INFERENTIAL CONTROL BASED ON A MODIFIED QPLS FOR AN INDUSTRIAL FCCU FRACTIONATOR

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Abstract: A modified Quadratic Partial Least Squares (MQPLS) algorithm based on nonlinear constrained programming is proposed. Sequential Unconstrained Minimization Technique (SUMT) is employed to calculate the outer input weights and the parameters of inner relationship. It was found that MQPLS can not only explain more of the underlying variability of the data, but also has improved modelling and predictive ability. An inferential control system is implemented on the Distribute Control System (DCS) of a fluid catalytic cracking unit (FCCU) main fractionator. A soft sensor MQPLS–based was developed to estimate solidifying point of diesel oil. The controller was established via constrained Dynamic Matrix Control (DMC) algorithm. Real time application results demonstrated the performance of the inferential control system based on MQPLS was much better than the original tray temperature control system. This resulted in a 1.0% increase in production rate, and a significant increase in profit.

Keywords: Partial Least Squares, Soft Sensor, Dynamic Matrix Control, Inferential Control.

1. INTRODUCTION

Many variables, which characterize the ‘quality’ of the final product in chemical processes, are often difficult to measure in real-time, and hence cannot be directly used in a feedback control. Most online quality analyzers, like gas chromatographs and NIR (Near-Infrared) analyzers, suffer from large measure delays and high investment and maintenance costs. Under these circumstances, a common alternative is to set up soft sensors to infer the product properties (primary variables) by employing some auxiliary measurements (secondary variables), and then build an inferential control scheme.

Statistic regression techniques have been extensively used in establishing soft sensing models from historical data. Among other related regression techniques, PLS has been proved to be a powerful tool for problems where data is noisy and highly correlated and where there are only a limited number of observations (Berglund and Wold, 1997; MacGregor et al., 1991). The power of PLS lies in the fact that it projects the input-output data down into a latent space, extracting a number of principle components with an orthogonal structure, while capturing most of the variance in the original data. Therefore, PLS can overcome the limitation that when dealing with highly correlated multivariate data, the traditional Least Squares (LS) regression will result in singular solution or imprecise parameter estimations.

However, in many practical situations, industrial processes exhibit significant nonlinear behaviors. As a linear regression method, PLS is inappropriate for modeling nonlinear systems.

Hence various kinds of nonlinear PLS (NLPLS) methods have been proposed in the literature which extend the PLS model structure to capture non-linearities of systems. A successful step towards

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nonlinear PLS modeling was the quadratic PLS (QPLS) proposed by Wold et al. (1989). In QPLS, second order polynomial (quadratic) regression is used to fit the function between each pair of input and output score vector, namely, the inner relation. The other ‘generic’ nonlinear PLS (NLPLS) such as spline PLS (SPLS) (Wold, 1992), neural networks PLS (NNPLS) (Qin and McAvoy, 1992) and Fuzzy PLS (FPLS) (Yoon et al., 2003) were developed. As their names suggest, SPLS uses spline function (quadratic or cubic) as inner model and NNPLS uses neural networks inner model. FPLS uses TSK (Takagi-Sugeno-Kang) fuzzy model as the inner model. All the algorithms above are developed from the nonlinear iterative partial least squares (NIPALS) algorithm (Geladi and Kowalski, 1986), which is called the ‘engine’ of the PLS methodology.

The problem of the input weight updating in NLPLS was firstly considered by Wold et al. (1989) and the benefit achieved by applying an updating procedure to the parameters of the NLPLS model was also proved. It has attracted the interests of many researchers. Especially, by modifying the input weight updating procedure of Wold et al., an error-based input weight updating approach was presented by G.baffi et al. (1999a, 1999b and 2000). In this paper, the input weight updating procedure is summarized to a constrained nonlinear optimal problem. Sequential Unconstrained Minimization Technique (SUMT) is utilized to calculate the outer input weights and the parameters of inner relation. It can make remedies of the shortcomings of the pseudo-inverse and large calculation burden that exist in the error-based input weight updating approach. Although this new kind of weight updating method is applicable to any nonlinear PLS algorithm, the new updating method is only combined with the original QPLS in this paper, leading to a modified quadratic Partial Least Squares (MQPLS) algorithm.

The paper is organised as follows. In Section 2, the basic principle of the NLPLS is introduced, and the error based input weight updating procedure by G. Baffi et al. (1999a) is briefly reviewed. Section 3 proposed a new input weight updating method and highlighted the details of the corresponding modified QPLS algorithm. Section 4 introduced the main structure of an inferential control system, in which the soft-sensor was built based on the modified QPLS to estimate diesel oil solidifying point, and the controller was established via a simplified Dynamic Matrix Control (DMC) algorithm. Section 5 gives the conclusions.

2. QUADRATIC PARTIAL LEAST SQUARES

PLS algorithm decomposes $\mathbf{X}$ and $\mathbf{Y}$ by projecting them to the directions (input weight w and output weight c) to extract several pair of input score vector t_h and output score vector u_h .The decomposition, known as the PLS outer relation, is formulated as follows:

$$\mathbf{X} = \sum_{h=1}^{k} t_h p_h^T + \mathbf{E}_h \qquad (1)$$

$$\mathbf{Y} = \sum_{h=1}^{k} \hat{u}_h q_h^T + \mathbf{F}_h \qquad (2)$$

Where p_h and q_h are loading vectors, $\mathbf{E}_h$ and $\mathbf{F}_h$ are residuals, and $\hat{u}_h$ is the estimator of u_h and calculated by the inner relation.

$$u_h = f_h(t_h) + e_h \qquad (3)$$

$$\hat{u}_h = f_h(t_h) \qquad (4)$$

The traditional linear PLS performs an ordinary LS regression between pair of corresponding score vectors, that is,

$$u_h = b_h t_h + e_h \qquad (5)$$

$$b_h = t_h^T u_h / t_h^T t_h \qquad (6)$$

while QPLS employs second order polynomial (quadratic) regression for inner mapping:

$$u_h = b_{0,h} + b_{1,h} t_h + b_{2,h} t_h^{\ 2} + e_h \qquad (7)$$

The appropriate number of components required to describe the data structure, k , is generally identified by means of cross-validation and chosen to be one which minimizes the Predictive Error Sum of Squares (PRESS). It is because most of the variance of the input and output matrixes can usually be accounted for by the first few score vectors, whilst the residuals are typically associated with the random noise in the data sets.

The problem of input weight updating procedure in NLPLS cannot be omitted. (Wold et al., 1989; Baffi et al., 1999a; Yoon et al., 2003). The input updating procedure proposed by Baffi et al. (1999a) is an error-based approach and listed as follows.

The mismatch e_h between the value of u_h , given by $u_h = \mathbf{Y} q_h$, and the value of $\hat{u}_h$, given by the nonlinear mapping, $\hat{u}_h = f_h(t_h, b_h)$, can be denoted by

$$e_h = u_h - \hat{u}_h \qquad (8)$$

Based on the first-order series expansion, equation (8) can be written as

$$e_h = u_h - \hat{u}_h = u_h - f_{00} = \frac{\partial f}{\partial w_{h\ 00}} \Delta w_h \qquad (9)$$

By combining the partial derivatives $\partial f / \partial w_h$ into a matrix $\mathbf{Z}_h$, e_h can be written as $e_h = \mathbf{Z}_h \Delta w_h$ and the correction Δw_h can be regressed directly as follows

$$\Delta w_h = (\mathbf{Z}_h^{\ T} \mathbf{Z}_h)^{-} \mathbf{Z}_h^{\ T} e_h \qquad (10)$$

$(\mathbf{Z}_h^{\ T} \mathbf{Z}_h)^{-}$ in equation (10) is the pseudo-inverse of the matrix $(\mathbf{Z}_h^{\ T} \mathbf{Z}_h)$. Then the input weight is updated

$$w_h = w_h + \Delta w_h \qquad (11)$$

And check convergence on t_h . The updating procedure is completed if a new input score vector t_h ($t_h = \mathbf{X} w_h$) is stable; otherwise repeat the steps mentioned above.

3. MODIFIED QPLS

In this section, a new input weight updating procedure based on nonlinear programming is presented. The new weight updating procedure combined with QPLS leads to QPLS based on nonlinear programming, whose NIAPLS algorithm is also given detailed.

3.1 A new input weight updating procedure

There are three points of the error based input weight updating procedure worthy to be investigated.

Firstly, $\mathbf{Z}_h$ in equation (10) is rank deficient under two conditions. One is input dimension is lager than number of samples, the other is the partial derivatives of the inner relation being linearly correlated with themselves or alternatively with the inner relation $f_h(\cdot)$ itself. In this case, the correction Δw_h cannot be obtained directly by equation (10). So the pseudo-inverse is necessary and numerical techniques are needed to evaluate the pseudo-inverse $(\mathbf{Z}_h{}^T\mathbf{Z}_h)^-$.

Secondly, w_h is updated iteratively until the input score vector t_h is converged, which result in large computation burden.

Thirdly, by applying the error based input weight updating procedure, the NLPLS model can catch larger output cumulative variance, but smaller input cumulative variance. It was also pointed out by Yoon et al. (2003).

In this paper, a new input weigh updating procedure was proposed on the basis of the method proposed by G.baffi et al. The core of the method is as follows.

The objective of the error based weight updating procedure by G..baffi et al. is to find proper input weights and parameters of nonlinear inner relation which can minimize the regression SSE of the each nonlinear inner relationship. It can be classified as a constrained nonlinear programming problem. In QPLS, the optimal weights and polynomial coefficients of inner relationship can be derived from nonlinear programming methods. The optimization problem, including the objective function and the constraints, can be described as follows:

$$\min\left\{(u_h-\hat{u}_h)^T(u_h-\hat{u}_h)\right\} \qquad (12)$$

$$\textbf{s. t.} \quad \|w_h\|=1$$

where $\hat{u}_h=[1 \quad t_h \quad t_h{}^2]^T\boldsymbol{b_h}$, $t_h = X\cdot w_h$.

In this problem, w_h and b_h are the decision variables, which should be found to minimize the objective function and satisfy the constraints. Herein Sequential unconstrained minimization technique (SUMT) is used to transform problem (12) into a series of unconstrained nonlinear programming problems. Then Hook-Jeevs method is employed to solve the unconstrained nonlinear programming problems. The initial values of w_h and b_h are obtained by NIPLAS algorithm.

By applying the proposed input weight updating procedure, the optimal w_h do not need to be calculated iteratively and the steps in NIPALS algorithm are simplified accordingly. Since the weight updating method improves the fitness of inner relation by changing the spread of score vectors, the proposed one is more precise than the error based one and can catch more cumulative variance. It will be illustrated in the application in Section 4.1.

3.2 Modified NIPALS algorithm:

The new weight updating procedure combined with QPLS leads to QPLS based on nonlinear programming, which is called the modified QPLS (MQPLS). Details of the steps of modified NIPALS algorithm are shown in Table 1.

<u>Table 1 Summary of the modified NIPALS algorithm</u>

It is assumed that **X** and **Y** blocks have been preprocessed, i.e., scaling around zero mean and unit variance. Proper scaling prevents the score vectors from being biased towards variables with larger magnitude. For each component h :

1 Take $u_h = y_j$ (if the column of $\mathbf{Y}$ equals to 1, set u equal to $\mathbf{Y}$)

2 Calculate the input weight $w_h{}^T = u_h{}^T\mathbf{X}/u_h{}^Tu_h$

3 Normalize $w_h = w_h / \| w_h \|$

4 Calculate the input score vector $t_h = \mathbf{X}w_h$

5 Fit the quadratic inner relationship $\boldsymbol{b}_h \leftarrow fit[u_h = [1 \quad t_h \quad t_h{}^2]^T\boldsymbol{b_h} + e_h]$

6 Calculate the nonlinear prediction of u_h $\hat{u}_h = [1 \quad t_h \quad t_h{}^2]^T\boldsymbol{b_h}$

7 Calculate the optimal input weight and parameters of inner relationship according to the new weight updating procedure described in Section 3.1

8 Calculate the new input score vector $t_h = \mathbf{X}w_h$

9 Calculate the input loading vector $p_h = t_h{}^T\mathbf{X}/t_h{}^Tt_h$

10 Normalize p_h to unit length $p_h = p_h/\|p_h\|$

11 Calculate the new nonlinear prediction of u_h $\hat{u}_h = [1 \quad t_h \quad t_h{}^2]^T\boldsymbol{b_h}$

12 Calculate the output loading vector $q_h{}^T = t_h^T\mathbf{Y}/t_h^Tt_h$

13 Normalize q_h to unit length $q_h = q_h/\|q_h\|$

14 Calculate the output score vector u_h $u_h = \mathbf{Y}q_h$

15 Calculate the input residual $\mathbf{E}_h = \mathbf{E}_{h-1} - t_hp_h{}^T$

16 Calculate the output residual $\mathbf{F}_h = \mathbf{F}_{h-1} - \hat{u}_hq_h{}^T$

17 If $h<k$ (k is the optimal number of components), step 1-17 are repeated ($\mathbf{X}$ and $\mathbf{Y}$ should be replaced by $\mathbf{E}_h$ and $\mathbf{F}_h$).

4. INFERENTIAL CONTROL OF A FCCU FRACTIONATOR

4.1 Soft sensor of diesel oil solidifying point

An industrial FCCU main fractionator is one of the key processes in modern petroleum refining. The function of the unit is to separate heavy distillates from FCC reactor like gas oils or residuals into gasoline, diesel oil and middle distillates. The MOPLS algorithms described above are applied to establish the soft sensors on the unit to predict diesel oil solidifying point.

Through mechanism analysis, fifteen process variables are chosen as secondary variables and measured online at one minute intervals. Secondary variables include top pressure，top temperature, the flow rate, temperature of the second reflux, etc. A data set including 720 samples are gathered from the DCS database of the FCCU main fractionator. The actual analysis value of product quality is only available from the lab with a frequency of 2 hours. The outliers have been removed beforehand. The data is split into a training data and a test data. Every fifth observation is placed in the test data set, totally 144 samples, and the remaining 576 observations form the training data. The optimal number of components is calculated by cross validation.

Slight nonlinearity is found in first pair of component of data gathered, which is suitable to be fit by quadratic polynomial. The cumulative variance of the $\mathbf{X}$ block and $\mathbf{Y}$ block captured by each model and their Mean Square Predictive Error (MSPE) is given in Table 2 for linear PLS, QPLS, error based QPLS and MQPLS，respectively. Figures 1-4 illustrate the final predication for the test data for the four algorithms.

The MSPE of the original QPLS is 1.3197, whilst the error based QPLS is 1.1651 and MQPLS is 1.0847. It is clearly evident that the three kinds of QPLS algorithms catch the main nonlinear characteristic in the data set. Although the predictive abilities of the error based QPLS and MQPLS are comparable, MQPLS shows a few better than the error based QPLS. The predictive results of MQPLS are used as a reference of the operators.

4.2 Predictive inferential control scheme

The product quality control of the fractionator has been a classical and difficult problem. Traditionally, the product quality is represented by tray temperature control, which has a wide application in the chemical plants. An inferential controller for quality control can be established once the solidifying point of diesel oil is available through the modified QPLS based soft sensor. Many papers (Kano et al., 2000; Kano et al., 2003) have proposed cascade inferential control system in which the set point of tray temperature controller is given by the output of quality inferential controller. However, in such control scheme, the inner temperature controller has a greater influence on the performance of the whole system, and its complex structure brings some difficulties to operators.

In this paper, a new inferential control system is proposed in which tray temperature controller and quality inferential controller can be switched without producing any disturbance. The configuration of the proposed inferential control system is showed in Figure 5. Temperature controller (denoted as TC in Figure 5) still uses the original tray temperature controller. Inferential controller (denoted as AC in Figure 5) adopts constrained Dynamic Matrix Control (DMC) algorithm.

Table2. Model comparison: Cumulative variance (%)

LV	Linear PLS		Original QPLS		Error based QPLS		MQPLS	
	X	Y	X	Y	X	Y	X	Y
1	69.75	56.37	74.40	72.47	29.42	78.61	34.56	82.70
5	70.85	62.14	93.61	75.51	37.17	80.24	53.56	84.96
10	92.45	65.06	99.40	78.24	52.08	91.73	87.26	92.57
15	100.00	68.85	100.00	78.62	62.58	92.55	88.83	93.79
MSPE	1.4687		1.3197		1.1651		1.0847	

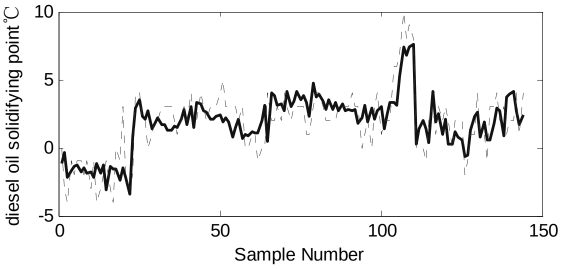

Fig.1 Actual versus Predicted values for the Linear PLS (……actual; ——predicted)

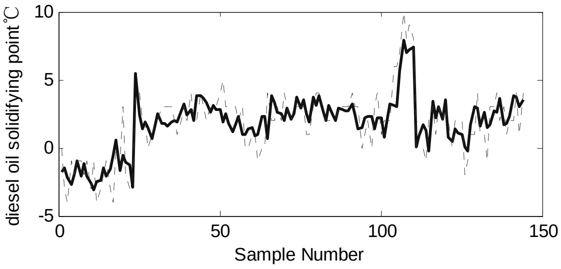

Fig.2 Actual versus Predicted values for the QPLS (……actual; ——predicted)

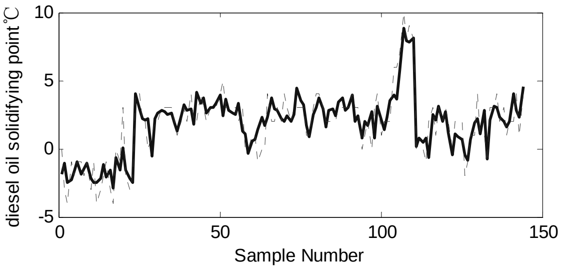

Fig.3 Actual versus Predicted values for the error based QPLS (……actual; ——predicted)

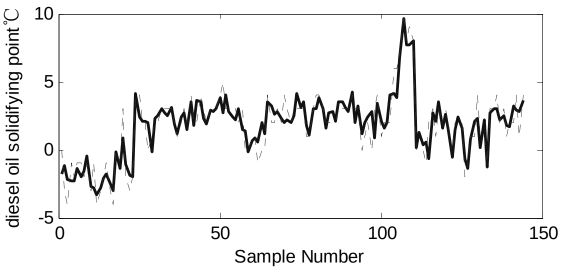

Fig.4 Actual versus Predicted values for MQPLS (……actual; ——predicted)

DMC uses the step response model for predicting the process output P step into the future in the absence of further control action. The model is also used to calculate the present and future M control actions which minimizes the following objective function:

$$J = \{[y_r(k+p) - y_c(k+p)]^2 q + \sum_{i=0}^{m-1} [\Delta u(k+i)]^2 r_i\} \quad (13)$$

s. t. $|\Delta u(k)| \le \Delta u_{\max}, u_{\min} \le u(k) \le u_{\max}$

Where $y_r(k+p)$ is the set objective value.

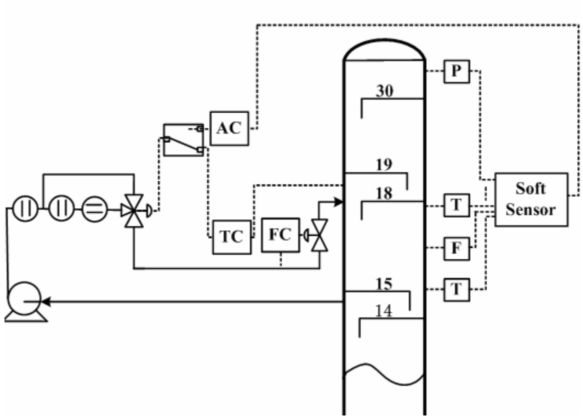

Fig. 5 Schematic diagram of a FCCU main fractionator

This kind of design scheme can make use of the original system module, and is easy to be implemented on the DCS system, and gives facilities for operating. However, there are some questions to pay attention to in practice. When step response of process is made for DMC, it must be sure that step response starts from some steady state. Also the inferential control system should consider some abnormalities from DCS and process to guarantee the safety of the process. Because the running performance of chemical plants is often in change, predictive model updating is another key point.

4.3 Real-time implementation Results

The designed soft sensor and the predictive inferential controller were implemented on the Distribute Control System (DCS) of an industrial FCCU main fractionator using CL (Control Language) programming. The sequential predicting results are shown in Figure 6, in which the dotted line is gathered from the laboratory and the solid line is computed by MQPLS soft sensor. The MSPE is 1.1055 and the predicted result is satisfactory to be used as the set point of the inferential controller.

Figure 7 compares the diesel oil quality control performance for both before and after implementing predictive inferential control system. It can be seen that the control variance decreases clearly when inferential control system is employed. Figure 8 show closed loop response of predictive inferential control system. When the set point step change of solidifying point is from -7.5℃ to -6℃, the control system can quickly trace the desired value.

Application results indicate that inferential control system has a better performance than tray temperature control system.

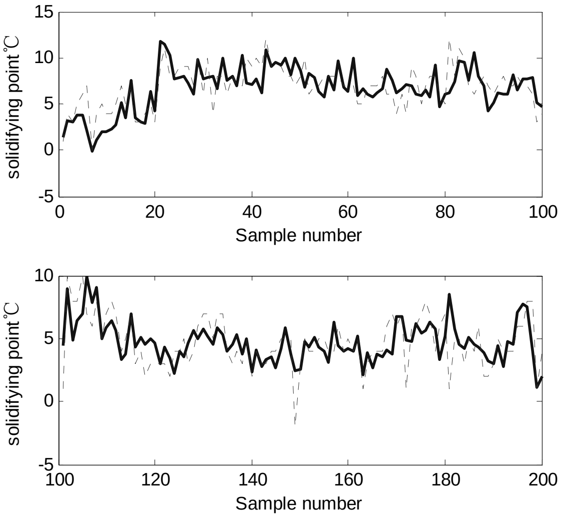

Fig. 6 Validation data set. Comparison between the actual value of solidifying point and its estimates provided by MQPLS (——predicted; ……actual)

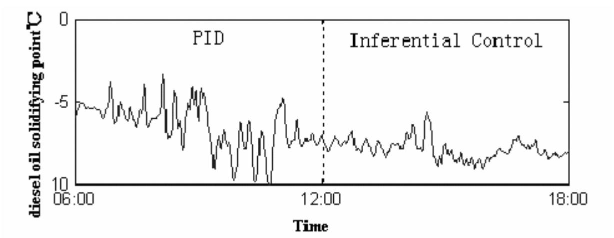

Fig 7 Comparison of the tray temperature control and inferential control system

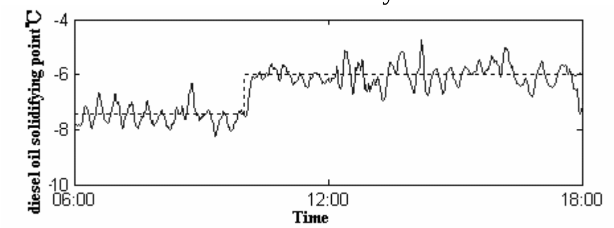

Fig 8 Closed-loop response of predictive inferential control system by step set point change

5 CONCLUSIONS

In this paper, the error based weight updating procedure of G. Baffi et al. is studied. A new weight updating procedure based on nonlinear programming is formulated. MQPLS algorithms are proposed. In comparison with existing QPLS algorithms, MQPLS can catch much higher percentage of input and output cumulative variance, avoid the problem of the pseudo-inverse of matrix and reduce the calculation burden. To realize online measurement, a soft sensor is built based on the MQPLS to estimate the solidifying point of diesel oil for an industrial FCCU main fractionator. An inferential control scheme is proposed. This control scheme can switch between usual tray temperature controller and inferential controller based on constrained DMC algorithm. The practical results obtained from an industrial plant show that the proposed system has a better performance than the traditional tray temperature control system.

6. ACKNOWLEDGEMENTS

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