The Application of Nonlinear Partial Least Square to Batch Processes

Lipeng Yan* and Barry Lennox**

* School of Electrical and Electronic Eng., The University of Manchester, M13 9PL, UK (lipeng.yan@postgrad.manchester.ac.uk)

** School of Electrical and Electronic Eng., The University of Manchester, M13 9PL, UK (barry.lennox@manchester.ac.uk)

Abstract: Multivariate statistical process control (MSPC) techniques play an important role in industrial batch process monitoring and control. One particularly popular approach to MSPC is partial least squares (PLS), which has been successfully applied many times in the modelling, estimation and control of batch processes. However, the nonlinear nature of many real, complex chemical systems means that traditional linear PLS is not always suitable. In this paper, the use of a nonlinear multi-way PLS is proposed to address the issues of non-linearity in batch processes. By analysing and comparing linear multi-way PLS, Neural network multi-way PLS, Type I and Type II nonlinear multi-way PLS models, the advantages and limitations of these methods are identified and summarised.

Keywords: Partial least square, Nonlinear PLS, Neural network, Modelling, Batch process

1. INTRODUCTION

Batch processes are widely used in industry as they outperform continuous operations in the manufacturing of certain chemicals and materials (Korovessi et al., 2006). In particular, batch processing is frequently used in the manufacture of low volume, high value products, such as pharmaceuticals or specialty chemicals. In batch processing, the materials are processed over a finite period of time, where the operational conditions are typically specified to follow a pre-determined recipe. To ensure safe and efficient operation of these processes and to improve or maintain product quality, it is important that these processes be continuously monitored during operation. However, as a result of disturbances to the process, such as changes in the initial conditions of the batch, and the frequent absence of on-line quality measurements, this can be challenging.

In an attempt to monitor processes such as this, the chemical industry has seen a rapid increase in the number of sensors that have been made commercially available. Unfortunately, because of the large amounts of data available and the highly correlated nature of these measurements, it can be difficult to interpret the data once it has been collected. To help with the interpretation of large quantities of process measurements, many researchers have successfully applied data analysis tools, such as those available within the field of Multivariate Statistical Process Control (MSPC) (Martin et al., 1996). Within MSPC, there are two techniques which have received considerable interest. These are Principal Component Analysis (PCA) and Partial Least Squares (PLS). For the monitoring of batch processes, both techniques have proven to be useful (Piovoso et al., 1996; Lennox et al., 2001). However, when there exist measurements of the output quality from the batch, even if these measurements are only available at the end point of the batch, PLS has been shown to be a highly useful tool for monitoring the process, as it is able to detect features within the data that highlight process changes that may have a direct impact on product quality.

The PLS method was originally developed and applied in the area of econometrics by H. Wold (Wold, 1982). Since then it has been applied in many other industries, including chemical (Martens et al., 1989; Wold et al., 1984). The properties of PLS that have made it so popular in process monitoring can be stated as follows (Ferrer et al., 2008): It is a good alternative to classical multiple linear regression and principal component regression methods as it has been shown to have robustness to limited sized data sets and highly collinear data.; it has relatively low computational requirements; it is efficient in dealing with situations where there are missing measurements.

A major limitation with PLS is that industrial processes are always nonlinear to some extent. This is not always a problem as many processes are only operated around limited operating regions, where linear PLS techniques tend to provide acceptable accuracy. However, batch processes are often operated over relatively large spaces and hence nonlinear extensions to PLS may be required. When PLS is applied to batch processes, a technique referred to as multiway PLS (MPLS) is frequently applied. This technique analyses the behaviour of the process relative to the mean trajectories of the process variables. In doing so, a major nonlinearity in the data is removed. However, there remain situations when this approach is insufficient to track the nonlinear behaviour of the process.

Several nonlinear PLS methods have been proposed and these tend to be divided in to Type I and Type II methods. A detailed overview of these methods is provided by Wold (1989). In Type I methods, the inputs in to the PLS model are specified to be cross and squared terms of the input variables. However, for Type II methods, non-linear functions are implemented in the inner structure of the PLS model. For example, Wold (1989) used quadratic functions of the inner variables. For increased functionality, the use of a neural network was proposed in the inner structure of the model (Qin et al., 1992). This was extended further by Baffi et al (2000), who utilised Radial Basis Functions. Related works in this area included that by Frank, 1990 & Wold, 1992, who used smoothing splines to provide the non-linear function within the model and Hiden et al., 1998, who proposed the use of genetic programming. In this paper, non-linear PLS modelling techniques are integrated within a multi-way model to provide a mechanism to track the nonlinear behaviour of general batch processes.

The paper is organised as follows: section 2 outlines the basic PLS algorithm and discusses several of its extensions, including MPLS, nonlinear PLS and neural network PLS (NNPLS). In section 3 and 4, linear MPLS is applied as a predictive tool to provide long term estimates for both linear and nonlinear systems and its performance compared with that obtained using nonlinear MPLS and multiway NNPLS. The capabilities of the non-linear PLS techniques are further illustrated through their application to a benchmark simulation of a fermentation process. Finally, some concluding remarks are made in section 5.

2. FUNDAMENTALS OF PLS, NONLINEAR PLS AND NNPLS

2.1 Partial Least Squares Regression (PLS)

PLS, also known Projections onto Latent Structures, was proposed by Herman Word (Wold et al., 1984) as a regression tool that could be applied to ill-conditioned data sets. It can be considered to be a more robust alternative to classical multiple linear regression. PLS is a projection method that models the relationship between a response matrix, Y and a predictor matrix, X. These matrices are decomposed as follows:

$$X = \sum_{a=1}^{A} t_a p_a^T + E \tag{1}$$

$$Y = \sum_{a=1}^{A} u_a q_a^T + F \tag{2}$$

These equations can also be expressed as:

$$X = TP^T + E \tag{3}$$

$$Y = UQ^T + F \tag{4}$$

Where X is a data matrix of independent variables, Y is a data matrix of dependent variables, T and U are the score matrices, P and Q are the loading matrices, and E and F are the residual matrices for X and Y. In the PLS model, the original descriptors are transformed to a new variable space based on a small number of orthogonal factors (latent variables). The number of latent variables that are retained in the model, A, is determined by cross-validation.

To enable PLS to track the dynamics of batch processes, multiway PLS has been proposed. MPLS is an extension of PLS that enables it to handle 3-Dimensional data arrays (Nomikos. et al., 1994). Measurement data from a batch process is typically stored as a 3-dimensional matrix (X) of size IxJxK, where I is the number of batches, J is the number of measured observations in a complete batch and K is the number of measured variables. If MSPC is to be applied, 3-Dimensional data must be transformed to a 2-Dimensional matrix. There are different approaches for rearranging the data sets. The most common approach, and the one adopted in this paper is batch-wise unfolding, which unfolds the matrix in accordance to the direction of batches by Nomikos. et al. (1994). PLS is then applied to the unfolded matrix, which has dimension IxJK.

2.2 Nonlinear PLS model

To improve the modelling capabilities of PLS, several nonlinear extensions have been proposed to enable it to better handle nonlinear systems. These methods can be divided into two categories: Type I and Type II Nonlinear PLS methods.

2.2.1 Type I nonlinear PLS

In the Type I Nonlinear PLS method, the observed variables are appended with nonlinear transformations. Following this, traditional linear PLS is then applied. For example, the Xmatrix can be augmented with transformed terms. The addition of transformed terms in X within PLS models was firstly proposed by Wold (1989), where he proposed the use of quadratic terms in the PLS model. Other studies involving this technique have utilised quadratic and higher order polynomial terms, while ignoring cross-terms (Berglund,et al., 1997 & 1999). The capabilities of the technique were illustrated through its application to some nonlinear systems.

2.2.2 Type II nonlinear PLS

In contrast to the Type I nonlinear PLS method, Type II nonlinear PLS method assumes a nonlinear relationship within the latent variable structure of the model. Type II Nonlinear PLS model, was first proposed by Wold et al. (1989) and has been shown to be able to provide an accurate fit to more complex nonlinear relationships than Type I PLS (Hiden et al., 1998).

In this paper, the Type I and II non-linear structures are integrated within MPLS models to enable them to more accurately approximate non-linear batch processes. In the studies described in Section 3, the Type II nonlinear PLS models were constructed using the technique proposed by Baffi et al. (2000). The principle of this algorithm is as follows:

In traditional PLS, the inner relation between t and u is defined as follows, where t and u are score vectors and h denotes residuals:

$$u = bt + h \tag{5}$$

In the algorithm proposed by Baffi et al (2000), the inner relation is replaced by a quadratic polynomial (2nd order):

$$u = c_0 + c_1 t + c_2 t^2 + h \tag{6}$$

A limitation with this approach is that by choosing a second order polynomial, the type of relationship that can be modelled is restrictive. Therefore, in the applications described in Section 3 of this paper, higher order terms are also included. The relationships are provided in equation 7.

$$u = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + h$$

$$u = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + c_5 t^5 + c_6 t^6 + h$$
(7)

2.3 NNPLS

An alternative to using polynomials in the inner relationship of the PLS model is to use a neural network to describe this relationship. In this case, the PLS inner model can be represented as follows: $U_1 = N(t_1) + r_1$

Where $N(\bullet)$ denotes the nonlinear relation represented by a neural network, which is determined by minimizing the residual r_1 (Qin et al., 1992).

The residual matrices are derived as

 $E_{1} = X - t_{1}J_{1}^{T}$ $F_{1} = Y - N(t_{1})G_{1}^{T}$ (8)

J and G are the loading matrices.

The neural network used in the NNPLS method can be trained using the back-propagation algorithm. However, using this method the learning can be slow to converge and in this work the Levenberg-Marquardt method was used instead. The number of hidden layers and hidden units are important factors when designing a neural network. In this work, cross-validation was used to determine the size of the neural networks (Qin et al., 1992).

NNPLS can be expressed as:

$$U_{h}^{test} = E_{h-1}^{test} M_{h}$$

$$t_{h}^{test} = F_{h-1}^{test} G_{h}$$
and
$$E_{h}^{test} = E_{h-1}^{test} - t_{h}^{test} J_{h}^{T}$$

$$F_{h}^{test} = F_{h-1}^{test} - N(t_{h}^{test}) G_{h}^{T}$$
(10)

Where M_h , G_h and J_h have been determined in the NNPLS method. M is weight.

3. SIMULATED STUDIES

3.1 Application of Linear PLS to example systems

To demonstrate its capabilities, linear MPLS was applied to four example systems. These systems were: *system 1*: Linear time invariant; *system 2*: Nonlinear time invariant; *system 3*: Linear time varying; *system 4*: Nonlinear time varying.

The linear time invariant system was defined as:

$$y(t) = 0.3x_1(t) - 0.2x_2(t) + 0.1y(t-1)$$
(11)

The linear time varying system was defined as:

$$y(t) = 0.5t \cdot x_1(t) + 0.7t^{0.6} \cdot x_2(t) + 0.1y(t-1)$$
(12)

The nonlinear time invariant system was defined as:

$$y(t) = 0.9x_1^2(t) - 0.6x_1(t) + 0.2x_2^2(t) - 0.4x_2(t) + 0.1y(t-1) (13)$$

The nonlinear time varying system was defined as:

 $y(t) = 1.2t \cdot x_1^2(t) - 0.8t^{0.3} \cdot x_1(t) + 0.9t^{0.5} \cdot x_2^2(t)$ $-0.7t^{0.6} \cdot x_2(t) + 0.1y(t-1)$ (14)

In each system, x_1 and x_2 were specified to be equal to a PRBS signal with amplitude between -1 and 1, and switching time of 1 sample. The initial value of y was 0. White noise with a standard deviation of 0.3 and 0.4 was added to the measurements of x_1 and x_2 respectively. Each of the systems was considered to operate as a batch. With each batch containing 50 samples. For each system, 200 batches of data were collected for training the models, and 20 batches were collected for testing purposes. Cross validation was used to determine the number of latent variables, which in each case was found to be 25. The accuracy of the models was measured using the sum of square error (SSE) which was calculated over the testing data sets. The results are displayed in Figures 1(a)-(d). In these figures, the dotted line is the predicted value for the output, y, and the solid line is the actual value.



Fig.1. PLS model prediction

Figures 1(a) and 1(b) show that linear MPLS is able to approximate the output of both the linear time invariant and linear time varying systems reasonably well. The SSE for these two systems was 28.5 and 29.7, respectively. However Figures 1(c) and 1(d) show that the MPLS model was not as accurate when used to predict the output of the nonlinear time invariant and nonlinear time varying systems. The SSE in these two cases was 151.4 and 198.2, respectively.

The results show that as might be expected, linear MPLS can predict the linear systems very well. However, this algorithm was not able to track the dynamics contained in the two nonlinear systems. These systems demonstrate that linear MPLS is suitable for modelling linear, time-varying systems. However, problems may be encountered when this algorithm is used to model non-linear systems.

3.2 Nonlinear Multiway PLS model

To illustrate the capabilities of the non-linear extensions to MPLS, these algorithms were applied to the nonlinear systems, defined by Equation 15 to Equation 19.

3.2.1 Application of Type I Nonlinear MPLS to the simulated systems

Before investigating the simulated systems introduced in section 3.1, the limitation of using Type 1 Nonlinear MPLS is

first illustrated through its application to two simple nonlinear systems. These are defined as follows:

System 5:
$$Y_1 = 2.5X^2 + 1.5X + 3$$
 (15)

System 6:
$$Y_2 = 2.5X^3 + 1.5X + 3$$
 (16)

X was specified to be white noise with a mean of 0 and a standard deviation of 1. For each system, 50 batches of data were collected for training the models, and 20 batches were collected for testing purposes. With each batch containing 20 samples. For each system a Type I Nonlinear MPLS model, using second order polynomials only was used to predict the endpoint.

The accuracy of the models over the testing data are shown in Figure 2(a). In this figure, the predicted endpoint value is seen to be very close to the actual endpoint value suggesting high accuracy. However, figure 2(b) shows that in the situation where the order of the non-linearity does not match that of the process, then problems are introduced and the accuracy of the prediction is reduced significantly. In real studies, the exact order of any nonlinear relationship will not be known a-priori and hence the required expansion of x will be difficult to determine. Hence, Type I MPLS is not recommended.



Fig.2. The predicted endpoint of the simple nonlinear system by Type I nonlinear MPLS model

3.2.2 Application of Type II Nonlinear MPLS model to simulated systems

In this section, 4th order Type II Nonlinear MPLS is used to approximate system 6, as defined in section 3.2.1. To provide a comparison, linear MPLS is also applied.



Fig.3. The predicted endpoint of the simple nonlinear system by Type II nonlinear MPLS model

In Figure 3, the red dots are the endpoints predicted by the Type II nonlinear MPLS model and the diamonds are endpoints predicted by linear MPLS. The accuracy of the Type II model is significantly greater than the accuracy of the linear model. In the Type II nonlinear MPLS model, the predicted endpoint value is very close to the real endpoint value. This shows that the Type II Model can be used to predict this simple nonlinear system.

To illustrate the capabilities and limitation of Type II nonlinear MPLS, the ability of this model to approximate three different modifications to system 3 is now presented. The systems used for this test are defined as follows:

4th order nonlinear system:

(15)

$$y(t) = 0.6x_1^{4}(t) + 0.9x_1^{2}(t) - 0.6x_1(t) + 0.2x_2^{2}(t)$$

$$-0.4x_2(t) + 0.1y(t-1)$$
5th order nonlinear system:

$$y(t) = 0.4x_2^{5}(t) + 0.6x_1^{4}(t) + 0.9x_1^{2}(t) - 0.6x_1(t)$$

$$+0.2x_2^{2}(t) - 0.4x_2(t) + 0.1y(t-1)$$
(18)

6th order nonlinear system:

$$y(t) = 0.5x_1^6(t) + 0.4x_2^5(t) + 0.6x_1^4(t) + 0.9x_1^2(t)$$

-0.6x_1(t) + 0.2x_2^2(t) - 0.4x_2(t) + 0.1y(t-1) (19)

Table 1 shows the errors that result when Type II (defined with second, fourth and sixth order polynomials) MPLS models are used to approximate each of these systems. The errors provided are the sum square error over the testing data sets.

Table 1. The List of SSE (when Type II nonlinear MPLS is applied in the nonlinear testing systems)

Type II	Testing system		
nonlinear			
MPLS			
	4th order	5th order	6th order
	nonlinear	nonlinear	nonlinear
	system	system	system
2nd order	577	3.1e+004	2.1e+005
4th order	3.5e-025	4.2e+004	4.0e+004
6th order	3.6e-024	1.7e-021	1.0e-019

The results in Table 1 show that when the system is known, the order of the Type II nonlinear MPLS model can be precisely determined. For example, when the testing system is a 4th order nonlinear system, 4th and 6th order Type II nonlinear MPLS can predict the end-point values very well. However, there are large errors for the 2nd order Type II nonlinear MPLS.

4 CASE STUDIES

To illustrate the capabilities of the non-linear extensions to MPLS, the Type 2 algorithms were applied to a benchmark simulation of a penicillin batch fermentation process. The fermentation process investigated is the Pensim simulator (Birol et al 2002), details for which are provided in Appendix A. There are two primary quality output variables in this process, biomass and penicillin, which are each affected by the primary manipulated variable, substrate feed rate. By analysing the response of this system it can be determined that the relationship between substrate and biomass is linear and time invariant, and for penicillin the relationship is nonlinear and time varying. Because of space constraints, the results for the estimation of biomass are not provided here. However, because this has a linear, time invariant relationship to substrate, this relationship can be approximated with high accuracy using linear MPLS.

In the following data, Pseudo-Random Binary Signals (PRBS) with high/low values of -0.005 and 0.005, were applied to the nominal feedrate of substrate (0.045 l/h) in order to excite process dynamics. The training data consisted of 50 batches, with 20 batches used for testing each model. Each batch was allowed to run for 200 samples, with a sample time of 1 hour. The number of latent variable, selected using crossing validation, was found to be 13.

4.1 Application of Type I Nonlinear MPLS model to Estimation of Penicillin

The ability of linear MPLS and Type I nonlinear MPLS to predict penicillin for one particular unseen test batch is shown in Figure 4. The expansion of the X matrix is still considered with the quadratic term x^2 only.



Fig.4. Penicillin prediction using Linear MPLS and Type I nonlinear MPLS

The results illustrate that the Type I nonlinear MPLS model did not significantly improve the accuracy of the prediction. The reason is that in the Type I nonlinear model, the expansion of the X matrix is only considered with the quadratic term x^2 . However, the actual relationship of the Penicillin system is of a higher order.

4.2 Application of Type II Nonlinear MPLS model to Pensim

In this section the ability of linear MPLS and 2nd, 4th and 6th order Type I nonlinear MPLS to estimate the final endpoint concentration of penicillin is illustrated. The end-point measurement is used because in most fermentation processes, quality measurements, such as penicillin concentration will only be available at the end of a batch. The results are shown in Figure 5.



Fig.5. The application of Type II nonlinear MPLS

Linear MPLS, as shown in Figure 5(a), produced a SSE of 0.0826. The 2nd order Type II nonlinear PLS, shown in Figure 5(b), produced a SSE of 0.0557, the 4th order Type II nonlinear MPLS, shown in Figure 5(c), produced a SSE of 0.0257 and the 6th order Type II nonlinear MPLS, shown in Figure 5(d), produced a SSE of 0.0072. This result shows that as the order of the model improves so too does the accuracy of the model.

4.3 Application of Multi-way Neural Network PLS to Pensim

To illustrate the benefit of using multi-way NNPLS, the ability of this model to predict the endpoint of penicillin concentration is presented. Figure 6 shows a comparison of the predictions made using Type II non-linear MPLS (the red dots) with that obtained using the multi-way NNPLS. For the multi-way NNPLS (the diamonds), the SSE was calculated to be 2.94e-04, which compared favourably with the SSE for the Type II MPLS, which was 0.0072.



Fig.6. 6th Type II nonlinear MPLS model and Multi-way NNPLS are used to predict the end-point value of Penicillin

The primary advantage in using the multi-way NNPLS is that it provides high accuracy without the need to determine the order for the model, which can be a critical parameter with Type II MPLS models.

5. CONCLUSIONS

This paper has shown that for modelling batch processes, it is not always appropriate to use MPLS models. Whilst such models have been shown to be very useful, when the dynamics of the process are highly non-linear then, nonlinear extensions to MPLS can offer significant benefits. Of the non-linear extensions to MPLS that were tested, it was found that the multi-way NNPLS produced the most accurate results and had the added advantage that no a-priori information regarding the order of the dynamics was required. When applying Type II nonlinear MPLS, it was shown that specifying the order of the model was vital to producing an accurate model.

Appendix A. PENSIM

Pensim is a benchmark simulation of a fed-batch fermentation system. The simulator is based on a series of detailed mechanistic models that describe an industrial fed-batch fermentation process used for the production of penicillin. The original models have been proposed by the Control Group at Illinois Institute of Technology (Briol et al, 2002)

18 measurements are collected at each sampling instant and in this study, the following measurements were used in the model: aeration rate, agitator power, substrate feed rate, substrate feed temperature, substrate concentration, dissolved oxygen concentration, biomass concentration, penicillin concentration, culture volume, carbon dioxide concentration, pH, fermentor temperature, generated heat, acid flow rate, base flow rate, cooling water flow rate. The functional relationships between the process variables are summarized in Table 2.

Table 2. Functional relationship among the process variables

Model	Structure

$X = f(X, S, C_L, H, T)$
$S = f(X, S, C_L, H, T)$
$C_L = f(X, S, C_L, H, T)$
$P = f(X, S, C_L, H, T, P)$
$CO_2 = f(X, H, T)$
H = f(X, H, T)

In Table 2, X is biomass concentration; S is substrate concentration; C_L is dissolved oxygen concentration; P is penicillin concentration; CO_2 is carbon dioxide concentration; H is hydrogen ion concentration for PH; T is temperature.

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