A PARTICLE FILTER BASED DYNAMIC GAUSSIAN MIXTURE MODEL FOR PROCESS FAULT DETECTION AND DIAGNOSIS

Jie Yu*
Department of Chemical engineering
McMaster University
Hamilton, Ontario L8S 4L7, Canada

Abstract

Complex multimode processes may have dynamic operation scenario shifts and strong transient behaviors so that the conventional monitoring methods become ill-suited. In this article, a new particle filter based dynamic Gaussian mixture model (DGMM) is developed by adopting particle filter re-sampling method to update the mixture model parameters in a dynamic fashion. Then the particle filtered Bayesian inference probability index is established for process fault detection. Furthermore, the particle filtered Bayesian inference contributions are decomposed among different process variables for fault diagnosis. The proposed DGMM monitoring approach is applied to the Tennessee Eastman chemical process with dynamic mode shifting and the results show its superiority to the regular Gaussian mixture model in terms of fault detection and diagnosis accuracy.

Keywords

Dynamic Gussian mixture model, Particle filter, Fault detection and diagnosis, Time-varying operating mode shifts, Non-Gaussian process.

Introduction

Industrial process monitoring is essential to safeguard process operation, ensure product quality and improve manufacturing profit. In literature, multivariate statistical process monitoring (MSPM) methods have been widely applied to various kinds of industrial processes with some success (Kourti and MacGregor, 1995, Qin, 2003, Bakshi, 2004, Yu, 2011). The most well-known MSPM techniques include principal component analysis (PCA) and partial least squares (PLS) (Nomikos and MacGregor, 1994; Piovoso and Kosanovich, 1994; MacGregor and Kourti, 1995). The monitoring statistics of PCA/PLS methods require the process data to follow multivariate Gaussian distribution approximately in order for their confidence limits are valid. In practice, however, the normal process data may not follow non-Gaussian distribution so that the traditional PCA/PLS monitoring approaches become inappropriate.

More recently, different types of non-Gaussian process monitoring techniques such as independent component analysis (ICA) and Gaussian mixture model (GMM) have been developed and applied to complex chemical process monitoring (Lee et al., 2004, Yoo et al., 2004, Yu and Qin, 2008, Yu and Qin, 2009, Yu, 2011). The ICA method takes into account the higher-order statistics in order to extract the non-Gaussian features from process data. The industrial processes are often characterized by shifting operation modes so that the data shows strong multimodality. In such situations, the objective function of negentropy used in ICA does not necessarily capture the multi-Gaussianity in multimode

* To whom all correspondence should be addressed

process data. Though the GMM based monitoring approach can nicely handle the multi-Gaussianity, it assumes that the multiple operating conditions and their corresponding prior probabilities remain unchanged during the entire plant operation. The issue may arise when the collected training data are not representative of all the operation scenarios under the actual prior probabilities or the mode shifting periods have strong transient behavior.

In this paper, a new particle filter based dynamic Gaussian mixture model is proposed to monitor multimode processes with transient mode shifting or operation strategy changes. The initial mixture model is first estimated by the modified Expectation-Maximization (E-M) algorithm. Then the particle filter is adopted to dynamically update the mixture model parameters and predict the time-varying operation shifts. The inferential monitoring statistics can thus be computed from the dynamic GMM and used to detect the abnormal events in the process. Furthermore, the inferential contribution indices are estimated to diagnose the process faults and identify the faulty variables. The utility of the present DGMM monitoring method is demonstrated through the application example of Tennessee Eastman process (TEP) with operating scenario changes and the monitoring results are compared to those of GMM approach.

Review of GMM

The multiple operating modes in normal process can be characterized by different Gaussian components in GMM and the prior probability of each Gaussian component represents the percentage of total operation when the process runs at the particular mode. The probability density function of Gaussian mixture model is equivalent to the weighted sum of the density functions of all Gaussian components as given below:

$$p(x \mid \Lambda) = \sum_{i=1}^{K} \beta_i g(x \mid \lambda_i) \tag{1}$$

where x is a l-dimensional measurement sample, β_i denotes the prior probability of the ith Gaussian component and $g(x \mid \lambda_i)$ is the multivariate Gaussian density function of the ith component. For each component, the model parameters to be estimated are β_i and $\lambda_i = \{\mu_i, \Sigma_i\}$, the latter of which include the mean vector μ_i and covariance matrix Σ_i (Duda et al., 2001). During the model learning, the following log-likelihood function is used as objective function to estimate the parameter values

$$\log L(x \mid \Lambda) = \sum_{j=1}^{N} \log\left(\sum_{i=1}^{K} \beta_i g(x_j \mid \lambda_i) \right) \tag{2}$$

where x_j is the jth training sample among the total N measurements.

The static Gaussian mixture model can be estimated by the modified E-M algorithm through the following iterative procedure:

- E-Step: compute the posterior probability of the jth training sample x_j at the sth iteration

$$P^{(s)}(C_i \mid x_j) = \frac{\alpha_i^{(s)} g(x_j \mid \lambda_i^{(s)})}{\sum_{l=1}^{K} \beta_l^{(s)} g(x_j \mid \lambda_l^{(s)})} \tag{3}$$

where C_i denotes the ith Gaussian component.

- M-Step: update the model parameters at the (s+1)th iteration

$$\mu_i^{(s+1)} = \frac{\sum_{j=1}^{N} P^{(s)}(C_i \mid x_j) x_j}{\sum_{j=1}^{N} P^{(s)}(C_i \mid x_j)} \tag{4}$$

$$\Sigma_i^{(s+1)} = \frac{\sum_{j=1}^{N} P^{(s)}(C_i \mid x_j)(x_j - \mu_i^{(s+1)})(x_j - \mu_i^{(s+1)})^T}{\sum_{j=1}^{N} P^{(s)}(C_i \mid x_j)} \tag{5}$$

$$\beta_i^{(s+1)} = \frac{\sum_{j=1}^{N} P^{(s)}(C_i \mid x_j)}{N} \tag{6}$$

To overcome the drawback of traditional E-M algorithm, the minimum message length (MML) criterion is used as model selection index to search for the optimal number of Gaussian components (Figueiredo and Jain, 2002).

Particle Filter Based DGMM

As the operation scenario may change over time, the Gaussian components and their model parameters need updates accordingly. Particle filter is a sequential model estimation technique and suitable for dynamic processes with non-Gaussian state-space latent variables, while the conventional Kalman filter is based upon the assumption that the state-space variables are Gaussian distributed. In this study, particle filter is employed to update the initial model parameters of Gaussian components and then trigger the mixture model re-learning.

For the estimated mixture density function prior to the updates $p(x \mid \Lambda)$, first generate a set of particle samples $y_t^{(m)}$ with $1 \le m \le N_s$. The posterior probabilities of those particles are set as the corresponding weights $\omega_t^{(m)}$, which can be normalized as

$$\hat{\omega}_t^{(m)} = \omega_{t-1}^{(m)} \frac{p(x_t \mid y_t^{(m)}) p(y_t^{(m)} \mid y_{t-1}^{(m)})}{\sum_{i=1}^{K} \beta_i g(y_t^{(m)} \mid y_{1:t-1}^{(m)}, x_{1:t})} \tag{7}$$

The particle weights may be further approximated as

$$\hat{\omega}_t^{(m)} = \omega_{t-1}^{(m)} p(x_t \mid y_t^{(m)}) \tag{8}$$

Then the effective number of particles may be adjusted as

$$\hat{N}_{eff} = \frac{1}{\sum_{m=1}^{N_s} (\omega_t^{(m)})^2} \tag{9}$$

The posterior filtered density function can be approximated as

$$p(x_t \mid y_{1:t}^{(m)}) = \sum_{m=1}^{N_s} \omega_t^{(m)} \delta(x_t - x_t^{(m)}) \tag{10}$$

where $\delta(\bullet)$ stands for the Dirac delta function.

If the value of $\hat{N}_{eff}$ is less than N_s, resample the particles and repeat the above calculations. After the re-sampling stops, update the parameters of Gaussian components by plugging the particle samples into Eqs. (3)-(6).

The step-by-step procedure of DGMM method is summarized below:

(i). Estimate the Gaussian mixture model with the modified E-M algorithm;

(ii). Generate initial particle samples $\{y_1, y_2, \cdots, y_t\}$ from the estimated mixture density function from Step (i);

(iii). Compute and normalize the corresponding weights $\{\hat{\omega}_1, \hat{\omega}_2, \cdots, \hat{\omega}_t\}$

(iv). Calculate $\hat{N}_{eff}$ and compare with N_s. If $\hat{N}_{eff} < N_s$, go back to Step (ii) and repeat. Otherwise, stop and update model parameters of Gaussian components using the particle samples.

Fault Detection and Diagnosis using DGMM

With the particle filtered Gaussian components, the Bayesian inference based monitoring statistic can be computed and compared against the pre-specified confidence level for fault detection. The particle filtered Bayesian inference probability (PFBIP) index is expressed as

$$\text{PFBIP} = \sum_{i=1}^{\tilde{K}} P(\tilde{C}_i \mid x_T) P_M^{(i)}(x_T) \tag{11}$$

where x_T is the test sample, $\tilde{K}$ is the updated number of Gaussian components after particle filter, $P(C_i \mid x_T)$ represents the posterior probability of x_T within the ith particle filtered Gaussian component $\tilde{C}_i$, and $P_M^{(i)}(x_T)$ denotes the probability of the test sample x_T outside of the Mahalanobis-distance based ellipsoid under the pre-set confidence level $(1-\alpha)\times 100\%$, as computed from the following equation

$$P_M^{(i)}(x_T) = \Pr\{D_r((x, \tilde{C}_i) \mid x \in \tilde{C}_i) \le D_r((x_T, \tilde{C}_i) \mid x_T \in \tilde{C}_i)\} \tag{12}$$

It is noted that D_r is the regularized Mahalanobis distance and follows a χ^2 distribution with l degrees of freedom (Mao and Jain, 1996; Yu and Qin, 2008). During fault detection, the process is identified as faulty operation when the PFBIP value is less than the confidence level. Otherwise, the process operation is determined as normal.

To further diagnose the faulty variables once an abnormal event is detected, the regularized Mahalanobis distance metric can be decomposed as follows

$$\begin{aligned} D_r((x_T, \tilde{C}_i) \mid x_T \in \tilde{C}_i) &= (x_T - \tilde{\mu}_i)^T (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (x_T - \tilde{\mu}_i) \\ &= \sum_{j=1}^{l} \left\{ s^{(j)} (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (x_T - \tilde{\mu}_i) \right\}^2 \end{aligned} \tag{13}$$

where $s^{(j)}$ denotes the jth unit vector and ε is a small number to remove the ill condition of particle filtered covariance matrix $\tilde{\Sigma}_i$. Thus the particle filtered Bayesian inference contribution (PFBIC) index can be defined as

$$\text{PFBC} = \sum_{i=1}^{\tilde{K}} \left\{ P(\tilde{C}_i \mid x_T) \left\{ s^{(j)} (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (x_T - \tilde{\mu}_i) \right\}^2 \right\} \tag{14}$$

which is used to diagnose the leading faulty variables from the contribution plots. In practice, the above contribution index can be normalized so that the sum of all variable contributions equals one.

Case Study

In this research, the Tennessee Eastman process (TEP) (Downs and Vogel, 1993) is simulated to evaluate the effectiveness of the proposed DGMM based monitoring approach and the results are compared to those of regular GMM.

The process includes 12 manipulated variables and 41 measurement variables, among which there are 19 composition variables sampled infrequently. The total 33 continuous variables are selected as monitored variables and the sampling interval for data collection is 3 min. During normal operation, the process may run at any of the six modes as listed in Table 1. The process flow diagram and the list of monitored variables are shown in Figure 1 and Table 2, respectively.

Based on the above possible operating modes, a test scenarios is designed to examine the performance of DGMM monitoring approach. In the test case, the entire operation period consists of three stages. During the first stage, the process is operated between Modes 1 and 4 with equal possibility. Then in the second stage, it runs at either Mode 3 or 6 with 60% possibility under Mode 3 while 40% of Mode 6. In the last stage, the process is among Modes 4, 5 and 6 with equal possibility. Total 4500 training samples are collected from the three operation stages with 1500 observations at each stage. In the test set, 100 normal samples from either Mode 3 or 6 are generated and then followed by 200 faulty ones, which involve a slow drifting error in reaction kinetics.

Table 1. Six operating modes in TEP

Mode	G/H Mass Ratio	Production Rate
1	50/50	7038 kg/h G/H
2	10/90	1408 kg/h G 12669 kg/h H
3	90/10	10000 kg/h G 1111 kg/h H
4	50/50	Maximum
5	10/90	Maximum
6	90/10	Maximum

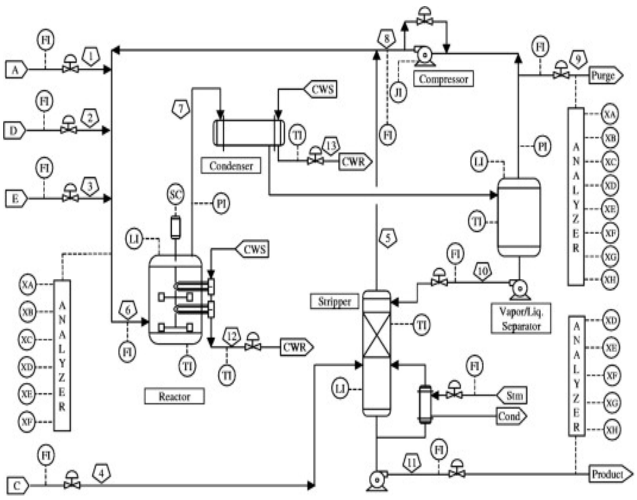

Figure 1. Flow Diagram of Tennessee Eastman Chemical Process (Downs and Vogel, 1993)

Table 2. Monitored Variables in TEP

No.	*Monitored Variable*
1	A feed rate
2	D feed rate
3	E feed rate
4	A+C feed rate
5	Recycle flow rate
6	Reactor feed rate
7	Reactor pressure
8	Reactor level
9	Reactor temperature
10	Purge rate
11	Separator temperature
12	Separator level
13	Separator pressure
14	Separator underflow
15	Stripper level
16	Stripper pressure
17	Stripper underflow
18	Stripper temperature
19	Steam flow rate
20	Compressor work
21	Reactor cooling water temperature
22	Condenser cooling water temperature
23	D feed valve
24	E feed valve
25	A feed valve
26	A+C feed valve
27	Recycle valve
28	Purge valve
29	Separator valve
30	Stripper valve
31	Steam valve
32	Reactor cooling water flow
33	Condenser cooling water flow

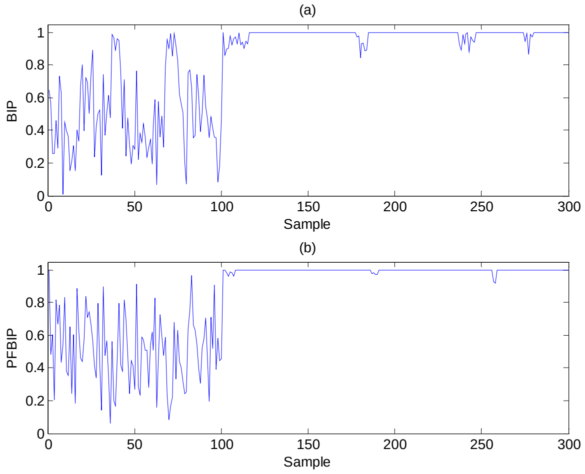

Figure 2. GMM Based BIP and DGMM Based PFBIP Plots for Fault Detection

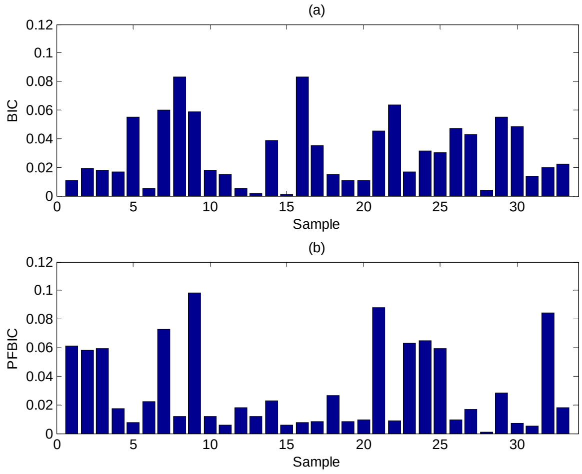

Figure 3. GMM Based BIC and DGMM Based PFBIC Contribution Plots for Fault Diagnosis

Table 3. Quantitative Comparison of GMM and DGMM Approaches in Fault Detection

Method	Fault Detection Rate	False Alarm Rate
GMM	86.5%	8%
DGMM	95.5%	2%

The detected faulty samples are further fed into the diagnosis scheme to identify the leading abnormal variables. The GMM and DGMM based contribution plots are shown in Figure 3(a) and (b). When the slow drift error on reaction kinetics occurs, the reactor temperature and pressure drift away from the steady-state values. Subsequently, the reactor cooling water outlet temperature changes and causes the reactor cooling water flow to respond. Furthermore, the feed flows of reactants A, D and E should change in order to balance the reaction and catch up with the new steady states. The PFBIC plot in Figure 3(b) successfully points out the leading variables including reactor temperature, pressure, coolant flow and reactant feeds. The BIC plot in Figure 3(a), however, does not capture the faulty variables accurately due to the dynamic shifting effects of different operating modes. The mixture model identified from the training data in this situation is biased without mode trajectory updates. Therefore, both the fault detection and diagnosis results of regular GMM method suffer from the static operating scenario assumption.

Conclusions

In this article, a new dynamic Gaussian mixture model based fault detection and diagnosis method is proposed for complex multimode processes with time-varying operation scenario shifts. The particle filter algorithm is adopted to account for the dynamic mode trajectory and update the mixture model parameters. Then the particle filtered Bayesian inference probability index and contribution metric are derived to detect abnormal operation events and diagnose major faulty variables, respectively.

The particle filtered DGMM approach is applied to the Tennessee Eastman process with shifting operation scenarios and the monitoring results are compared to those of GMM method. The superior performance of DGMM approach in terms of fault detection rate, false alarm rate and variable diagnosis demonstrates that it is a powerful technique to monitor non-Gaussian process with complicated operation scenario shifts and strong transient behaviors.

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