$$
$$VnMAX = \max\left\{\left|w_s(\mathbf{v})\right|\right\}$$

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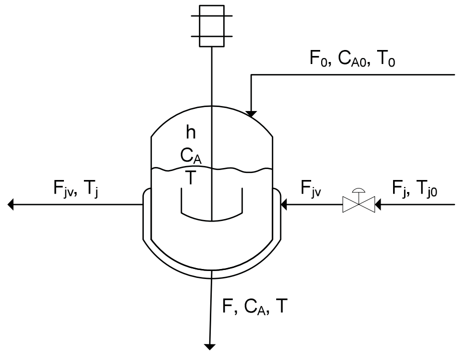
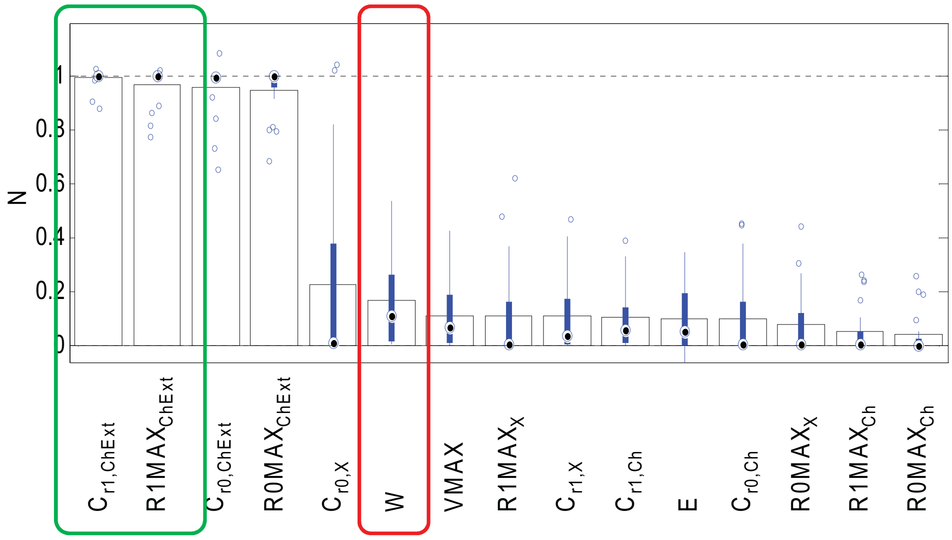
SPM based on partial correlations





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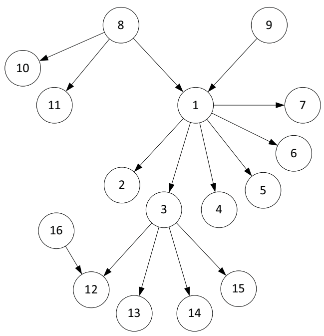
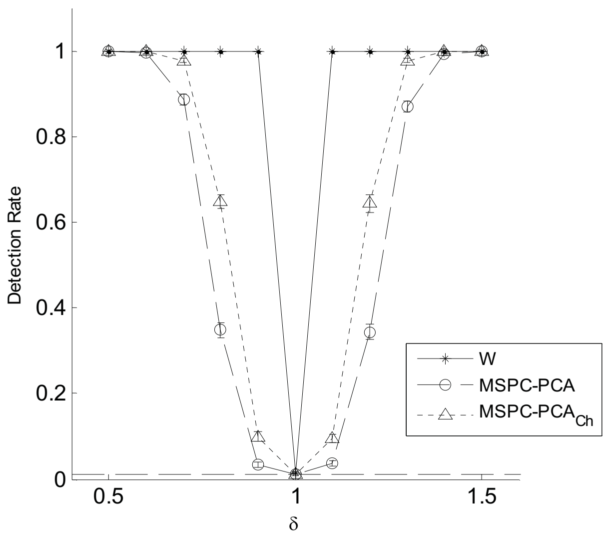
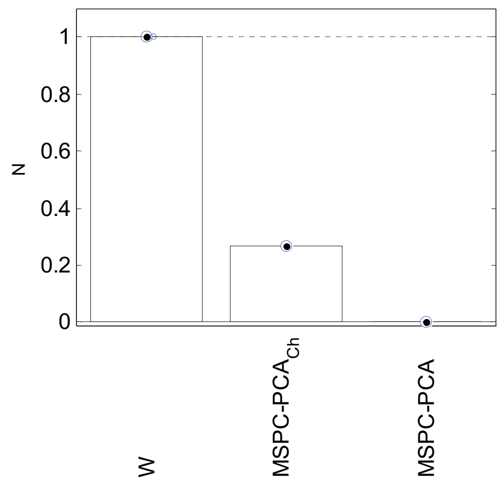


- PCA performs rather poorly in detecting localized changes in correlation
- A conventional approach, based on the marginal covariance (W), performs much better





SPM based on partial correlations

- Rato, T. J., & Reis, M. S. (2014a). Non-causal data-driven monitoring of the process correlation structure: a comparison study with new methods. Computers & Chemical Engineering, 71, 307-322.
- Rato, T. J., & Reis, M. S. (2014b). Sensitivity enhancing transformations for monitoring the process correlation structure. Journal of Process Control, 24, 905-915.
- Rato, T. J., & Reis, M. S. (2015a). Multiscale and Megavariate Monitoring of the Process Networked Structure: M2NET. Journal of Chemometrics, 29(5), 309-322.
- Rato, T. J., & Reis, M. S. (2015b). On-line process monitoring using local measures of association. Part I: Detection performance. Chemometrics and Intelligent Laboratory Systems, 142, 255-264.
- Rato, T. J., & Reis, M. S. (2015c). On-line process monitoring using local measures of association. Part II: Design issues and fault diagnosis. Chemometrics and Intelligent Laboratory Systems, 142, 265-275.

From stationary, to dynamic, to non-stationary

PCA – assumes i.i.d. observations

X1	X2	X3	X4		Xm
X1(0)	X2(0)	X3(0)	X4(0)		Xm(0)
X1(1)	X2(1)	X3(1)	X4(1)		Xm(1)
X1(2)	X2(2)	X3(2)	X4(2)		Xm(2)
X1(3)	X2(3)	X3(3)	X4(3)		Xm(3)
X1(4)	X2(4)	X3(4)	X4(4)		Xm(4)
X1(5)	X2(5)	X3(5)	X4(5)	…	Xm(5)
X1(6)	X2(6)	X3(6)	X4(6)		Xm(6)
X1(7)	X2(7)	X3(7)	X4(7)		Xm(7)
X1(8)	X2(8)	X3(8)	X4(8)		Xm(8)
X1(9)	X2(9)	X3(9)	X4(9)		Xm(9)

→ PCA

Dynamic PCA – Ku et al. (1995)

X1	X1 (L=1)	X1 (L=2)	X2	X2 (L=1)	X2 (L=2)		Xm	Xm (L=1)	Xm (L=2)
X1(0)			X2(0)				Xm(0)		
X1(1)	X1(0)		X2(1)	X2(0)			Xm(1)	Xm(0)	
X1(2)	X1(1)	X1(0)	X2(2)	X2(1)	X2(0)		Xm(2)	Xm(1)	Xm(0)
X1(3)	X1(2)	X1(1)	X2(3)	X2(2)	X2(1)		Xm(3)	Xm(2)	Xm(1)
X1(4)	X1(3)	X1(2)	X2(4)	X2(3)	X2(2)		Xm(4)	Xm(3)	Xm(2)
X1(5)	X1(4)	X1(3)	X2(5)	X2(4)	X2(3)	…	Xm(5)	Xm(4)	Xm(3)
X1(6)	X1(5)	X1(4)	X2(6)	X2(5)	X2(4)		Xm(6)	Xm(5)	Xm(4)
X1(7)	X1(6)	X1(5)	X2(7)	X2(6)	X2(5)		Xm(7)	Xm(6)	Xm(5)
X1(8)	X1(7)	X1(6)	X2(8)	X2(7)	X2(6)		Xm(8)	Xm(7)	Xm(6)
X1(9)	X1(8)	X1(7)	X2(9)	X2(8)	X2(7)		Xm(9)	Xm(8)	Xm(7)
	X1(9)	X1(8)		X2(9)	X2(8)			Xm(9)	Xm(8)
		X1(9)			X2(9)				Xm(9)

PCA →

Dynamic Principal Components Analysis (DPCA)

- However, the DPCA scores still present autocorrelation …

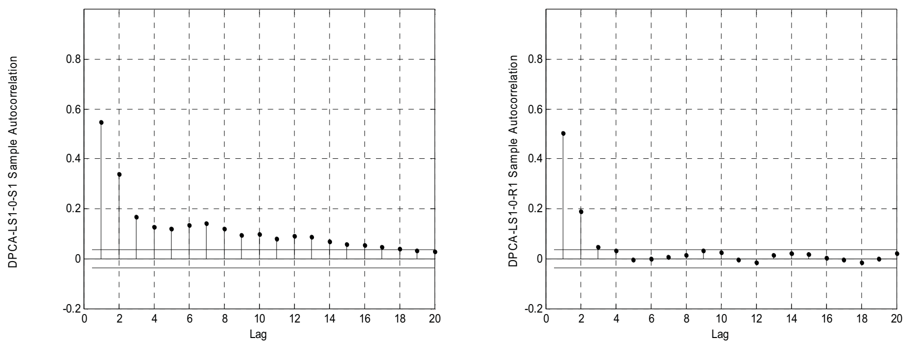


Figure. Sample autocorrelation function for the DPCA-LS1-0-S1 and DPCA-LS1-0-R1 statistics.

Dynamic PCA with Decorrelated Residuals: DPCA-DR (Rato & Reis)

$$\mathbf{X} = [\mathbf{X}(k)\ \mathbf{X}(k–1)\ \ldots\ \mathbf{X}(k–l)];$$

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}^{\#} \\ \mathbf{x}^{*} \end{bmatrix}, \quad \mathbf{S} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^{\mathrm{T}}, \quad \mathbf{P} = \begin{bmatrix} \mathbf{P}^{\#} \\ \mathbf{P}^{*} \end{bmatrix}$$

$$\hat{\mathbf{t}}_{1:k} = \begin{bmatrix} \mathbf{I}_k & \mathbf{0}_{k\times(n-k)} \end{bmatrix} \mathbf{\Lambda}\mathbf{P}^{*\mathrm{T}} \left(\mathbf{P}^{*}\mathbf{\Lambda}\mathbf{P}^{*\mathrm{T}}\right)^{-1} \mathbf{x}^{*}$$

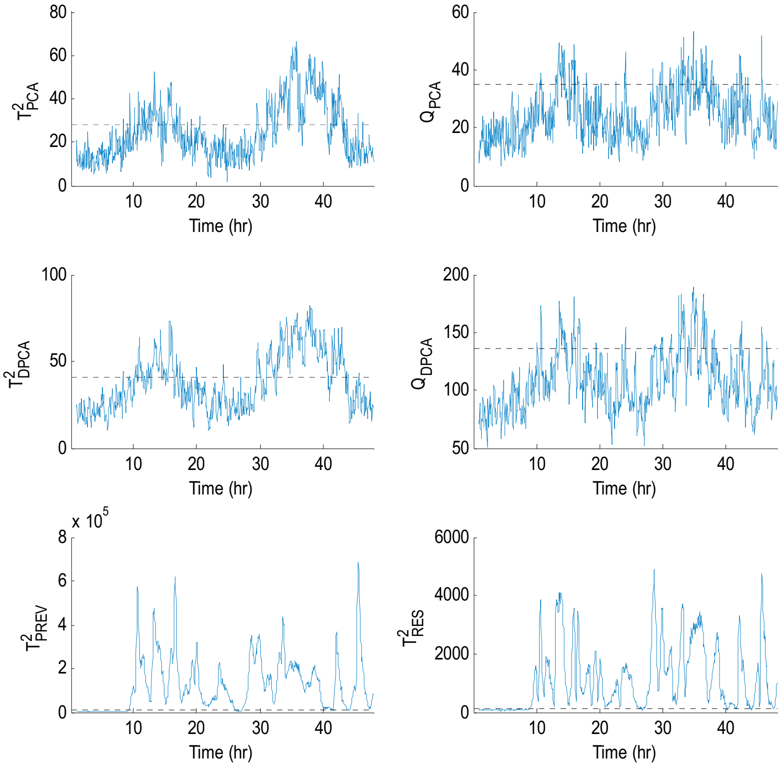
Scores

$$T^2_{PREV} = \left(\mathbf{t} - \hat{\mathbf{t}}\right)^{\mathrm{T}} \mathbf{S}^{-1}_{\mathbf{t}-\hat{\mathbf{t}}} \left(\mathbf{t} - \hat{\mathbf{t}}\right)$$

Residuals

$$T^2_{RES} = \left(\mathbf{x} - \mathbf{P}\hat{\mathbf{t}}\right)^{\mathrm{T}} \mathbf{S}^{-1}_{\hat{\mathbf{t}}} \left(\mathbf{x} - \mathbf{P}\hat{\mathbf{t}}\right)$$

Tennessee Eastman process



Dynamic DPCA-DR

- DPCA-MD scores for the same system present a significantly lower level of autocorrelation.

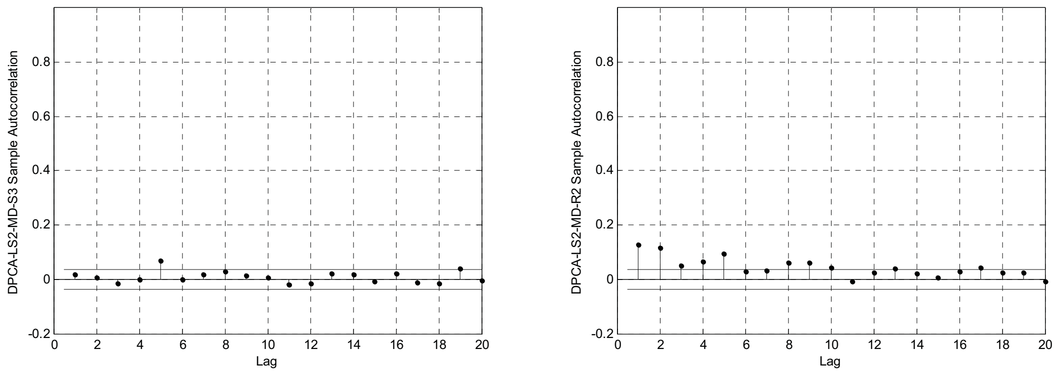


Figure. Sample autocorrelation function for T^2_{Prev} and T^2_{Res} statistics.

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From sensor data to higher-order profiles

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Monitoring Profiles (1D, 2D, 3D, …)

"(…) *We view the monitoring of process and product profiles as the most promising area of research in statistical process control*. (…)"

Woodall, W. H., Spitzner, D. J., Montgomery, D. C., and Gupta, S. (2004). Using Control Charts to Monitor Process and Product Quality Profiles. *Journal of Quality Technology*, 36(3), 309-320.

- Definition [Profile, ***P***]:

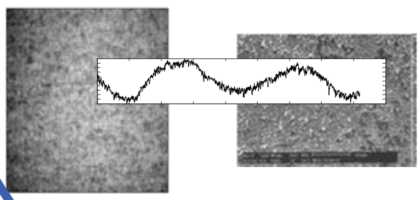
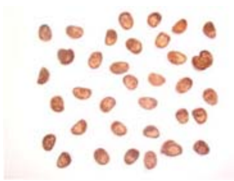
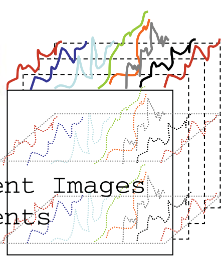
An array of data, indexed by time and/or space, that characterizes a given entity (product, process).

$$P:\left\{\mathbf{Y}\left(ix,iy,iz,it\right)\right\}_{\underbrace{ix,iy,iz}_{\text{Spatial indices}},\underbrace{it}_{\text{Time index}}\in\Omega_x\times\Omega_y\times\Omega_z\times\Omega_t}$$

$$\left\{\mathbf{Y}\right\}_{ix,iy,yz,it}\in\Re^n$$

"Dual domain" classification

Frequency domain localization

	Low (Time/Space localization)	High (Time/Space localization)
High	Frequency Localized Random Profiles 	Fully Localized Profiles More: Acoustic signals Seismic signals "Hard" constraint: $\sigma(g)\cdot\sigma(\hat{g})\geq\frac{1}{2}$ 
Low	Delocalized Random Profiles 	Time-Space Localized Random Profiles   More: Analysis of Coherent Images Perfusion experiments fMRI, …

Time/Space localization

Monitoring paper formation*
(Reis, MS & Bauer, A.)

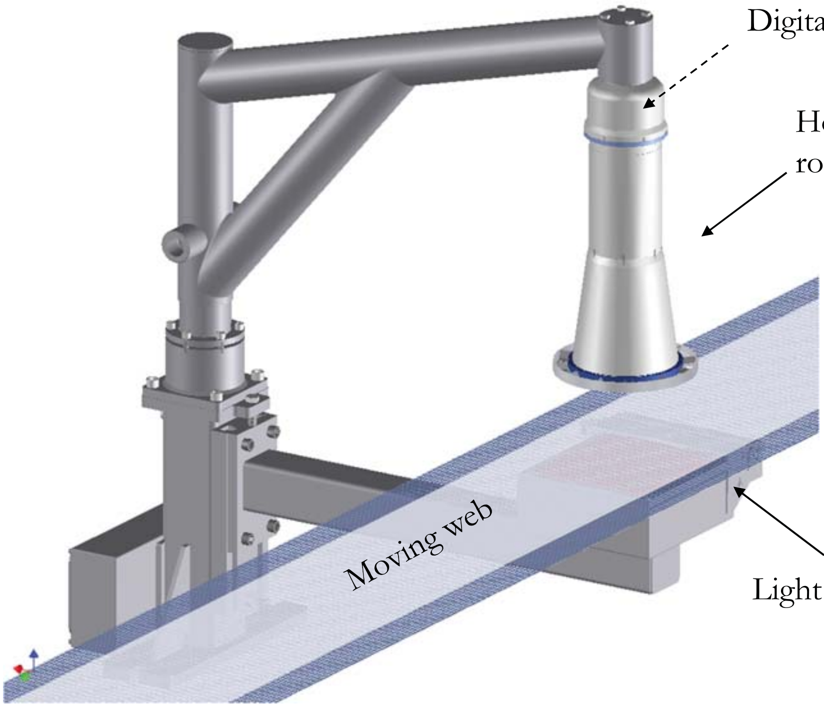
- Currently is evaluated off-line: few times per day (e.g. after each paper reel production)
  - Very high delay, regarding the production speed of current paper machines (**~100 Km/h!**)

* Level of uniformity in the way fibres are distributed across the paper surface.

Goal

Develop a technology for on-line monitoring of the paper formation.

Experimental: Measurement Sensor



Experimental

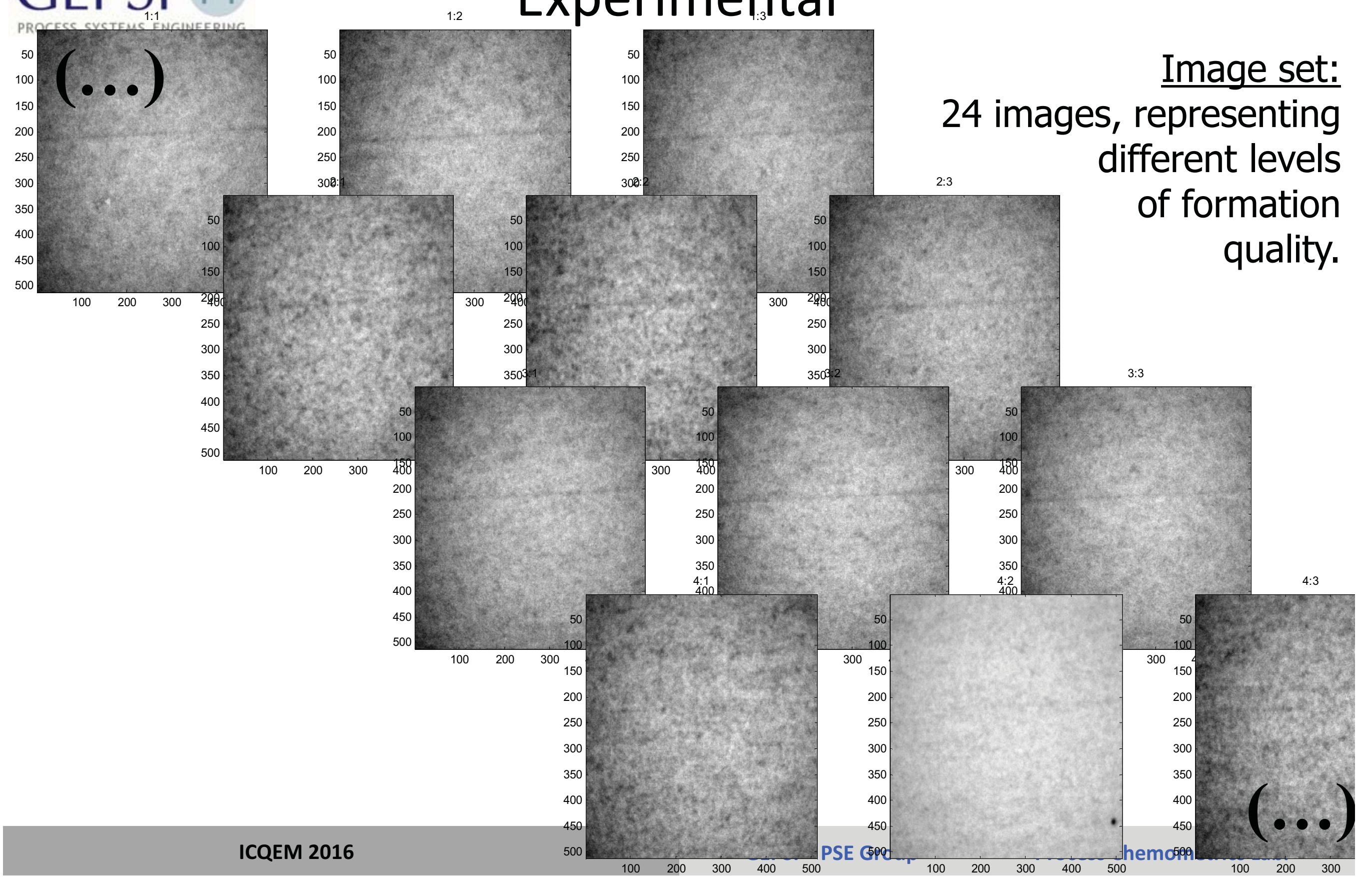
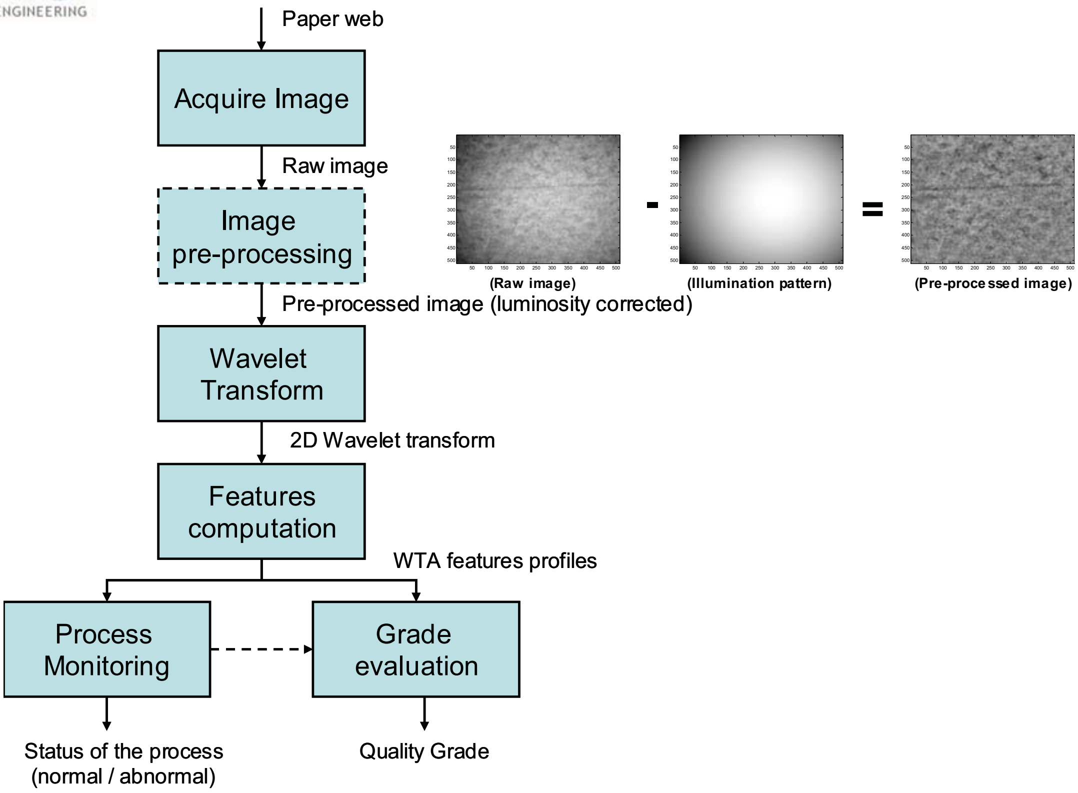


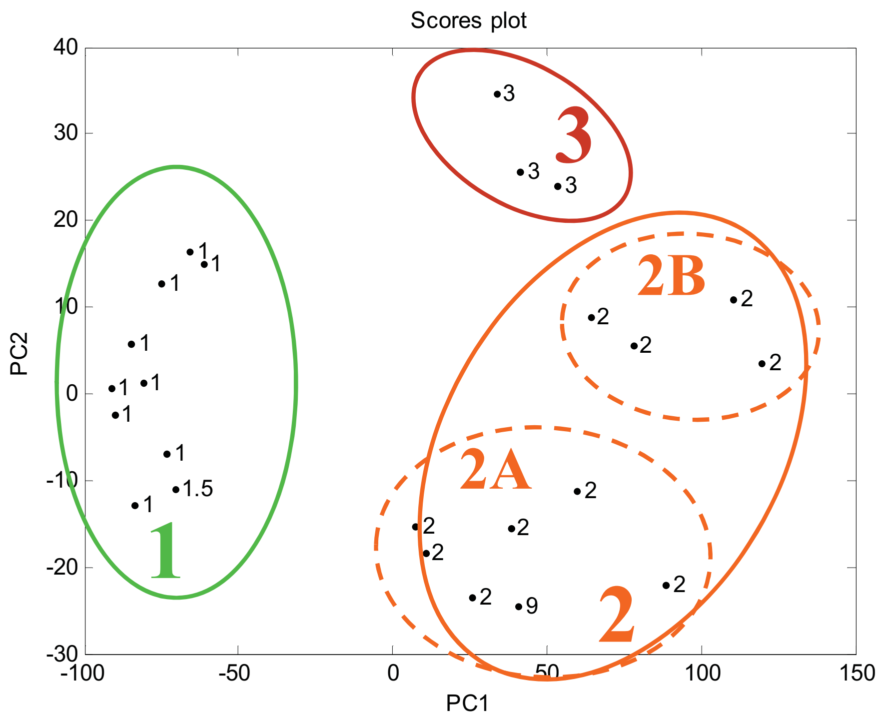
Image set:
24 images, representing different levels of formation quality.

Methods



Results (RQ1)

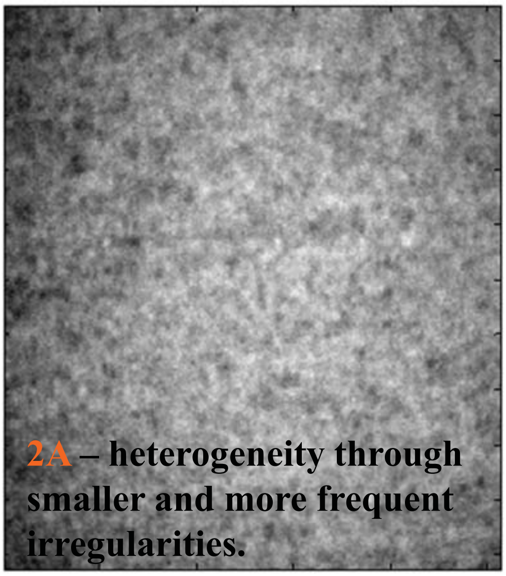
- PCA analysis of wavelet signatures

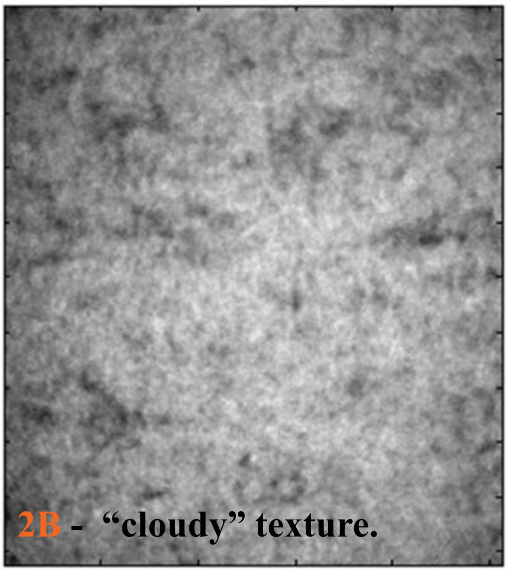


2PC's – 97.96% of the overall variability

Results (RQ1)

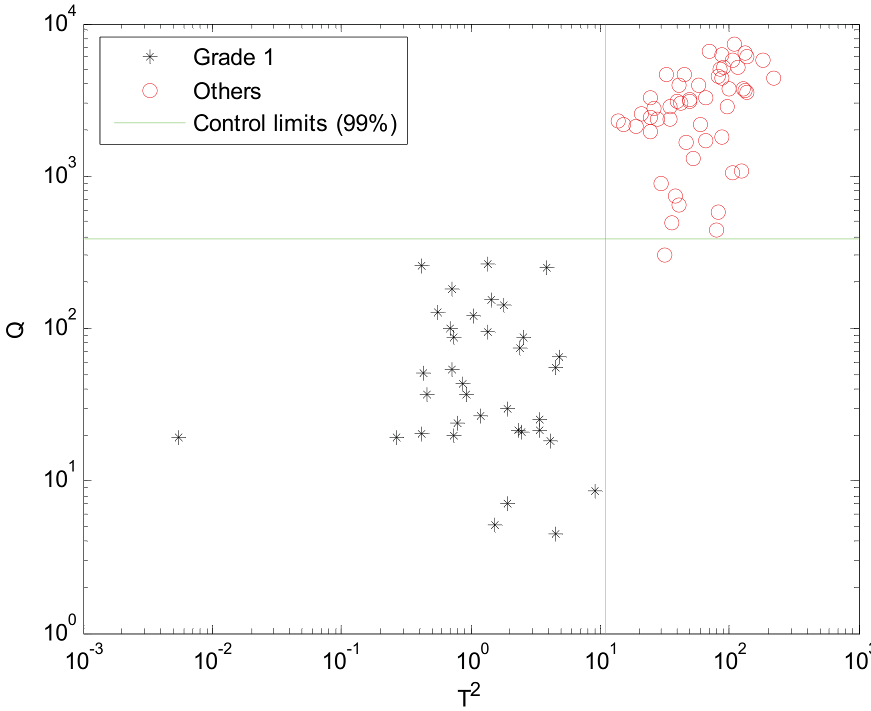
- Prototypes of clusters 2A and 2B





Results (RQ2)

Analysis 2 (sub-images)



Note: Half of the Grade 1 samples were used to estimate the NOC region.

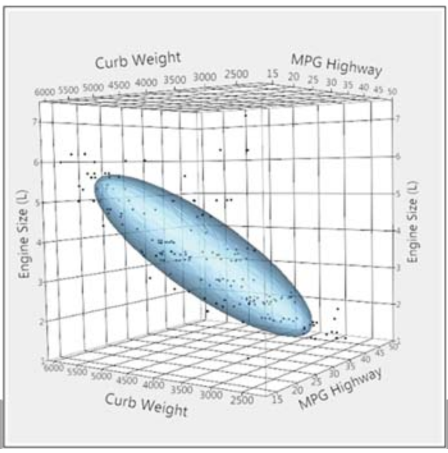
GEPSI PROCESS SYSTEMS ENGINEERING

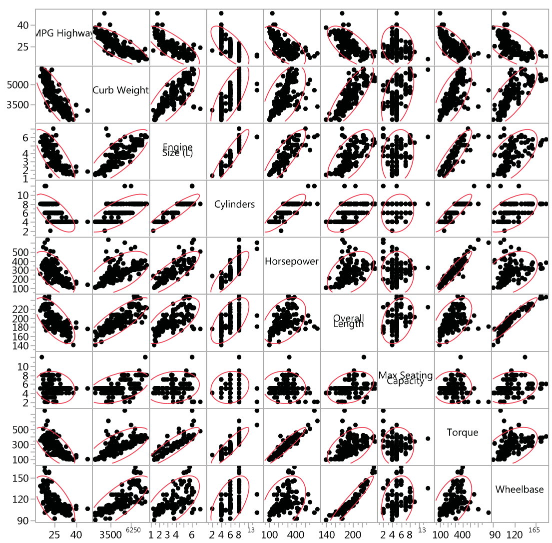
From detection, to diagnosis, to prognosis

GEPSI PROCESS SYSTEMS ENGINEERING

Detection

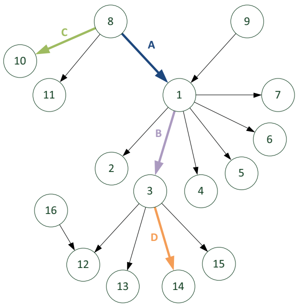
- Basic requirement: a good description of the Normal Operating Conditions
  - Mean levels and main correlations between variables
  - Non-causal associations





Diagnosis

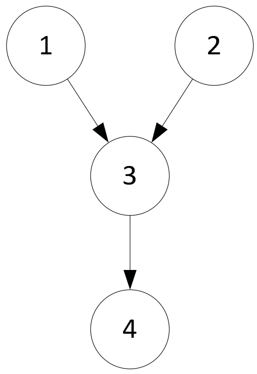
- To find the root cause, causal information is needed!
- However, **most SPM models are acausal**, and therefore cannot provide all the information required for a thorough diagnosis
- They may also point to variables that are not directly involved in the fault
  - The smearing-out effect of PCA-MSPC is a well-known manifestation



One solution

- Plug-in causality into conventional NOC models through an adequate pre-processing of the variables
- This can be done using the concept of **Sensitivity Enhancing Transformations (SET)**
  - Rato, T. J., & Reis, M. S. (2014a). Non-causal data-driven monitoring of the process correlation structure: a comparison study with new methods. Computers & Chemical Engineering, 71, 307-322.
  - Rato, T. J., & Reis, M. S. (2014b). Sensitivity enhancing transformations for monitoring the process correlation structure. Journal of Process Control, 24, 905-915.

Sensitivity enhancing transformation (SET)



1. Network Identification

$$x_1 \to x_3$$
$$x_2 \to x_3$$
$$x_3 \to x_4$$

2. Regress each variable onto its parents

$$y_1 = x_1$$
$$y_2 = x_2$$
$$y_3 = x_3 - x_1 b_{1,3} - x_2 b_{2,3}$$
$$y_4 = x_4 - x_3 b_{3,4}$$

3. Final model

$$\mathbf{Y} = \mathbf{X}\mathbf{B}$$

$$\mathbf{B} = \begin{bmatrix} 1 & 0 & -b_{1,3} & 0 \\ 0 & 1 & -b_{2,3} & 0 \\ 0 & 0 & 1 & -b_{3,4} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

4. Apply the Cholesky decomposition to the regression residuals thus obtained.

Plug-in approach:

Process Data

↓

SET

↓

Uncorrelated data

↓

Monitoring statistics (PC, T^2)

↓

Statistics

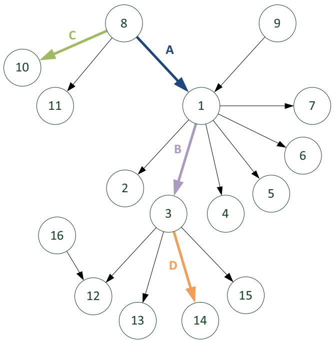
↓

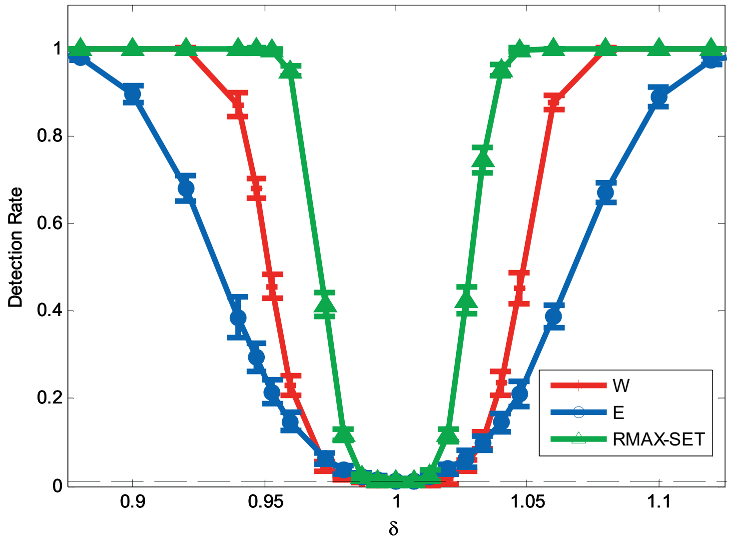
MSPC

↓

Process State (Normal / Abnormal)

Detection

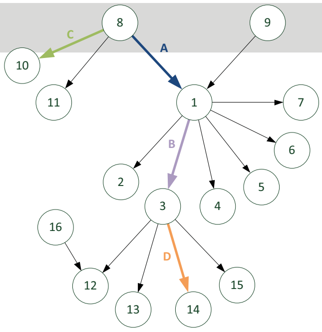


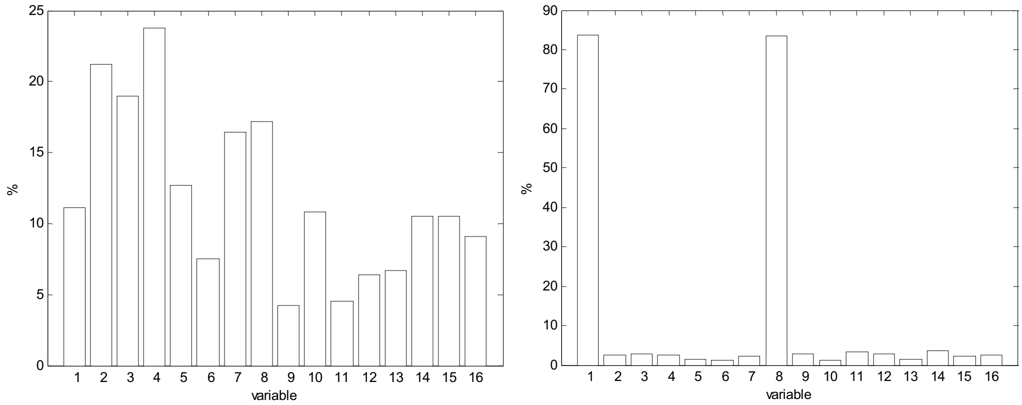


Rato, T.J. and M.S. Reis, *Sensitivity enhancing transformations for monitoring the process correlation structure.* Journal of Process Control, 2014. **24**: p. 905-915.

Rato, T.J. and M.S. Reis, *On-line process monitoring using local measures of association. Part I: Detection performance.* Chemometrics and Intelligent Laboratory Systems, 2015. **142**: p. 255-264.

Diagnosis

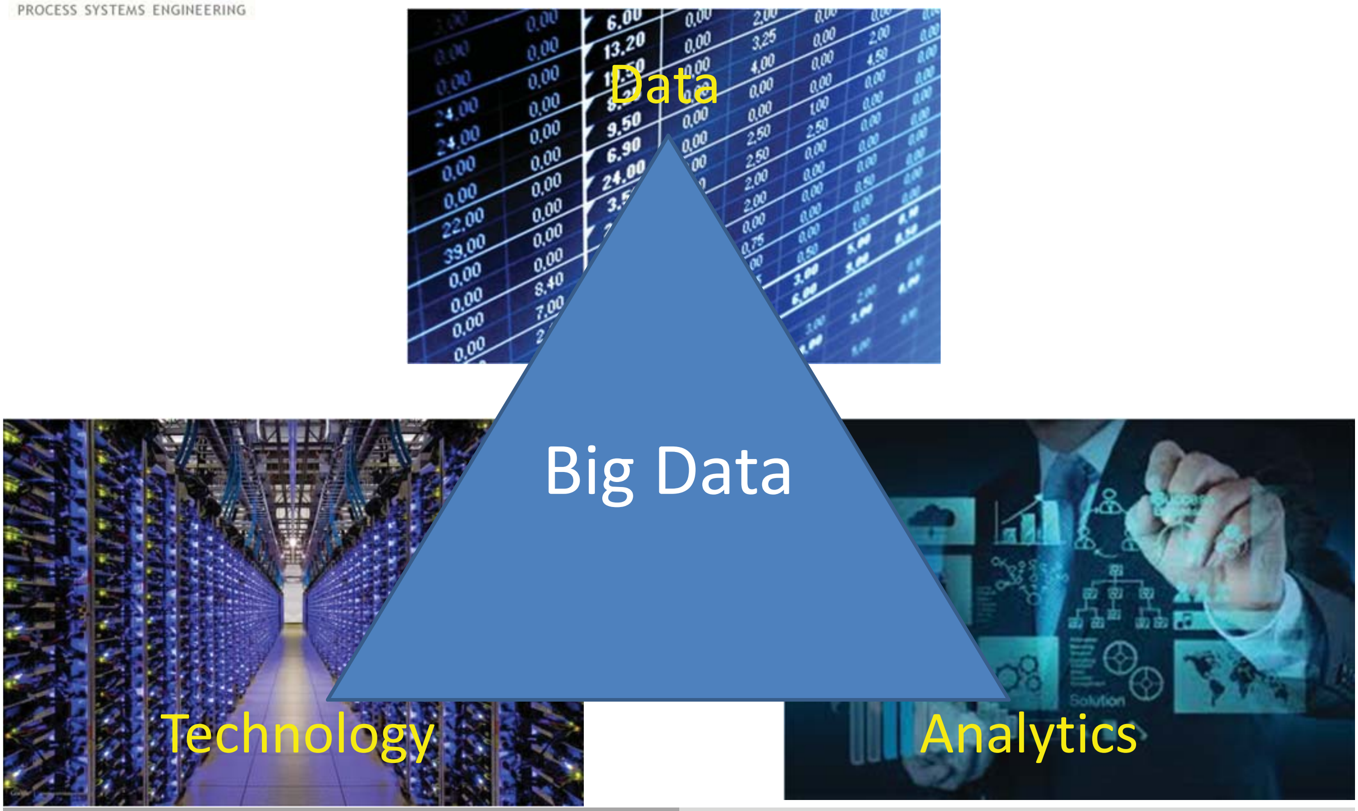




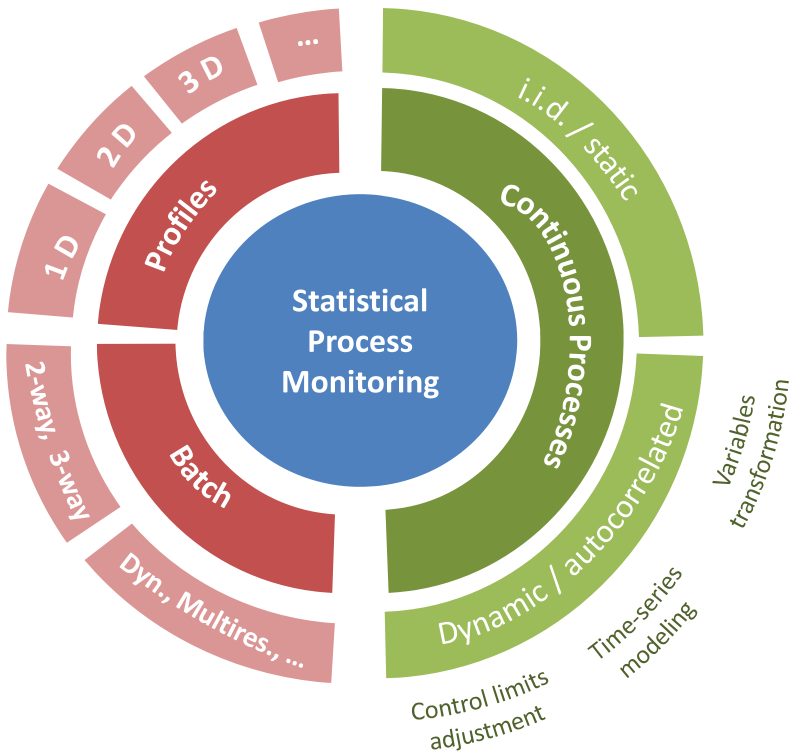
(a) (b)

Figure . Percentage of times that each variable was considered as the faults' root cause by the marginal correlation procedure on a **fault in the relationship between variables 1 and 8**: (a) marginal correlation of the original variables; (b) marginal correlation of the transformed variables.

SPM in the big data era



Typology of SPM applications



Conclusions

- 90+ years after its introduction, SPC is still an exciting and evolving field!
- SPC should be complemented with effective Diagnosis tools
- New challenges include
  - Move focus from Detection to Diagnosis
  - Handling complex dynamics: multiscale methods
  - Integrating the structure of the system and existing domain knowledge: SET, Bayesian methods
  - Handling multiple data structures (profiles): multi-block methods
  - Monitoring time-varying systems: adaptive methods, …

and … making everything **simple to use** and **robust**!

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http://www.eq.uc.pt/~marco/research/pclab/