On-line monitoring of batch processes: Does the modelling structure matter?

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1 Introduction

Principal Component Analysis (PCA) is a bilinear modelling tool which has been successfully applied to batch process data for process understanding and statistical monitoring. Since batch data are three-way, the data matrix $\underline{\mathbf{X}}$ containing J process variables measured at K sampling times in I batches has to be conveniently rearranged in a number of two-way matrices to apply PCA. There are at least three methods to do this: i) To unfold the three-way matrix of data [1, 2, 3]; ii) To use an adaptive approach where current and past information are combined, e.g. by using hierarchical models [4]; and iii) To fit K PCA local models [5], each one modelling exclusively the information corresponding to a sampling time. Additionally, both the unfolding and splitting in K models -options i) and iii), respectively- can be combined in approaches such as the evolving modelling [5, 6] or the moving window approach [7]. Finally, the multi-stage approach is based on the calibration of independent models for different stages of a batch process [8]. For a theoretical discussion on what kind of process dynamics is captured by the different methods see [9]. All these approaches lead to modelling structures which are very similar to autoregressive models [10]. When modelling continuous processes using autoregressive models, it is customary to identify the model structure -i.e., the order of the dynamics- from the data used for calibration. Nonetheless, this simple and sensible approach is usually forgotten when dealing with batch processes. All the approaches cited are based on using always the same modelling structure, no matter the dynamic nature of the process. In an attempt to overcome this limitation, the Multi-Phase Framework [11] is aimed at identifying the convenient model structure for a specific process at hand. Recent investigations performed by the authors [11, 12] have shown that the use of an inappropriate modelling structure in a process has negative consequences in the performance of a monitoring system. In this paper, a comparative study of the performance of several on-line monitoring methods is performed using a simplified simulation of a batch process with particular, *a priori* known, process dynamics.

2 Materials and Methods

A Simulink system has been designed to simulate data from a simplified batch process (see Figure 1). Data are obtained for a null average trajectory in the variables. Therefore, the Simulink system is supposed to simulate the data obtained after the subtraction of the average trajectory of the process variables, which is a common data preprocessing step in PCA-based batch monitoring. Those approaches that do not perform this subtraction -eg. [13]- are not assessed in this comparative. The batches take 150 sampling times to be processed and 10 variables are collected every sampling time. The first 100 sampling times correspond to the first phase of the process, where two latent variables (LVs) are simulated using autoregressive exogenous (ARX) models of order 1. The last 50 sampling times correspond to the second phase, where four LVs are simulated using ARX models of orders 1,2 and 3. The LVs are converted into observable variables (OVs) using a random matrix of dimension 2×10 and 4×10 for the first and the second phases, respectively. The following data-sets are simulated:

Data-set	# batches	Description
Calibration	30	Data for the calibration of the monitoring system
Test-NOC	15	Data for the validation of the monitoring system
Test-Ab$_a$	5	Upset in the interval $[90, 110]$ not coherent with PCA sub-space
Test-Ab$_{a+}$	5	Large upset in the interval $[90, 110]$ not coherent with PCA sub-space
Test-Ab$_b$	5	Upset in the interval $[90, 110]$ coherent with PCA sub-space
Test-Ab$_{b+}$	5	Large upset in the interval $[90, 110]$ coherent with PCA sub-space
Test-Ab$_c$	5	First phase lasts 20 sampling times more than usual (from 1 to 120)
Test-Ab$_d$	5	Abnormal (excessive) content of initial raw materials
Test-Ab$_e$	5	Different dynamics in the batch (change of ARXs in the model)
Test-Ab$_f$	5	Different sub-space in the batch (change of LVs in the model)

The following modelling approaches are under study:

- The approaches of Nomikos and Macgregor [14], based on the batch-wise unfolding of the data (Figure 2(a)) and zero-deviations (ZD), current-deviations (CD) and Projection to Model Plane (PMP).
- The variable-wise unfolding (Figure 2(b)) after trajectory centering (TC) [15].
- The local modelling (Figure 2(c)) [5].
- A 2-phases model matching the actual phases, obtained from variable-wise unfolding after TC.
- A 2-phases model matching the actual phases, obtained from batch dynamic unfolding (Figure 2(d)) after TC. One and three lagged measurement vectors (LMVs) are used for the first and the second phases, respectively, in order to meet the order of the dynamics simulated.

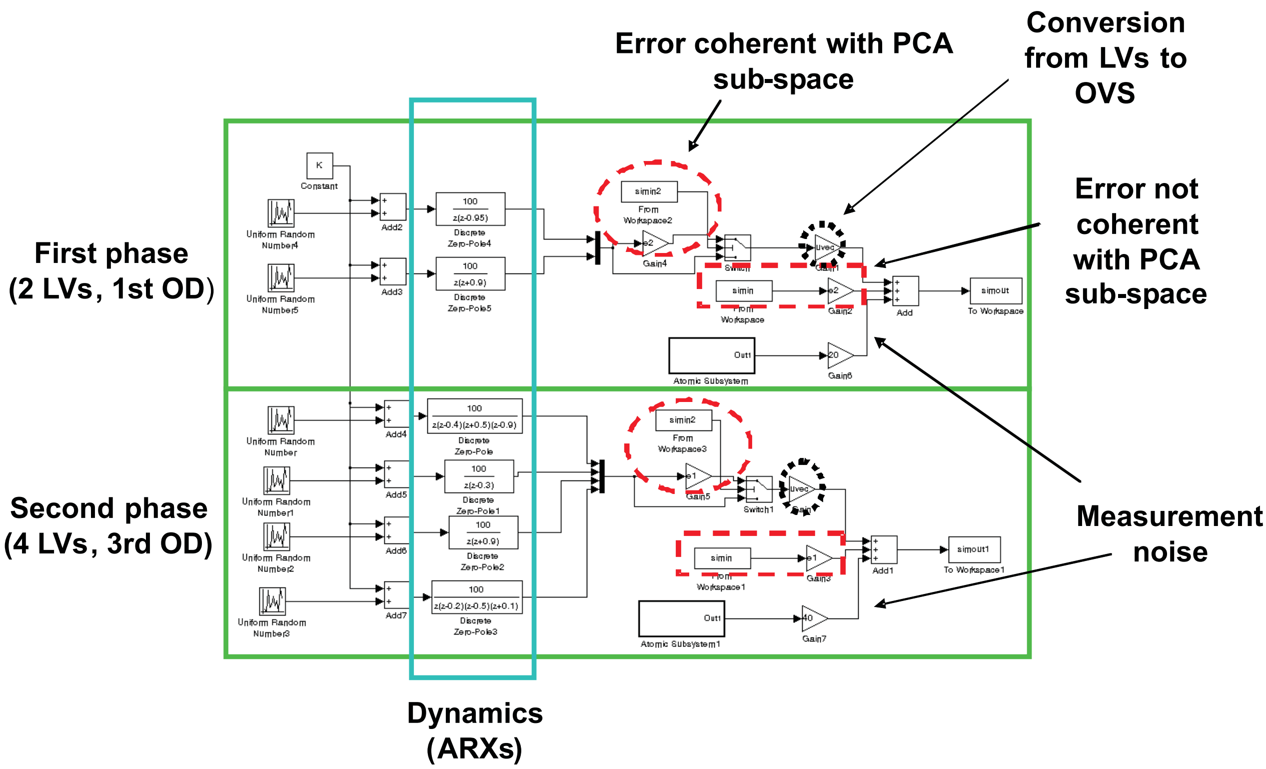
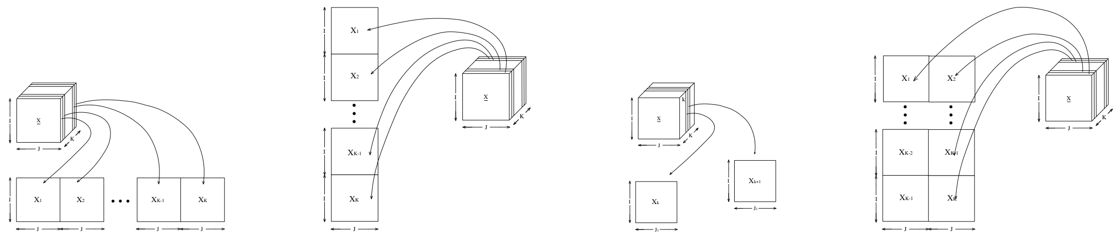


Figure 1: Simulink system used for simulation. The first 100 sampling times of a batch are obtained from the first phase and the remaining 50 from the second phase. OD stands for order of dynamics, LVs for latent variables, OVs for observable variables and ARXs for autoregressive exogenous model.



(a) Batch-wise (b) Variable-wise (c) Local (d) Batch Dynamic

Figure 2: Different arrangements of the three-way batch data in two-way form. d) presents a batch dynamic unfolding for 1 lagged measurement vector (LMV).

The difference between the two last choices is that the former does not include dynamic information whereas the latter does [9]. The monitoring systems consist of two monitoring charts built from the D-statistic and the SPE [14]. The control limits in these charts are adjusted using a leave-one-out approach [12, 16] for an Imposed Significance Level (ISL) of 1%. This value is the expected percentage of faults for a batch under Normal Operation Conditions (NOC).

The performance of the models will be compared using several indices. The adjustment of the control limits is assessed by computing the Overall Type I (OTI) risk. Following the definition in [14], the OTI is the actual percentage of faults in the NOC batches:

$$OTI = 100 \cdot \frac{nf}{I_{NOC} \cdot K}\% \tag{1}$$

where nf is the total number of faults and I_{NOC} is the number of NOC batches considered. For a coherent monitoring system, the OTI -actual percentage of faults under NOC- should be close to the ISL -expected percentage of faults under NOC. The accuracy of detection of the faults is assessed using two indices: a) the Overall Type II (OTII) risk and b) the OTI risk after a fault (OTI^f). The OTII follows:

$$OTII = 100 \cdot \frac{nnf}{I_{ab} \cdot l}\% \tag{2}$$

where nnf is the number of non-signaled faults, I_{ab} is the number of abnormal batches considered and l is the length of the faulty interval. The OTII should be as close to 0 as possible. The OTI^f is computed using (1) in NOC intervals that follow a faulty interval in a batch. This value should be as close to the OTI as possible. If the OTI^f is much higher than the OTI, this may mean that the monitoring system is not accurately signaling the end of a fault [12]. Finally, the Type I (TI) risk stands for the percentage of batches under NOC detected as abnormal batches and the Type II (TII) risk measures the percentage of abnormal batches detected as NOC batches. Three consecutive sampling times exceeding the control limits in any chart are sufficient for a batch to be determined as abnormal.

3 Results and discussion

Three simulations were performed for different values of the random matrices used for transforming the LVs into OVs. Each simulation represents a different imaginary process. The results of the comparative, averaged for the three simulations, are presented in the following table:

	Test-NOC			Test-Ab$_{a+}$ & Test-Ab$_{b+}$	
Model	TI	OTI$_D$	OTI$_{SPE}$	OTI^f_D	OTI$^f_{SPE}$
NMG-PMP	**2.2%**	**0.81%**	**1.39%**	**52%**	**23%**
NMG-CV	**2.2%**	**0.06%**	**1.70%**	**53%**	**40%**
NMG-ZV	**4.4%**	**0.96%**	**1.08%**	**58%**	**46%**
VW	**0%**	**1.02%**	**1.08%**	**4%**	**1.6%**
Local	**0%**	**0.47%**	**1.38%**	**1.2%**	**1.2%**
VW-2ph	**0%**	**0.95%**	**1.04%**	**2.8%**	**1.8%**
BD-2ph	**0%**	**0.81%**	**1.99%**	**9%**	**10%**

	Test-Ab	Test-Ab$_a$	Test-Ab$_b$	Test-Ab$_c$	Test-Ab$_d$	Test-Ab$_e$	Test-Ab$_f$
Model	TII	OTII	OTII	OTII	OTII	OTII	OTII
NMG-PMP	**26%**	**18%**	**28%**	**81%**	**22%**	**98%**	**60%**
NMG-CV	**22%**	**18%**	**28%**	**72%**	**48%**	**98%**	**57%**
NMG-ZV	**24%**	**14%**	**27%**	**75%**	**31%**	**98%**	**65%**
VW	**20%**	**0%**	**35%**	**59%**	**67%**	**96%**	**15%**
Local	**19%**	**4%**	**25%**	**59%**	**53%**	**98%**	**51%**
VW-2ph	**14%**	**0%**	**28%**	**8%**	**60%**	**97%**	**4%**
BD-2ph	**17%**	**0%**	**6%**	**26%**	**58%**	**97%**	**15%**

The proposals of Nomikos and MacGregor [14] -NMG-PMP, NMG-CV and NMG-ZD- based on batch-wise unfolding present one principal drawback: The D-statistics are highly positively autocorrelated and so the evolution in the D-statistic of a batch is smooth. Because of this, NOC batches are more likely to present several consecutive faults. Also, this reduces the performance of the monitoring system in the detection of faults. This can be observed in a generalized way in the TII and OTII results, where the batch-wise methods are outperformed by other approaches except for faults of the type Test-Ab$_d$. Batch-wise models are specially suited for this type of faults, in which the batch process is in a different operational point than the NOC -for instance, because it starts from different initial conditions than usual. Finally, the autocorrelation of the D-statistics prolongs the detection of a fault, so that the monitoring systems keep on signaling a fault for several sampling times once this fault has already finished. This can be observed in the large difference between the OTI^f_D and OTI$^f_{SPE}$ with respect to the OTI$_D$ and OTI$_{SPE}$, respectively, in the batch-wise methods.

The monitoring system based on variable-wise unfolding (VW) presents an intermediate performance. This performance, nonetheless, may be reduced for more complex process dynamics than those considered here. Anyway, the results show that even in this simplified situation VW is outperformed by other approaches in terms of TII and OTII. This discussion is also valid for the local approach.

The 2-phases model based on variable-wise unfolding (VW-2ph) is, in general terms, the approach which gives the best outcomes. This is true except for the case of faults of the type Test-Ab$_b$ and Test-Ab$_d$. The 2-phases batch-dynamic model (BD-2ph) also presented a good performance in general terms and outperformed the rest in front of Test-Ab$_b$ faults. Thus, the addition of dynamic -lagged- information is improving the performance of the monitoring system for detecting faults which are coherent with the PCA subspace. Nonetheless, this addition has the negative consequence of prolonging the detection of the faults (compare the OTI^f_D and OTI$^f_{SPE}$ results with the OTI$_D$ and OTI$_{SPE}$ results, respectively, for the BD-2ph approach).

Finally, faults of type Test-Ab$_e$ cannot be detected by any of the approaches under study. This means that the addition of dynamic information in the model is not enough for the monitoring system to detect the changes in the dynamics considered here.

4 Conclusion

The simulation analysis performed shows that the model structure influences the performance of the statistical monitoring system of a batch process. The time-varying dynamics of a process should be taken into account by using a piece-wise modelling solution. Although these time-varying dynamics can be modelled using batch-wise unfolding, the results evidence that this approach presents several drawbacks.

All the results obtained in simulation are coherent with those obtained from real batch processes in previous comparatives performed by the authors [10, 11, 12].

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