PROCESS MONITORING BASED ON NONLINEAR WAVELET PACKET PCA

Xiuxi Li, Junfeng Wang, Yu Qian*, and Yanbin Jiang

School of Chemical Engineering, South China University of Technology, Guangzhou, 510640, China

Abstract: For using process operational data to realize process monitoring, kinds of improved PCA are applied to cope with complexity of industrial processes. In this paper, a novel nonlinear wavelet packet PCA (NLWPPCA) method, which combines input training network with wavelet packet PCA, is proposed. Wavelet packet PCA integrates ability of PCA to de-correlate the variables by extracting a linear relationship with what of wavelet packet analysis to extract auto-correlated measurements. Then the paper gives the methodology of process monitoring based on NLWPPCA. Finally, the proposed approach is successfully applied to an eight variables nonlinear process with noise and Tennessee Eastman process for process monitoring. *Copyright © 2003 IFAC*

Keywords: Process monitoring; Wavelet packet analysis; Principal components analysis

1. INTRODUCTION

With the increase in on-line data acquisition systems in industrial processes, the collection of process operational data is becoming routine. Then process plants are becoming data rich but information poor. There is therefore a need to extract the inherent information within the data. Data mining techniques, which mining inherent useful knowledge from kinds of databases or data warehouses, are introduced to process monitoring. Then process monitoring based on data mining is to collect raw data from time-series database or data sets, reprocess data using data reconciliation method, mine outliers and classification or clustering analyze these outliers. Principal components analysis (PCA) as an effective method of data mining techniques has been widely applied in process monitoring. However, many industrial processes exhibit significant nonlinear behaviour and industrial data is also synonymous with process measurement noise. In these cases the application of PCA is not strictly appropriate. Then many improved methods are proposed and applied. Kramer (1991) used an auto-associative neural network, trained using backpropagation to produce a nonlinear PCA. Dong and McAvoy (1994) integrated

principal curves with a neural network to build a nonlinear PCA. Tan and Mavrovouniotis (1995) proposed a nonlinear PCA based on input-training neural network. Bakshi (1998) introduced the principle of multiscale PCA, which combines the attractive properties of linear PCA and wavelet analysis by computing the PCA of wavelet coefficients at each scale and then combining the results at relevant scales. Chen, et al. (1999) combined neural networks and multiscale wavelet analysis in a modified version of the adaptive resonance theory for diagnostic system development. Shao, et al. (1999) proposed a nonlinear PCA algorithm for process monitoring based on an input-training neural network and also applied wavelet denoising and non-parametric control limits. Fourie and Vaal (2000) gave an on-line nonlinear multiscale principal component analysis methodology.

Wavelet packet PCA integrates PCA and wavelet packet analysis. Wavelet packet analysis decomposes the high-frequency part further, which wavelet analysis not does, and adaptively selects relative frequency bond based on character of signal to be analyzed. To further improve denoising character of multiscale PCA, the paper describes a wavelet packet PCA, which combines the ability of PCA to decorrelate the variables by extracting a linear

^{*} Corresponding author: +87112046, Email:ceyuqian@scut.edu.cn

relationship with that of wavelet packet analysis to extract autocorrelated measurements. Then, a novel nonlinear wavelet packet PCA is proposed by combining input-training neural network with wavelet packet. Finally, the nonlinear wavelet packet PCA will be used to analyze two simulated systems to verify its operation.

2. WAVELET PACKET PCA

In the WPPCA, signals are decomposed first using wavelet packet to get wavelet packet decomposition coefficients matrixes. Then these coefficients matrixes use PCA to confirm the retain number of principal components and compute principal components score matrixes and load matrixes. Wavelet packet coefficients are obtained by rebuilding the score matrixes and the load matrixes. These coefficients are de-noised by using wavelet packet de-noise limit method, Rebuild signals are obtained by using wavelet packet rebuild algorithm. Finally, These rebuild signals are analyzed by PCA. The steps in the WPPCA methodology are shown in Figure 1, and the detailed procedures are given as follows.

- (1) For each column in data matrix, select wavelet packet function $\Psi_{j,k,n}(t)$ and wavelet packet dividing level L and compute wavelet packet decomposition coefficients $\{W_{L,0}, W_{L,1}, ..., W_{L,2}^{L}, 1\}$;
- (2) For each variable, use the same best full wavelet

packet base algorithm to process wavelet packet decomposition tree and find best wavelet packet decomposition coefficients;

- (3) Select these coefficients as column vector to build wavelet packet coefficients matrixes with different tree nodes $\{X_{L,0}, X_{L,1}, \dots, X_{L,2}^{L}, 1\}$, the row number of these matrix is $n/2^{L}$ and the column number is *m*;
- (4) For these coefficients matrixes, respectively use conventional PCA to confirm the retain number of principal components and compute principal components score matrixes $\{T_{L,0}, T_{L,1}, \dots, T_{L,2}^{L}, 1\}$ and load matrixes $\{P_{L,0}, P_{L,1}, \dots, P_{L,2}^{L}, 1\}$;
- (5) Use retain score matrixes and load matrixes to rebuild wavelet packet coefficients matrixes {X'_{L0}, X'_{L1},...,X'_{L2}^L,1};
- (6) For each column in {X'_{L,0}, X'_{L,1},...,X'_{L,2}, }, combines corresponding column vectors to get rebuild wavelet packet coefficients;
- (7) For these coefficients, respectively use wavelet packet de-noise limit method to process these coefficients and get de-noising coefficients;
- (8) Use wavelet packet rebuild algorithm to get each variable samples $\{x'_1, x'_2, \dots, x'_m\}$;
- (9) Build new data matrix X' and use PCA to select the retain number of principal components and compute score matrix T' and load matrix P'.

The WPPCA combines the ability of PCA to de-correlate the variables by extracting a linear relationship with that of wavelet packet analysis to extract auto-correlated measurements.



Figure 1 Methodology of wavelet packet PCA

3. NONLINEAR WAVELET PACKET PCA

Nonlinear PCA is an extension of linear PCA. Nonlinear PCA can extract both linear and nonlinear correlations, while PCA identifies linear correlations between process variables. Neural networks have long been recognized as a useful tool for extracting features from highly nonlinear data. Some researchers have proposed different approaches based on kinds of neural networks. Malthouse (1998) discussed these approaches and recommended the techniques developed from the principal curve method and the input-training network to overcome the continuous function projection constraint. The nonlinear wavelet packet PCA (NLWPPCA) method proposed in this paper is based upon the input-training neural network (IT-net). In the IT-net each data input pattern is not fixed but adjusted in conjunction with the internal network parameters to reproduce a corresponding output pattern using the steepest gradient descent optimization rule. In the approach, the process observation data are defined as the output layer pattern and the nonlinear principal scores are identified from the input layer. The architecture of the IT-net is shown in Figure 2.



Figure 2 Structure of IT-net



Figure 3 Methodology of nonlinear wavelet packet PCA

The NLWPPCA enables both nonlinear characters and noise characters to be analyzed. Figure 3 illustrates the NLWPPCA methodology. The implement steps of the NLWPPCA algorithm is as followed:Collect normal operation data matrix *X*;

- For each column in X, use wavelet packet PCA algorithm to compute linear principal scores matrix T' and principal loads matrix P';
- (2) Let linear principal scores matrix T' as the IT-net output layer pattern, let nonlinear principal scores matrix T as the IT-net input layer pattern, select input layer nodes k and determine hidden layer nodes q and other network initial values;
- Use extend backpropagation algorithm to optimize network parameters and input values, then get the IT-net model *F*(.);
- (4) Let the IT-net input layer values, which be trained, as the forward feedback neural network output layer, let linear principal scores matrix T' as the forward feedback neural network (FF-net) input layer, and select similar structure as the IT-net;
- (5) Use backpropagation algorithm to train the parameters, then get the FF-net model G(.);
- (6) Determine the nonlinear principal scores matrix T,

load matrix *P*, and get the NLWPPCA model as $X=F(T)P^{T}+E$, where *E* is an error matrix.

4 PROCESS MONITORING BASED ON NLWPPCA

Algorithm implement of process monitoring based on NLWPPCA is illustrated in Figure 4. It includes two parts: off-line model determination and on-line process monitoring. Where off-line model determination includes: select best full wavelet packet base, select appropriate denoising threshold, determine the retain principal components number, compute linear principal scores matrix and loads matrix, determine the IT-net structure and initial parameters, use extend backpropagation algorithm to get nonlinear principal scores matrix, train the forward network to get the NLWPPCA model, determine statistical value limitation to monitor process. Where on-line process monitoring includes: reprocess real-time operation data to input the normal NLWPPCA model, compute each statistical value SPE and T², compare these values with the corresponding thresholds, determine abnormal situation.



Figure 4 Algorithm of process monitoring based on NLWPPCA

5. CASE STUDY

In this Section, the proposed process monitoring based on NLWPPCA is demonstrated and tested by applying in an eight variables nonlinear process with noise and a recognized chemical process tested base Tennessee Eastman process. We will demonstrate the use of NLWPPCA approach for nonlinear monitoring purposes first with respect to a simple multivariate process as well as with the much more complex and realistic Tennessee Eastman process.

5.1 An eight variables nonlinear process with noise

Consider the following process:

 $\begin{array}{l} x_1 = 8 + 0.1*randn(n,1) + 0.8*wnoise; \\ x_2 = 11 + 0.2*randn(n,1) + 0.8*wnoise; \\ x_3 = 17 + 0.3*randn(n,1) + 0.8*wnoise; \\ x_4 = 5 + ((-1.3*x_1^3 + 0.2*x_2^2)/(x_2*x_3)) + 0.8*wnoise; \\ x_5 = 120 + 0.8*(-3.8*x_1^2 + 0.8*x_2^2 + 0.9*x_3*x_4) \\ + 0.8*wnoise; \\ x_6 = 5 + x_2 - 0.3*x_3 + 0.8*wnoise; \\ x_7 = -x_1 + 0.8*x_2 + x_4 + 0.8*wnoise; \\ x_8 = x_2 + x_3 + 0.8*wnoise; \end{array}$

where *wnoise* is a white noise with zero mean and variance 1. 1000 samples are selected as normal operation data for analysis. The initial data matrix consists of as follow:

 $X = [x_1^{T} x_2^{T} x_3^{T} x_4^{T} x_5^{T} x_6^{T} x_7^{T} x_8^{T}]$

For data matrix X, use the proposed NLWPPCA algorithm to build off-line model. Where structure of the IT-net is 1-3-2, and hidden layer function is

Sigmoid function. The IT-net is trained by extend Levenberg-Marquardt (LM) algorithm. When train step is 56, train error is 0.005. Similar, select structure of the FF-net is 2-3-1 and use LM algorithm to train the FF-net. When train step is 18, the error is 0.005. Determine the statistical limitation: $SPE_a=0.1234$, $T^2_a=6.0060$. The NLWPPCA model is used to monitor 200 real-time samples of the eight variables nonlinear process. To verify performance of monitoring, introduces mean error disturbance at 160 sample time and cancels it at 180. The process real-time trend is illustrated in Figure 5. Figure 6 shows the SPE plot and T^2 plot.

The relationship between the first principal component and the second one is shown in Figure 7. Figure 8 describes the contribution plot of the first and the second principal component. From Figure 5, it is not easy to identify the process operational situation because of nonlinear character. However, from SPE plot, SPE values before 160 times step is clearly below the SPE limitation and out of control after 160. So, SPE plot successfully finds the abnormity. Similarly, T^2 plot also finds the abnormity. From scores plot, finds some outliers away from the clustering points, which directly shows the trend. In addition, some projection points are overlapped for wavelet packet denoising. Figure 8 shows that contribution of the second and 7th variables to the first pc is biggish and contribution of the second, 5th and 7th variables to the second pc is biggish. Then, it is inferred that the abnormity is brought by the second, 5th and 7th variables. The conclusion is consistent with process model. The simulation illustrates the proposed approach is valid for nonlinear process with noise monitoring.



Figure 5 Real-time trends with mean error



Figure 7 Scores plot with mean error

5.2 Tennessee Eastman process

Table 1 Process disturbance

Case	Disturbance	Туре
IDV(1)	A/C feed ratio, B composition	Step
	constant	
IDV(2)	B composition, A/C ratio	Step
	constant	
IDV(3)	D feed temperature	Step
IDV(4)	Reactor cooling water inlet	Step
	temperature	
IDV(5)	Condenser cooling water inlet	Step
	temperature	
IDV(6)	A feed loss	Step
IDV(7)	C header pressure loss –	Step
	reduced availability	
IDV(8)	A, B, C feed composition	Random
IDV(9)	D feed temperature	Random
IDV(10)	C feed temperature	Random
IDV(11)	Reactor cooling water inlet	Random
	temperature	
IDV(12)	Condenser cooling water inlet	Random
	temperature	
IDV(13)	Reaction kinetics	Slow drift
IDV(14)	Reactor cooling water valve	Sticking
IDV(15)	Condenser cooling water valve	Sticking
IDV(16)	Unknown	Unknown



Figure 6 SPE and T^2 plots with mean error



Figure 8 Contribution plot with mean error

Tennessee Eastman process, which was developed by Downs and Vogel (1993), consists of five major unit operations: a reactor, a condenser, a vapor-liquid separator, a recycle compressor, and a product stripper. The process has 41 measurements, including 22 continuous process measurements and 19 composition measurements, and 12 manipulated variables. Some disturbances are programmed for researching the characteristics of the control system, listed in Table 1.

The reference set contains 1000 samples from normal operation with a sampling interval of 3 min. A NLWPPCA model is developed from the data matrix. Nine principal components are selected, which capture 97.7% of the variation in the reference set. The control limits shown in every plot correspond approximately to the 95% confidence region, which is determined by using the methodology presented by Nomikos and MacGregor:

 $SPE_a = 7.1509, T^2_a = 75.0008.$

The simulation is run under the first disturbance IDV[1], which is loaded at the 300th time step. SPE plot and T² plot are shown in Figure 9. From these plots, disturbance is quickly and easily detected. Figure 10 shows the scores plot. The figure clearly

illustrates that process projection points are away from the normal situation. This result shows that for



Figure 9 SPE plot and T^2 plot for IDV[1]

6. CONCLUSIONS

In this paper, a nonlinear wavelet packet PCA approach has been proposed for process monitoring. The advantage of this method is that both linear and nonlinear correlations can be extracted from the process data with noise. Heavy noise and data spikes in the industrial data sets were first eliminated through wavelet packet denoising method. Whilst, input-training neural network was introduced to extract nonlinear character in industrial processes. The results of the application of the NLWPPCA algorithm to an eight nonlinear process and TE

REFERENCES

- Bakshi, B.R. (1998). Multiscale PCA with application to multivariate statistaical process monitoring. *American Institute of Chemical Engineering Journal*, 44(7),1596.
- Chen, B.H., X.Z. Wang, S.H. Yang, and C. McGreavy, (1999). Application of wavelets and neural networks to diagnostic system development. Part 1. Feature extraction. *Computers & Chemical Engineering*,23,899.
- Dong, D. and T.J. McAvoy, (1994). Non-linear principal component analysis based on principal curve and neural networks. *Computers & Chemical Engineering*, 20(1),65-78.
- Downs, J.J. and E.F. Vogel, (1993). A plant-wide industrial process control problem. *Computer & Chemica. Engineering*, 17, 245-255.
- Fourie, S.H. and P.de. Vaal, (2000). Advanced process monitoring using an on-line non-linear multiscale principal component analysis methodology. *Computers & Chemical Engineering*, 24(2000)755-760.

the TE process the proposed NLWPPCA will get well effect in process monitoring.



Figure 10 Scores plot for IDV[1]

process demonstrate the improved performance over that of linear methods for fault detection.

ACKNOWLEDGMENTS

Financial support from the National Natural Science Foundation of China (No. 29976015), the China Excellent Young Scientist Fund, China Major Basic Research Development Program (G20000263), and the Excellent Young Professor Fund from the Education Ministry of China are gratefully acknowledged.

- Kramer, M. A. (1991). Non-linear principal component analysis using autoassociative neural networks. A.I.Ch.E. Journal, 37(2),233-243.
- Ku, W., R. Storer, and C. Georgakis, (1995). Disturbance detection and isolation by dynamic principal component analysis. *Chemometrics* and Intelligent Lab. Systems 30, 179-196.
- Lin, Weilu, Y. Qian, and X.X. Li, (2000). Nonlinear dynamic principal component analysis for on-line process monitoring and diagnosis. *Computer & Chemical Engineering* 24, 423-429.
- Malthouse, E.C. (1998). Limitations of non-linear PCA as performed with generic neural networks. *IEEE Transactions on Neural Networks*, 9(1),165-173.
- Shao, R., F. Jia, E.B. Martin, and A.J. Morris, (1999). Wavelets and non-linear principal components analysis for process monitoring. *Control Engineering Practice*, 7,865.
- Tan, S., and M.L. Mavrovouniotis, (1995). Reducing data dimensionality through optimizing neural network inputs. A.I.Ch.E. Journal, 41(6), 1471-148.