Data-based Latent Variable Methods for Process Analysis, Monitoring and Control

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Abstract

This paper gives an overview of methods for utilizing large process data matrices. These data matrices are almost always of less than full statistical rank, and therefore latent variable methods are shown to be well suited to obtaining useful subspace models from them for treating a variety of important industrial problems. An overview of the important concepts behind latent variable models is presented and the methods are illustrated with industrial examples in the following areas: (i) the analysis of historical databases and trouble-shooting process problems; (ii) process monitoring and FDI; (iii) extraction of information from novel multivariate sensors; (iv) process control in reduced dimensional subspaces. In each of these problems latent variable models provide the framework on which solutions are based.

Keywords: Latent variables, PCA, PLS, subspace models, monitoring, control, digital imaging, machine vision

1. Introduction

Process data sets are often very large, and are not causal in nature (i.e. models built from them cannot be used to infer the causal effects of any variable on any other). The correlation among the measured variables is usually of such a high degree that the resulting data matrices are typically of very low statistical rank. Furthermore, in most process databases, there are usually large amounts of missing data and the signal to noise ratio is often quite low in any one variable. The objective of this paper is to present an overview of the important concepts behind multivariate latent variable models that are useful for treating such data and to illustrate the use of these reduced dimensional models for several classes of problems.

2. Latent Variable Models

Consider a dataset $\mathbf{x} = [x_1, x_2, ..., x_k]$ where k variables are measured. The concept behind a latent variable model for the data is that the process under observation is actually driven by a set of $a \ll k$ latent variables. This latent variable space can be represented by an orthogonal set of vectors $\mathbf{t} = [t_1, t_2, \ldots, t_a]$. Given data from two spaces

X ($n \times k$) and **Y** ($n \times m$) a latent variable multivariate regression (LVMR) model can be defined as follows:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \tag{4}$$

$$\mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{F} \tag{5}$$

where **E** and **F** are assumed to random error and the (nxa) matrix of latent variables **T** is modeled as linear combinations of the x's:

$$\mathbf{T} = \mathbf{X}\mathbf{W} \tag{6}$$

The latent variable space generated by the a columns of **T** is usually of much smaller dimension than **X** (and possibly **Y)**.

In the LVMR model, there is no intrinsic difference between the **X** and **Y** spaces. The LV model (4) and (5) is symmetric in **X** and **Y**, They are both functions of the latent variables, they are both measured with error, and there is no assumption of a causality direction. The division of the data into **X** and **Y** matrices is arbitrary, and arises mainly from the intended use of the model rather than in the features of the data modeled. The model can always be rearranged to express the prediction of **Y** in terms of **X** as:

$$\hat{\mathbf{Y}} = \mathbf{T}\mathbf{Q}^T = \mathbf{X}\mathbf{W}\mathbf{Q}^T = \mathbf{X}\hat{\mathbf{B}} \tag{7}$$

However, it is important to remember that equation (7) is not the model, rather just a rearrangement of the prediction equation for **Y**. A more complete discussion of the concept and importance of LVMR models is given in Burnham et. Al. (1999).

There are many nonlinear versions of latent variable models. The simplest just use transformations of the x and y's or simply expand the **X** matrix with quadratic or other nonlinear functions of the x variables. Dynamic ARX models are easily obtained by simply including lagged values of past x and y variables in the **X** matrix (e.g. MacGregor et al. 1991). Other nonlinear approaches (e.g. Wold et. al. 1989) use linear LV models for the **X** and **Y** spaces, but relate the latent variables of the two spaces by nonlinear models.

3. Estimation of LV Models

Different methods can be used to estimate score matrix (**T**) and loading matrices (**P**, **W**, **Q**) in the latent variable model. These include Principal Component Analysis (PCA) for a single data matrix **X**, and Principal Component regression (PCR), Partial Least Squares (PLS), Canonical Correlation Analysis (CCA), and Reduced Rank Regression (RRR) for the case of both **X** and **Y** matrices. Although all of the above estimation methods provide a set of orthogonal latent variables, they do so by optimizing quite different objective functions (Burnham et al., 1996), and these differences play a vital role in the appropriateness of the methods for use in various problems. In particular, PLS and PCA are the only latent variable models that provide a good model for the **X**-space, since this is part of their objective function. This is an extremely important point since, for many problems, the model for the **X**-space will be the most important part of the LV model (equations (3)-(6)). This may seem strange to the statistical and identification communities because they are used to working only with datasets in which the **X**-space is full rank, by virtue of the way in which the data were collected (e.g. using designed experiments). In such situations, a model for the **X**-space is unnecessary since it is fully explained by the **X**-data directly. However, with the large data sets that we are dealing with in this paper, that arise from routine operation of the plant, the **X**-space typically has a statistical rank a << Min (n, k), and any models built from such data are only valid in this reduced dimensional space of the latent variables, and even then only in the restricted region of this space spanned by the training data. The **X**-space model is essential for defining this valid model space, for treating missing data, for detecting outliers, and for monitoring processes. It is this modeling of the reduced dimensional spaces of both **X** and **Y** that make the latent variable methods of PLS and PCR so different from standard regression approaches such as multiple linear regression (MLR), neural networks (NN), etc., and makes them much more powerful for treating the problems being addressed here.

The number of principal components ($a << \min(n, k)$) required to adequately model the covariance structure of **X** is often decided by a cross-validation procedure [Wold, 1978] which yields statistical tests for their significance based on a prediction criterion.

4. Analysis of Process Databases

Perhaps the main area of industrial application for these LV models has been, and continues to be, the analysis of historical databases collected routinely by process computers. There are two common ways in which industrial engineers currently use these LV methods to analyze such data. The first is where nobody has every looked seriously at the historical data to see if things can be learned that might lead to process improvements. This retrospective analysis is often performed over several very different time scales. A second usage is for short term trouble-shooting. Immediately after a process upset, a local LV model can be built over the recent period leading up to and covering the upset, and the local model used to analyze for possible causes.

The tools for analysis consist of looking at score plots of the latent variables (e.g. t_1 vs. t_2) to study how the process has moved in the reduced dimensional space, and at the corresponding loading plots (p_1 vs. p_2) to interpret the groups of variables that are related to movements in certain directions. The squared prediction error (SPE) in the X and Y spaces are used to detect abnormal situations

$$\text{SPE}_i = \sum_{j=1}^{K} (x_{ij} - \hat{x}_{ij})^2 \tag{8}$$

where the predicted values are given by

$$\hat{\mathbf{X}} = \mathbf{T}\mathbf{P}^T \tag{9}$$

Contribution plots are particularly useful for highlighting which group of variables is highly related to a movement in the score space or the residual space [MacGregor et al., 1996; Kourti and MacGregor, 1996; Miller et al., 1998].

The contribution of variable x_j to the residual SPE_i is

$$\text{Contribution } (x_j) \text{ } to \text{ SPE}_i = x_{ij} - \hat{x}_{ij} \tag{10}$$

and the contribution of x_j to a movement in any latent variable Δt_l over any period is

$$\text{Contribution } (x_j) \text{ } to \text{ } \Delta t_l = \Delta x_j p_{jl} \tag{11}$$

where p_{jl} is the loading of the variable x_j in the loading vector p_l of the LV, and Δx_j is the change in x_j over that period. These contribution plots do not show causal relationships. They only reveal which group of variables, in which part of the plant, are related to the movement or event that occurred. However, by narrowing down the possible variables and location in the plant it is usually much easier for the engineer or operator to diagnose some possible reasons for the event.

There are numerous applications of this use of LV models to analyze industrial databases in both continuous processes [e.g. Yacoub & MacGregor, 2002] and batch processes [Nomikos, 1996; Garcia et al. 2003]. In this section, an industrial batch process will be used to illustrate the basic concepts. Typically data from batch processes are of the form illustrated in Fig. 2. For each batch one has data on initial conditions, prior processing history, etc. (**Z** matrix), histories on the time varying trajectories of process variables during each batch (**X̲** array), and data on the final product quality and productivity (**Y** matrix). Although the **Z**-matrix is important in this problem we ignore it here and illustrate the analysis using only **X̲** and **Y** data. The three dimensional **X̲** array can be unfolded to give an **X** matrix with each row containing the time histories of all the variables for a given batch.

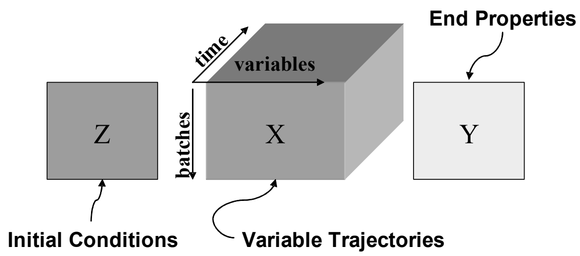

Figure 2: *Nature of batch data*

Although there are over 350,000 observations in this data set, a PLS model (using scaled and mean centered data) explains the statistically significant information with only a=2 latent variables. In other words, for each batch, the changing co-variation among all the variables, over the entire time history of the batch can be summarized by the score values of two latent variables (t_1, t_2). A score plot of these two LV's is shown in Fig. 3. It reveals a clear separation in the t_1 direction between batches with good **Y** results (high t_1 values – indicated by the region of the dark ellipse) and those with poor Y results (low t_1 values). A plot of the p_1 loading vector shown in Fig. 4 can be used to help interpret why these two groups of batches are different. For each process variable there are 350 loading values corresponding to the 350 time intervals during the batch. From this plot it is clear that good performance (a high value of t_1) is associated with trajectories of variables x_1 and x_3 lying above their mean trajectories throughout the last two thirds of the batch and with the trajectory of variable x_4 lying below its mean over the same period. Such information together with a more complete analysis of the (Z, X, Y) data provided great insights into improving the batch operation.

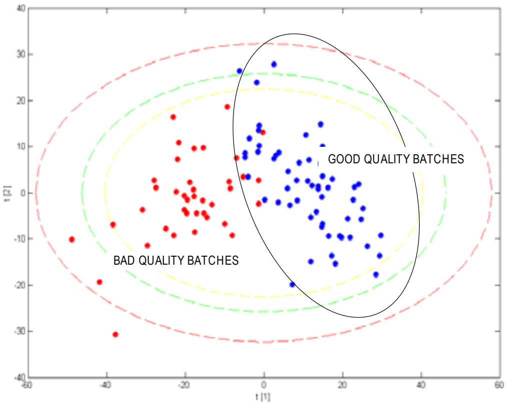

Figure 3: *Score plot for all the batches (good batches in solid elliptical region)*

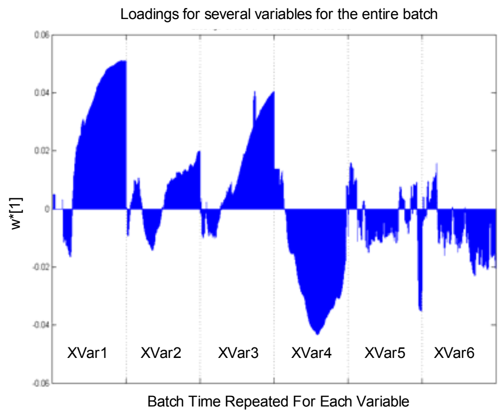

Figure 4: *Plot of the elements of the first loading vector p_1 consisting of a loading value for each variable at each time period over the time history of the batch*

5. Process Monitoring and FDI

Once the analysis of the historical process data is complete and improvements made to the process, one is interested in monitoring the process to ensure that any gains are maintained, and that any new problems are detected and identified as early as possible. The scope of process monitoring is wider than detecting simple hardware and sensor faults. Its purpose is to detect any type of complex atypical behavior such as might be associated with the effects of changes in impurities, surface chemistry, etc. on the performance of the process.

There is a large literature on FDI methods such as those based on analytical redundancy [Gertler, 1998] that involve the use of causal models from theory or identification experiments. However, multivariate statistical approaches based on LV models use non-causal models built from normal operating data. They are multivariate extensions of statistical process control (SPC) methods. They compare the behaviour of future operation of the plant against a LV model built from past behaviour where only "common cause variation" was present (i.e. from data collected where the performance was acceptable) [Kresta et.al., 1991; MacGregor and Kourti, 1995]. Any abnormal behaviour can be detected in the residual SPE plot or in the score plots or their Hotelling's T^2 equivalent

$$T^2 = \sum_{l=1}^{a} t_l^2 / s_l^2 \tag{13}$$

where s_l^2 is the variance of t_l from the training data. Control limits on these plots [MacGregor and Kourti, 1996; Nomikos and MacGregor, 1995] can be obtained using the F-distribution or using the empirical reference distribution of the training data. An abnormal situation is detected when any of the control limits on these charts is violated, and then contribution plots can be used to identify that group of variables associated with the fault.

To illustrate the concepts of the MSPC approach we again use the batch fermentation process of the last section. To develop a PLS model for monitoring, we now only use the cluster of batch data with good performance shown in Fig. 3. Control charts for the SPE and Hotelling's T^2 statistics for a new (bad) batch are shown in Fig. 5. An abnormal event is clearly detected by time 277 when the 99% control limit on both the T^2 and SPE charts are violated. The SPE contribution plot for the process variables at that time period is also given. High values of variables x_6 are clearly related to the fault.

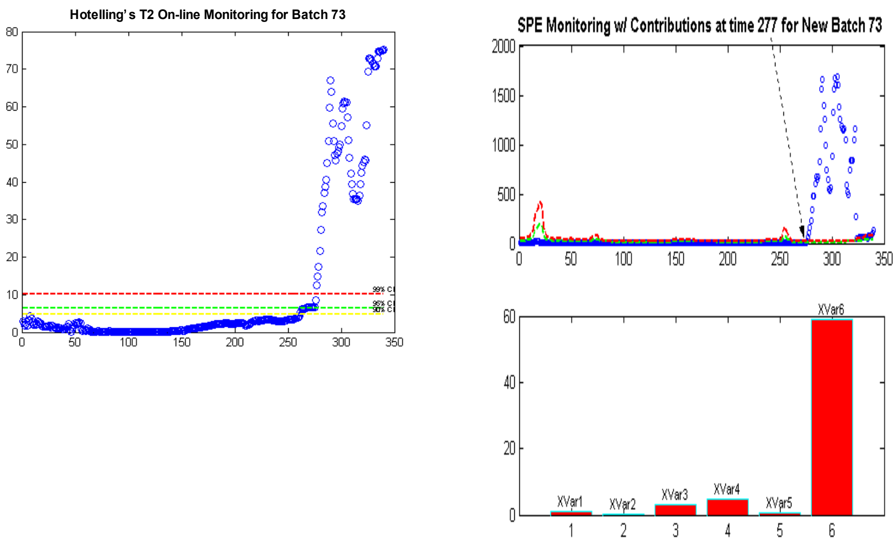

Figure 5: Batch # 73: Left: *Hotelling's T2 plot with control limits shown*
Right: SPE plot and contribution plot at time 277 where fault is first detected

6. Extracting Information From Multivariate Sensors

There is currently a major revolution occurring in new sensor technologies that will have major impacts on process control. In the chemical industry a whole new generation of sensors referred to as micro-sensors or molecular sensors are being developed by process analytical chemists. These sensors generate large amounts of data with information on the detailed molecular properties of the streams or products being sampled, and they do so at a greatly reduced cost per sample over traditional laboratory analysis. In the solids processing industries the lack of on-line sensors has greatly limited the ability to implement control systems, but digital imaging systems, based on the availability of inexpensive cameras and computers, are starting to have an impact.

As an illustration consider two applications of on-line digital colour imaging; the first involves the monitoring of a combustion process through imaging of the turbulent flame in a boiler system; the second involves the monitoring and feedback control of product quality in the snack food industry.

The monitoring of the off-gas pollutants (NO_x, SO_2, etc.) from combustion processes in boiler systems is an important environmental problem. Inferential models based on neural networks are well established for predicting these off-gas pollutants using process measurements taken around the boiler system. In this example we consider the use of colour (RGB) digital images of the turbulent flame in the boiler as a predictor variable [Yu and MacGregor, 2003a,c]. Figure 6 shows two flame images taken one second apart during a time when no changes were occurring. The difficulty in extracting information from these highly time varying flame images is obvious. However, by performing a PCA on these images and projecting them into the LV score space, the score plots of successive images are very stable at any given operating condition, but they do change significantly as the process conditions and waste fuel feeds change. Using masking methods, features can be extracted from the PCA score plots that summarize the changes in the flame [Yu and MacGregor, 2003a,c], and these can be used as predictors in a PLS model for the NO_x and SO_2 off-gas concentrations. The predicted versus observed plot for NO_x from a feasibility study is shown in Fig. 7. The predictions obtained from the flame data alone were as good as using both the flame and the process data and much better than just using the latter. Prediction of other important process and environmental variables was equally good.

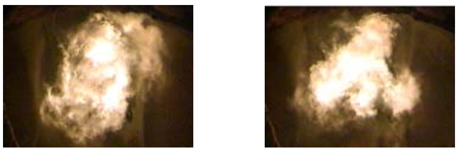

Figure 6: *Flame images taken 1 second apart in an industrial boiler*

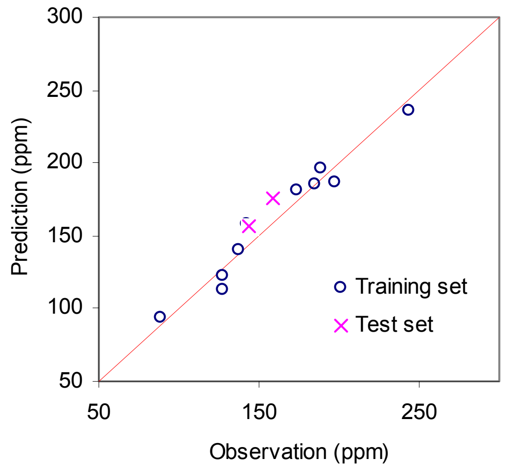

Figure 7: *Predicted* vs. *observed* NO_x *concentration in the off-gas. Prediction done using only RGB flame images*

The monitoring and feedback control of product quality in snack food production has been presented by Yu et al. (2003b,c). A schematic of the system showing the imaging of the randomly deposited chips on a moving belt is shown in Fig. 8. Multi-way PLA and PLS methods are used to extract information from the images that is related to both the concentration of coating materials on the base product and to the distribution of the coatings over the product. This image information is then used for the on-line feedforward/feedback control of the process. Feedback control of the coating concentration based on the imaging systems is currently in use on several industrial lines. Table 1 compares the results of the image-based control on one of the lines against the results from the previous operator-based control system.

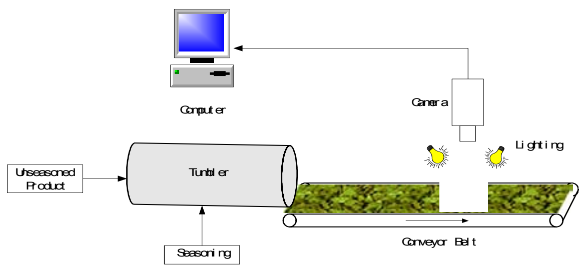

Figure 8: *Imaging system for feedback control of snack food quality*

Table 1: Mean Absolute Error (MAE) for the three cases

	Prior control	Image-based feedback control (regulation)	Image-based feedback control (set point tracking)
MAE	0.8523	0.4481	0.4769

7. Process Control In Reduced Dimensional LV Spaces

Latent variable methods are also useful in process control situations, particularly where the controlled (CV) and manipulated (MV) variable spaces are high dimensional, but of less than full rank. The simplest situation, where the CV space is high dimensional, but of low rank, include problems such as the cross-directional control of properties on paper machines or polymer films [Rigopoulos et. al., 1997], control of polymer molecular weight distributions [Clarke-Pringle and MacGregor, 1998] and particle size distributions [Flores-Cerrillo and MacGregor, 2003a], and control of polymer end properties in continuous reactors [Roffel et al., 1989]. In these cases some variation of PCA has usually been employed on the collected data to reduce the dimension of the CV space to a full rank space (e.g. use the latent variables of PCA, or a subset of the real variables which best define the PCA space, as new CV's), and the MV's are used to control this space.

A more complex situation occurs where the MV space is also of less than full rank. This situation will arise when there are operational constraints preventing all the MVs from acting independently. A classic example occurs in the control of batch reactors where the control at any time (θ_i) during the batch calls for the adjustment of the trajectories of all the MV's over the entire remainder of the batch (for example see the trajectories in Fig. 3). The MV vector therefore consists of an extremely high dimensional vector, but this vector of MV trajectories must respect many operational constraints both with respect to the shape of the trajectories over time, and with respect to the covariance among the MV's at all time points (e.g. see Fig. 9).

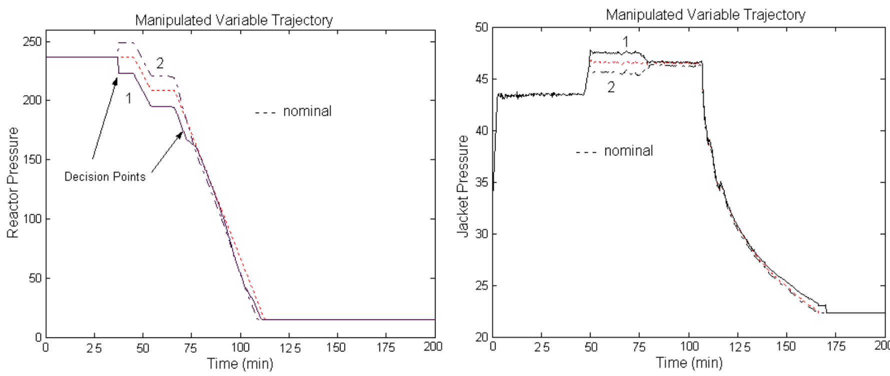

Figure 9: *Control of polymer quality using LV models to adjust the MV trajectories at two decision times*

This problem can easily be formulated and solved in the latent variable space of PLS models. An example from Flores-Cerrillo and MacGregor [2003b] on the control of product quality in batch nylon polymerization reactors is used here to illustrate the approach. A PLS model is built using historical batch data and a few designed experiments in the MV's at the decision points θ_i. This model allows for prediction of the vector of final product quality variables $(\hat{\mathbf{y}})$ using the measured trajectories on all the process and manipulated variables (e.g. Fig. 9) up to any decision time (θ_i) during the batch run. The missing data imputation feature of PLS models is used to impute the as yet unknown process variables for the uncompleted portion of the batch. A control action is then computed in the LV space (t_1, t_2, t_3) of the PLS model that will optimize the quadratic objective

$$\min_{\Delta \mathbf{t}(\theta_i)} [(\hat{\mathbf{y}}(\theta_i) - \mathbf{y}_{sp})\ R_1 (\hat{\mathbf{y}}(\theta_i) - \mathbf{y}_{sp})^T + \Delta\mathbf{t}\ R_2 \Delta\mathbf{t}^T]$$

where $\mathbf{y}$ is a (1xm) vector and $\mathbf{t}$ a (1xa) vector. The optimization is subject to the constraint that the new computed score values for the batch ($t_l = t_l(\theta_i) + \Delta t_l$; $l = 1, 2, \ldots, a$) fall within the range of historical values given by

$$T^2 = \sum_{l=1}^{a} \frac{(t_l + \Delta t_l)}{s_l^2} < \varepsilon$$

and

$$\mathbf{y}(\theta_i) = (\mathbf{t}(\theta_i) + \Delta\mathbf{t})\mathbf{Q}^T$$

Once the new score values have been computed from the control algorithm, the adjustments $\Delta\mathbf{u}$ to the remainder of all the actual MV's can then be computed using the PLS model for the **X**-space [Flores-Cerrillo and MacGregor, 2003b] as $\mathbf{x}_2^\mathbf{T} = (\mathbf{t}^\mathbf{T} - \mathbf{x}_1^\mathbf{T}\mathbf{W}_1)(\mathbf{P}_2^\mathbf{T}\mathbf{W}_2)^{-1}\mathbf{P}_2^T$ where $\mathbf{x}_1^\mathbf{T}$ is the vector of measurements on all process and MV's up to time θ_i and $\mathbf{x}_2^\mathbf{T}$ is the computed values for all process and MV's from time θ_i until the end of the batch. The matrices $\mathbf{W}_1$, $\mathbf{W}_2$ and $\mathbf{P}_2$ are the partitioned parts of **W** and **P** relating to $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively. The plots in Fig. 9 show the resulting trajectories of two MV's resulting from solving the control problem at two decision times (θ_1 = 35 min and θ_2 = 75 min) for the nominal conditions (0) and two disturbances (1 and 2). In both situations the final controlled variables were returned to their target values at the end of the batch.

Although a linear PLS model has been used in the above problem, it is important to note that the resulting controller is a nonlinear time varying one. This results from two factors. First, the batch PLS model is centered about the average or nominal trajectories of all variables and hence is modeling only variations about these (nonlinear) trajectories. Secondly, the PLS model captures the time varying covariance structure among the deviations in all the variables as this structure changes throughout the entire course of the batch.

8. Conclusions

An overview of data based methods for the analysis, monitoring and control of processes has been presented. In particular, emphasis has been placed on the use of latent variable models, based on PLS and PCA, to treat situations where the data matrices are less than full statistical rank. In essence all these problems are subspace problems where the analysis, control etc. must be confined to the low dimensional subspaces defined by the latent vectors. Such situations dominate most industrial data base problems.

Several industrial problems are discussed in this paper to illustrate the power of these approaches. These include the problems of analyzing large historical databases and trouble-shooting process problems; process monitoring and FDI; extracting information from multivariate image sensors for process monitoring and control; and control in reduced dimensional subspaces. Many other important problems based on using latent variable models and industrial databases have also been addressed in the literature.

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