커널주성분분석을 이용한 회분 공정모니터링 기술

(Fault Detection of Batch Processes Using Multiway Kernel Principal Component Analysis)

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현재까지의 대부분의 회분식 공정 모니터링 방법은 주 성분 분석을 이용하고 있으나 주 성분 분석은 선형 분석법이다. 일반적으로 회분식 공정은 비선형성이 강하기 때문에 비선형성을 고려한 새로운 모니터링 기술이 필요하다. 이를 해결하기 위해 비선형 주성분 분석을 토대로 하는 여러 방법이 제시되어 왔다. 1991 년 Kramer 가 auto-associative neural networks 를 이용한 비선형 주성분 분석을 제시하였으나 5 개의 layer 로 구성되어 있기 때문에 학습하기가 매우 어려우며 각 layer 마다 노드를 몇 개씩 설정해야하는지에 대한 문제점을 가지고 있다. 1996 년 Dong 과 McAvoy 가 principal curve 와 뉴럴넷을 이용한 비선형 주성분 분석법을 제시하였다. 하지만 이 방법은 optimization 과정이 필요하고 미리 주성분 개수를 정해서 학습을 시켜야하는 단점이 있다.

한편, 1998 년 Scholkopf 등이 커널 주성분 분석이라는 새로운 비선형 주성분 분석법을 발표하였다. 이 방법은 커널 함수라는 무한 차수의 비선형 함수를 이용하여 비선형데이터를 매핑시키는데 이 과정에 의해 비선형 데이터가 보다 선형 데이터를 이루게 된다. 선형화된 데이터에 기존의 주성분분석을 적용함으로써 비선형성을 고려할 수 있게 된다. 커널 함수로 매핑 시키고 주성분분석을 이용하여 데이터 차수를 떨어뜨리는 과정을 커널 함수를 미리 정의함으로써 아주 간단하게 수식화 할 수 있게 된다. Scholkopf 등은 이러한 장점을 이용하여 feature selection, classification

등에 적용하여 좋은 결과를 보여주었다. 커널 주성분 분석은 커널 함수만 정의해주면 계산절차가 매우 간단하고 주성분 개수를 미리 정해줄 필요없이 나중에 선택할 수 있기 때문에 기존의 방법보다 많은 장점을 가지고 있다.

1. Off-line Analysis of Batch Process Data Using MKPCA

Batch processes are, by nature, a 3-way matrix ($\underline{\mathbf{X}}(I \times J \times K)$) of data. In a typical batch run, $j = 1, 2, \ldots, J$ variables are measured at $k = 1, 2, \ldots, K$ time intervals throughout the batch. There exists similar data on several ($i = 1, 2, \ldots, I$) similar process batch runs. MPCA needs to unfold this matrix in order to obtain a two-way matrix, and then performing PCA. Fig. 1 shows the unfolding method for MPCA. By subtracting the mean of each column of unfolded matrix ($\mathbf{X}(I \times JK)$), the mean trajectory of each variable is removed, so that major nonlinear behavior of the process can be eliminated (Nomikos & MacGregor, 1994 and 1995). Once the matrix is mean centered and variance scaled and PCA is performed, then the results from PCA are the loading vectors and the calculated scores for each batch. The loading vectors have a weight for each variable at each time, which gives the history of the process. In this paper, we used KPCA instead of PCA to extract nonlinear structure of the unfolded matrix, $\mathbf{X}(I \times JK)$.

A measure of the variation within the MKPCA model is given by Hotelling's T^2 statistic. T^2 is the sum of the normalized squared scores, and is defined as

$$T^2 = [t_1, \ldots, t_p]\Lambda^{-1}[t_1, \ldots, t_p]^T \quad (1)$$

where t_k is obtained from KPCA, p is the number of PCs and $\mathbf{\Lambda}^{-1}$ is the diagonal matrix of the inverse of the variances associated with the retained principal components. The confidence limit for T^2 is obtained using the F-distribution.

$$T^2 \sim \frac{p(I^2-1)}{I(I-p)} F_{p,I-p,\alpha} \tag{2}$$

where I is the number of batches in the model, p the number of principal components, and α significance level.

The measure of goodness of fit of a sample to the PCA model is the squared prediction error (*SPE*), also known as the Q statistic. However, KPCA of Schölkopf, Smola, and Müller (1998) provides only nonlinear principal components and does not consider any reconstruction method of the data in the feature space. So, there is a problem to make a monitoring chart of *SPE*. In this paper, a simple calculation of *SPE* in the feature space F is suggested. Then *SPE* in the feature space is defined as

$$SPE = \left\| \Phi(\mathbf{x}) - \hat{\Phi}_p(\mathbf{x}) \right\|^2 \tag{3}$$

where $\hat{\Phi}_p(\mathbf{x}) = \sum_{k=1}^{p} t_k \mathbf{v}_k$ is the reconstructed with p principal components in the feature space. Here, $\Phi(\mathbf{x})$ is identical to $\hat{\Phi}_n(\mathbf{x}) = \sum_{k=1}^{n} t_k \mathbf{v}_k$ if p equals n where n is the number of nonzero eigenvalues generated from Eq. (8) among N. Therefore, *SPE* is obtained from the following equations.

$$\begin{aligned} SPE &= \left\| \Phi(\mathbf{x}) - \hat{\Phi}_p(\mathbf{x}) \right\|^2 = \left\| \hat{\Phi}_n(\mathbf{x}) - \hat{\Phi}_p(\mathbf{x}) \right\|^2 \\ &= \hat{\Phi}_n(\mathbf{x})^T \hat{\Phi}_n(\mathbf{x}) - 2\hat{\Phi}_n(\mathbf{x})^T \hat{\Phi}_p(\mathbf{x}) + \hat{\Phi}_p(\mathbf{x})^T \hat{\Phi}_p(\mathbf{x}) \\ &= \sum_{j=1}^{n} t_j \mathbf{v}_j{}^T \sum_{k=1}^{n} t_k \mathbf{v}_k - 2\sum_{j=1}^{n} t_j \mathbf{v}_j{}^T \sum_{k=1}^{p} t_k \mathbf{v}_k + \sum_{j=1}^{p} t_j \mathbf{v}_j{}^T \sum_{k=1}^{p} t_k \mathbf{v}_k \\ &= \sum_{j=1}^{n} t_j{}^2 - 2\sum_{j=1}^{p} t_j{}^2 + \sum_{j=1}^{p} t_j{}^2 = \sum_{j=1}^{n} t_j{}^2 - \sum_{j=1}^{p} t_j{}^2 \end{aligned} \tag{3}$$

where $\mathbf{v}_j{}^T \mathbf{v}_k = 1$ when $j = k$, $\mathbf{v}_j{}^T \mathbf{v}_k = 0$ otherwise.

In off-line batch analysis, the confidence limit for the *SPE* can be computed from its approximate distribution

$$SPE_\alpha = \Theta_1 \left[\frac{c_\alpha \sqrt{2\Theta_2 h_0^{\ 2}}}{\Theta_1} + 1 + \frac{\Theta_2 h_0 (h_0 - 1)}{\Theta_1^{\ 2}} \right]^{1/h_0} \tag{4}$$

where c_α is the standard normal deviate corresponding to the upper (1-α) percentile, λ_j is the eigenvalue associated with the j^{th} loading vector, $\Theta_i = \sum_{j=a+1}^{d} \lambda^i{}_j$ for $i = 1,2,3$ and $h_0 = 1 - \frac{2\Theta_1\Theta_3}{3\Theta_2^{\ 2}}$ (Nomikos & MacGregor, 1995).

2. Procedure for On-line Batch Monitoring using Multiway KPCA

A. 정상상태 공정 모델링 (NOC model)

1) Acquire normal operating data $\underline{\mathbf{X}}(I \times J \times K)$ and unfold it batch-wise $\mathbf{X}(I \times JK)$.

2) The data $\boldsymbol{X}(I \times JK)$ are normalized using the mean and standard deviation of each variable at each time in the batch cycle over all batches.

3) Given a set of *JK*-dimensional scaled normal operating data $\mathbf{x}_k \in R^{JK}$, $k = 1, \ldots, I$, we compute the kernel matrix $\mathbf{K} \in R^{I \times I}$ by $[\mathbf{K}]_{ij} = K_{ij} = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle = [k(\mathbf{x}_i, \mathbf{x}_j)]$.

4) Carry out mean centering in the feature space for $\sum_{k=1}^{I} \tilde{\Phi}(\mathbf{x}_k) = 0$,

$$\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_I \mathbf{K} - \mathbf{K} \mathbf{1}_I + \mathbf{1}_I \mathbf{K} \mathbf{1}_I \tag{5}$$

where, $\mathbf{1}_I = \frac{1}{I} \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \in R^{I \times I}$.

5) Carry out variance scaling in the feature space for $\frac{1}{I-1}\sum_{k=1}^{I}\tilde{\Phi}_{scl}(\mathbf{x}_k)^2 = 1$

$$\tilde{\mathbf{K}}_{scl} = \frac{\tilde{\mathbf{K}}}{\frac{trace(\tilde{\mathbf{K}})}{I-1}} \quad (6)$$

6) Solve the eigenvalue problem $I\lambda\,\boldsymbol{\alpha} = \tilde{\mathbf{K}}_{scl}\boldsymbol{\alpha}$ and normalize $\boldsymbol{\alpha}_k$ such that $\langle \boldsymbol{\alpha}_k, \boldsymbol{\alpha}_k \rangle = \frac{1}{\lambda_k}$.

7) For normal operating data $\mathbf{x}$ at each normal batch, we extract a nonlinear component via

$$t_k = \langle \mathbf{v}_k, \tilde{\Phi}_{scl}(\mathbf{x}) \rangle = \sum_{i=1}^{I} \alpha_i^k \langle \tilde{\Phi}_{scl}(\mathbf{x}_i), \tilde{\Phi}_{scl}(\mathbf{x}) \rangle = \sum_{i=1}^{I} \alpha_i^k \tilde{k}_{scl}(\mathbf{x}_i, \mathbf{x}) \quad (7)$$

where $\tilde{\Phi}_{scl}(\mathbf{x})$ is the mean centered and variance scaled feature vector of $\Phi(\mathbf{x})$.

8) Calculate the monitoring statistics (T^2 and *SPE*) of normal operating data at each batch

9) Determine control limits of T^2 and *SPE* charts

B. 실시간 공정 모니터링 (On-line Monitoring)

1) For new batch data until time k, $\mathbf{X}_t(k \times J)$, unfold it to $\mathbf{x}_t^T(1 \times Jk)$. Scale it with the mean and the variance obtained at step 2) of the modeling procedures.

2) Anticipate the future observations by the method mentioned earlier

3) Given *JK*-dimensional scaled test data $\mathbf{x}_t \in R^{JK}$, we compute the kernel vector $\mathbf{k}_t \in R^{1 \times I}$ by $[\mathbf{k}_t]_j = [k_t(\mathbf{x}_t, \mathbf{x}_j)]$ where $\mathbf{x}_j$ is the scaled normal operating data used in step 3) of the modeling procedures: $\mathbf{x}_j \in R^{JK}$, $j = 1, \ldots, I$.

4) The test kernel vector $\mathbf{k}_t$ is mean centered as follows;

$$\widetilde{\mathbf{k}}_t = \mathbf{k}_t - \mathbf{1}_t\mathbf{K} - \mathbf{k}\mathbf{1}_I + \mathbf{1}_t\mathbf{K}\mathbf{1}_I \quad (8)$$

where $\mathbf{K}$ and $\mathbf{1}_I$ are obtained from step 4) of the modeling procedures and $\mathbf{1}_t = \frac{1}{I}[1,\ldots,1] \in R^{1\times I}$.

5) The mean centered kernel vector $\widetilde{\mathbf{k}}_t$ is variance scaled

$$\widetilde{\mathbf{k}}_{tscl} = \frac{\widetilde{\mathbf{k}}_t}{\frac{trace(\widetilde{\mathbf{K}})}{I-1}} \quad (9)$$

6) For the test data $\mathbf{x}_t$, we extract a nonlinear component via

$$t_k = \left\langle \mathbf{v}_k, \widetilde{\Phi}_{scl}(\mathbf{x}_t) \right\rangle = \sum_{i=1}^{I} \alpha_i^k \left\langle \widetilde{\Phi}_{scl}(\mathbf{x}_i), \widetilde{\Phi}_{scl}(\mathbf{x}_t) \right\rangle = \sum_{i=1}^{I} \alpha_i^k \widetilde{k}_{tscl}(\mathbf{x}_i, \mathbf{x}_t) \quad (10).$$

7) Calculate the monitoring statistics (T^2 and SPE) of test data

8) Monitor whether T^2 or SPE exceeds its control limit calculated in the modeling procedure.