Combination of Statistical Process Control (SPC) methods and classification strategies for situation assessment of batch processes

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Abstract

The paper focuses on the development of a classification strategy to identify critic situation in batch process control. Data acquired from a batch execution is reduced by means of multiway principal component analysis in order to be assessed according to the statistical model of the process. Multiple situations have been categorized by a classification algorithm applied to the principal components in order to identify misbehaviour causes.

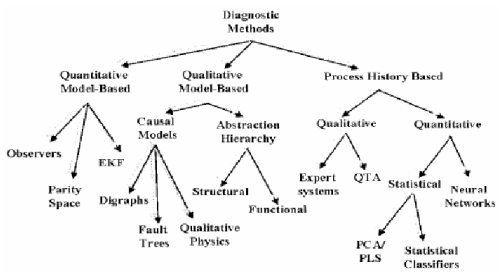

Figure 1: Classification of diagnostic algorithms, according to [27]

1 Introduction

Many strategies for fault detection and diagnosis are referenced in the bibliography. According to [27], fault diagnosis methods can been classify in three general categories: quantitative model based methods, qualitative model based methods and process history based methods, illustrated by figure 1.

The solution proposed in this work falls in the third category; and particularly in the subgroup of statistical methods. A biological batch process for the treatment of wastewater has been used to develop and test the supervision method.

Multivariate Statistic Process Control (MSPC) methods have shown to be effective in detecting and diagnosing events that cause a significant change in the dynamic correlation structure among the process variables [10] some examples are: polymerization reactor process [22], pharmaceutical process [16], the elaboration at industrial scale of the polymer polypropylene oxide [36], WasteWater Treatment Plant [13] among others. These variables utilize the information directly to systematically recognize the normal operation behavior of the process. Different applications has been proposed in the literature according to this principle. In [4] a strategy to isolate sensors that are affected by nonconforming operation is described. It allows to distinguish between failed sensors and process upsets. In [14] MSPC is combined with wavelet properties, in this way was created adaptive multiscale MPCA in order to detect abnormal behaviors and to identify the major sources of process disturbances.

In this work a combination between MSPC

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and a classification tool is proposed. The combination of both methods improves the results obtained using only MSPC. The paper describes the operation of the SBR process in section 2. Then, section 3 is focused on those MSPC extensions for process monitoring. Section 4, the classification method is presented. And finally in section 5 and subsequent a example is presented and evaluated using data acquired from the real plant.

2 Biological batch process

A Waste-water treatment pilot plant has been used in this work. The plant operates as a Batch Reactor (SBR) as Figure 2 depicts. In a SBR waste-water treatment plant nitrogen removal and elimination of organic matter is done with sludge. Sludge is responsible for the organic matter degradation and nitrogen removal. SBR Pilot plant is composed of a metal square reactor with a capacity of 200 of water to process. Waste-water is taken directly from a real station sited in Girona (Spain). Next, waste-water is pumped to the reactor where the treatment is performed.

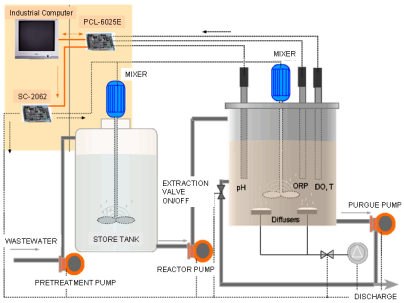

Figure 2: Real SBR pilot plant

In SBR pilot plant the nitrogen and organic matter are removed after a 8 hours cycle in which anoxic and aerobic stages are alternated. In an aerobic stage the ammonia is converted to nitrate and under anoxic condition nitrate is converted to nitrogen gas. Four process variables are monitored: pH, Oxidation Potential Reduction (ORP), Oxygen Dissolved (OD) and Temperature. The process is highly nonlinear, time-varying and subject to significant disturbances such as atmospheric changes, variation in the composition of influent. The process has been characterized statistically by its covariance matrix in order to study the correlation structure between variables and streams of them.

3 MSPC for batch processes

MSPC is a reduction technique based on classical statistical process control (SPC) theory extend to operate with multiple variables. Nowadys, it has also been adapted to characterise batch processes by considering as an additional dimension the number of batches (execution of a process according to a recipe) assuming the same length (same number of samples). The bases of MSPC for batch processes are the extensions of principal component analysis (PCA) and partial least squares (PLS) [21][13][20][12]. Extensions of principal component analysis are described in the next section.

3.1 Multiway principal component analysis (MPCA)

Consider a typical batch run in which j=1,2,...,J variables are measured at k=1,2,...,K time instants throughout the batch. Similar data will exist on a number of such batch runs i=1,2,...,I. All the data has been summarized in the $\underline{\mathbf{X}}$ (I x J x K) array illustrated in figure 3, where different batches are organized along the vertical side, the measurement variables along the horizontal side, and their time evolution occupant the third dimension. Each horizontal slice through this array is a (J x K) data matrix representing the time histories or trajectories for all variables of a single batch (i). Each vertical slice is an (I x J) matrix representing the values of all the variables for all batches at a common time interval (k) [20] [34].

MPCA is equivalent to performing ordinary PCA on a large two-dimensional $(2-D)$ ma-

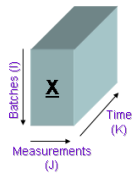

Figure 3: Arrangement of a three-way array $\underline{\mathbf{X}}$

trix constructed by unfolding the three-way. In this work the unfolding **IxKJ** is used [20] (See figure 4). This unfolding is particularly meaningful because, by subtracting the mean of each column of this matrix **X**, these procedures are subtracting the mean trajectory of each variable, thereby removing the main nonlinear and dynamic components in the data. A PCA performed on these mean-corrected data is therefore a study of the variation in the time trajectories of all the variables in all batches about their mean trajectories [19].

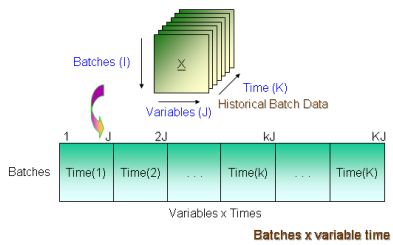

Figure 4: Decomposition of $\underline{X}$ to 2-D (I x KJ)

The objective of MPCA is to decompose the three-way $\underline{\mathbf{X}}$, into a large two-dimensional matrix **X**. This decomposition is accomplished in accordance with the principal of PCA and separates the data in an optimal way into two parts: The noise or residual part ($\underline{E}$), which is as small as possible in a least squares sense, and the systematic part ($\sum_{r=1}^{R} t_r \bigotimes P_r$), which expresses it as one fraction (t) related only to batches and a second fraction (P) related to variables and their time variation [20]. The MPCA algorithm derives directly from the NIPALS algorithm , resulting the matrix X. It is the product of score vector tr and loading matrices Pr, plus a residual matrix E, that is minimized in a least-squares sense:

$$\underline{\mathbf{X}} = \sum_{r=1}^{R} t_r \bigotimes P_r \tag{1}$$

$$X = \sum_{r=1}^{R} t_r P_r^T + E = \hat{X} + E \tag{2}$$

MPCA decomposes the three-way $\underline{\mathbf{X}}$ array where $\bigotimes$ denotes the Kronecker product ($\underline{\mathbf{X}} = t \bigotimes P$ is $\underline{\mathbf{X}}(i,j,k) = t(i)P(j,k)$) and R denotes the number of principal components retained. The equation (1) is the 3-D decomposition while the equation (2) displays the more common 2-D decomposition [32].

3.2 Multiblock multiway principal component analysis (MMPCA)

In this case the data matrix $X(IxKJ)$ is divided into K blocks $(X_1, X_2, ..., X_K)$ in such a way that the variables from each time instant can be blocked in the same block (see figure 5) [13][32]. This approach has significant benefits because the latent variable structure is allowed to change at each phase in the batch processes. In the lower layer of the model, each data block is considered as a separate source of information and the details of the blocks are modelled by corresponding block model. In the upper layer, information from all blocks on the lower data level is combined and the relative importance of the different blocks, $X_{b.}$, for each dimension is obtained. In the upper layer information from the previous block, block scores $t_{b(k-1)}$, is combined with the block score vector from the lower layer [38][37].

3.3 Control charts

Abnormal behavior of batch can be identified by projecting the batch onto the model. Control charts that are used in monitoring batch processes are generally based on the the

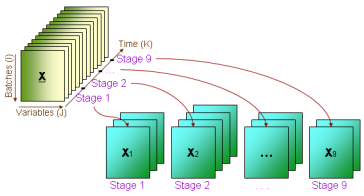

Figure 5: Dividing batch data into different phases

Q-statistic and D-statistic, in which control limits are used to determine whether the process is in control or not. The assumption behind these approximate confidence limits is that underlying process exhibits a multivariate normal distribution with a population mean of zero. This is to be expected, because any linear combination of random variables, according to the central limit theorem, should follow a normal distribution.

The Q-statistic is a measure of the lack of fit with the established model. For batch number i, Q_i is calculated as:

$$Q_i = \sum_{j=1}^{J} \sum_{k=1}^{K} (e_{jk})^2 \sim g x^2_{(h)} \qquad (3)$$

where e_{jk} are the elements of E. Q_i indicates the distance between the actual values of the batch and the projected values onto the reduced space.

The D-statistic or Hotelling T^2 statistic, measures the degree to which data fit the calibration model:

$$D_i = t_i^T S^{-1} t_i \sim \frac{I(I-R)}{R(I^2-1)} F_{R,I-R} \qquad (4)$$

where S is the estimated covariance matrix of the scores. The D-statistic gives a measure of the Mahalanobis distance in the reduced space between of batch and the origin that designates the point with average batch process behavior.

4 Classification method

For classification, the Learning Algorithm for Multivariate Data Analysis (LAMDA) has been used [1]. This method takes advantage of hybrid logical connectives to perform a soft bounded classification.

LAMDA is proposed as a classification technique to apply to principal components selected for monitoring. The goal is to assess the actual situation according to profiles previously learned [1][18].

Input data is presented to LAMDA as a set of observations or individuals characterized by its descriptors or attributes and recorded as rows. Principal components obtained in the MPCA step are used as input variables to be classified. Once, the descriptors are loaded, every individual is processed individually according to the desired goal [1]:

1. To classify the individuals according to a known and fixed set of classes.

2. To learn and adapt from a previous given set classes which can be modified according to the new individuals.

3. To discover and learn representative partitions in the training set.

The basic assignment of an individual to a class follows the procedure represented by figure 6. In this, MAD and GAD stand for Marginal (it takes into account only one attribute) and Global Adequacy Degree (obtained from the hybrid logical combination of the previously obtained MADs) respectively, of an individual to a given class. Equations (5) and (eq:GAD)are used to calculate them. This classifying structure resembles that of a single neuron ANN [1].

$$MAD(d_i x_j / \rho_{i/k}) = \rho_{i/k}^{d_i x_j} (1 - \rho_{i/k})^{1 - d_i x_j} \qquad (5)$$

where

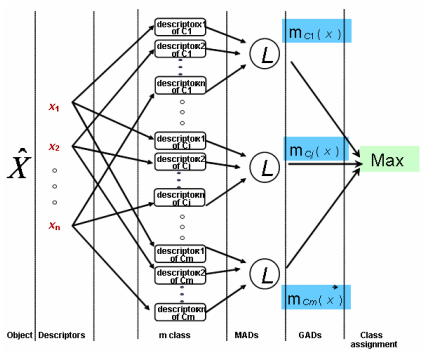

Figure 6: Basic LAMDA recognition methodology

$d_i x_j$ = Descriptor i of the object j $\rho_{i/k}$ =ρ of descriptor i and class k

$$GAD = \beta T(MAD) + (1-\beta)S(MAD) \quad (6)$$

Formalizing the description of LAMDA, it is possible to define an individual as a series of descriptors values d_1, ...,d_n such that each d_j takes values from the either finite or infinite set D_j. We will call universe or context to the Cartesian product $U = D_1$ x D_2 ... x D_j. Thus, any object or individual is represented as a vector $x = (x_1,..., x_n)$ from U, such that each component x_j expresses the value for the descriptor d_j in the object x. The subset of U gathering all these vectors will be called data base or population. To assign individuals to classes MAD step will be calculated for each individual, every class and each descriptor, and these partial results will be aggregated in order to get the GAD of an individual to a class. The simplest way to build this system would be by using probability distributions functions, and aggregating them by the simple product, but that would force us to impose a series of hypothesis on the data distribution and independence which are too arbitrary. Finally, MAD and GAD have been used according to definitions of equation 5 and equation 6 respectively [1]. The hybrid connective used for GAD is a combination between a t-norm and a t-conorm by means of the β parameter. $\beta = 0$ represents the intersection and $\beta = 1$ means the union. This parameter will -inversely- determine the exigency level of the classification, so it can be identified as a tolerance or exigency parameter.

5 Results

5.1 Types of batch process

The data obtained from the SBR process was analyzed under two points of view. The first one, based on analytical methods proposed in [24] where the sludge reaction is explained. The second one, was a preliminary MSPC analysis where some batches are detected to be outside the control limit. This study created five types of batches, or executions : Electrical fault, variation composition, atmospheric changes, equipment misbehaviour and normal behavior. According to this classification it is possible to quantify the number of batches for each group. Table 1 resumes this information. There are 60 (equivalent to 33.5%) batches with abnormal behavior, which are divided into electrical faults, variation in the composition, equipment defects and atmospheric changes (basically rainy days). The normal behavior was the most common type (66.5%) with a higher nitrogen efficiency than legally required effluent standards, which are classified according to the final quality of the wastewater.

Type of batch process	Quantity	%
Atmospheric changes	17	9.50
Equipment defects	8	4.47
Variations in the composition	33	18.44
Electrical Fault	2	1.12
Normal behavior	119	66.48

Table 1: Batch classification by group.

5.1.1 MPCA: Batch direction

Each batch lasts 8 hours (5760 samples for each variable sampled every 5 seconds). Only

392 samples from each one of the four acquired variables have been used in order to reduce computational cost resulting a $IxKxJ =$ 179x4x392 array, ($\underline{\mathbf{X}}$) for the collection of 179 available batches. MPCA algorithm was applied to the three-way data array, $\underline{\mathbf{X}}$ unfolded in the batch direction (I x KJ) resulting 8 principal component. So, the new dimensionality becomes (179 x 8). The statistical model was created with eight components, which explain 92.79% of the total variability. To examine the process data in the reduced projection spaces (defined by a small number of latent variables), the variables contribution analysis are made; as is shown in Figure 7 the temperature variable is positively correlated with loadings 1 where can be appreciate that in sample 1153 had a increase of the temperature. From the Figure 8 represents loadings 2 where Load2 represents at ORP variable.

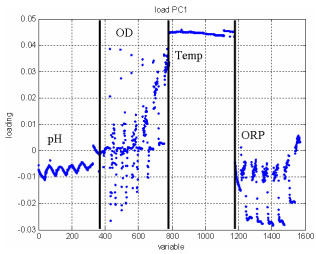

Figure 7: Variable loadings for the principal component

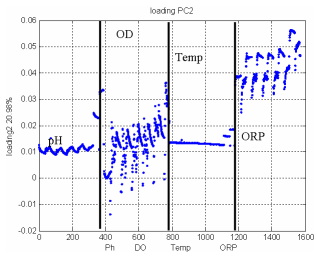

Figure 8: Variable loadings for the second component

Figure 9 shows the Q and T^2 charts for all process batches. In the Q chart, it can be seen that some batches exceed its limits. These batches have several behaviors. In T^2, two batches are outside. These batches had electrical fault (EF).

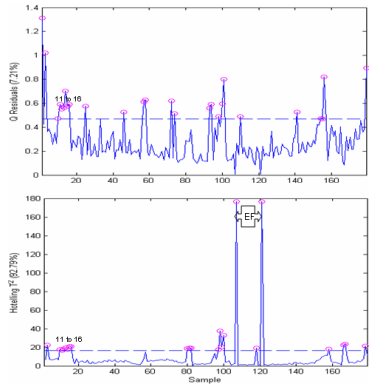

Figure 9: Multiway PCA. Q and T^2 charts with 92.79% confidence limits

In Table 2 the batches outside the model are summarised. In the Q chart, only a third of the total the abnormal behavior is detected, furthermore there are 8 false alarms. The T^2 chart has 20 batches with abnormal behavior (without false alarm), distributed as follows: 4 are atmospheric changes, 6 are equipment defects, 8 are variation of the composition and 2 are electrical faults. 39 about 60 of the abnormal behavior can be detected, 9 batches are in both charts.

Type of batch process	Q		T	
	Quantity	%	Quantity	%
Atmospheric changes	9	5.03	4	2.23
Equipment defects	0	0.00	6	3.35
Variations in the composition	11	6.15	8	4.47
Electrical Fault	0	0.00	2	1.12
Normal behavior	8	4.47	0	0.00

Table 2: MPCA classification.

5.1.2 Multiblock MPCA

The SBR pilot plant consists of 6 stages in which the latent variable structure can change

due to different environments. Applying Multiway MPCA, the data matrix $\underline{\mathbf{X}}$ can be break. In this way, it is possible to work with the total three-way data array, $\underline{\mathbf{X}}$, with dimensions 179 x 4 x 5760. Data array for each stage are: cycle 1 (179 x 4 x 780);cycle 2 (179 x 4 x 780);cycle 3 (179 x 4 x 780);4 (179 x 4 x 780);cycle 5 (179 x 4 x 780);cycle 6 (179 x 4 x 804);purge cycle (179 x 4 x 36);settling cycle (179 x 4 x 720);draw cycle (179 x 4 x 300). Using the control charts by each stage, it is possible to observe the following: Batches 11 to 17 have variation in the composition and these batches are identified by the Q and T^2 control charts. The alarms by each stage are summarized in Table 3 (common batches are discounted). Purge, settling and draw are stages without nitrogen removal, they have more false alarms than other stages.

	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6	Purge	Settling	Draw
outside	26	31	34	26	28	21	16	20	35
false alarm	8	3	5	3	4	1	5	8	23

Table 3: Alarms by each stage

These Multiblock charts supply knowledge about stages which potentially help to fault location and diagnosis. Moreover, the data interpretation is easier. Some types of batch process with large duration fault have been found to be present in the 6 stages models, for example the batches 10 to 16.

5.2 Classification for situation assessment

Initially, MPLS was used for classification purposes. This technique is a dimensionality reduction that maximises the relation between the matrix X (I x JK) and the predicted matrix Y [30] (179 x 5) where 179 is the number of historical data batches and 5 are the types of batch process. The model made did not describe the process because matrix Y was created with the results obtained of the preliminary MSPC analysis. Matrix Y should be constructed with quality variables which are obtained each three days, finding now the missing problem. Thus, a classification tool for situation assessment was used: MPCA + classification tool.

5.3 MPCA classification

$\hat{X}$ is the principal components by each batch with dimensions 8 x 179. These were sued as descriptors to feed into LAMDA algorithm to discover relevant classes under an unsupervised schema. The tool automatically classified the data in eleven classes (11). Table 4 compares the classes and the types of batch process. According to these results, it was possible to identify classes that only contain batches with equipment defects, electrical faults, atmospheric changes and variation in the composition. The classes 1,9 and 10 correspond to normal behavior. The group 6 is associated to atmospheric changes. Classes 3 and 11 represent variations in the composition while classes 7 and 8 include electrical fault. Finally, the classes 2, 4 and 5 groups different types of batchs. The predominant class (class 1) represents the 48.04% of the total historical data, this class represents the normal behavior. The class 5 is abnormal behavior due to atmospheric changes and equipment defects.

	Class 1	Class 2	Class 3	Class 4	Class 5	Class 6	Class 7	Class 8	Class 9	Class 10	Class 11
normal	79	17	0	8	0	0	0	0	17	4	0
atmospheric changes	2	1	0	10	3	1	0	0	0	0	0
equipment defects	1	3	0	0	2	0	0	0	0	0	2
variation composition	4	11	7	1	0	0	0	0	3	1	0
Electrical Fault	0	0	0	0	0	0	1	1	0	0	0
total	86	32	7	19	5	1	1	1	20	5	2

Table 4: Composition by class

The relationship between the class and principal components is another observation. The 8th component is less predominant because it does not change. It indicates that $\hat{X}$ can be computed using only seven descriptors. Then, the total variability will be 90.54%. Consequently, only 7 principal components are used in the analysis Multiblock MPCA.

5.4 MMPCA classification

According to previous analysis, there are seven principal components (seven descriptors for each stage). Classification tool is used individually at every stage taking the whole set of batches. It resulted that at different stages the numbers of classes was very aslo different. Likewise to MPCA classification, the classes

were marked (Table 5). Table 6 summarises the error for this classification. Other observation: electrical Fault is present in cycles 2 and 6 because one batch experimented a sags in two cycles (Remember Table 1). Types of normal behavior are the classes more populated.

	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6	Stage 7	Stage 8	Stage 9
Electrical Fault		11				7,8			
Variation in the compositio	3,6,7	3,5,19	2,5,6,17, 18	2,6,16,17	2,3,7,17, 18	2,4	2,4,5,6,9, 15,16	2,5,14	2
Equipment defects	9,18	8	8	9	12	12			
Atmospheric changes	15	9,10,14	11,14	11,12,14, 19	10,11,19, 21	6	11	7,8,11,18, 19	8
Normal behaviour	1,2,4,5,8, 10,11,13, 14,17,21, 22, 23,24,25	2,4,7,12, 15, 17,18	1,3,4,7,12 13,15,16, 18	1,3,4,5,7,8 , 10,13,18	1,4,5,6,8,9 , 13,15,16	1,3,9,11	1,7,8,10, 13, 14	1,3,4,6,9, 10,12,13, 15,17	1,3,5,6,7,9 10,11,12, 13,15,16, 19
Not classified	2,16,19,20	1,6,13,16	9, 10	15	14, 20	5, 10	3,12	16	4,14,17,18

Table 5: Classes by each cycle

	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6	Stage 7	Stage 8	Stage 9
Quantity not classified	20	28	9	6	9	8	9	6	47
% not classified	11,17%	16,20%	5,03%	3,35%	5,03%	4,47%	5,03%	3,35%	26,26%
Batch wrongly classified	4	8	7	9	8	13	12	10	14
% mistake	2,23%	4,47%	3,91%	5,03%	4,47%	7,26%	6,70%	5,59%	7,82%

Table 6: Classes by each cycle

6 Conclusions and future work

Multivariate Statistical Process Control has been used to detect abnormal behavior in SBR process by projecting the data into a lower dimensional space that accurately characterizes the state of the process. Therefore, the new variable matrix is smaller. The use of a classification tools has been tested with previously known data to verify the utility of it to discover clusters of data in the historical registers useful for further situation assessment. Splitting data into meaningful groups allows a faster localization and identification of faults reporting similar experiences. .

In order to improve the results and to process the data faster, it is necessary to developed a technique that combine the dimensionality reduction and nonlinear classification instead of the classical strategy. The use of a classification tool applied to the new variables allows a simple identification and grouping of similar situations according to a matching criteria.

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