Journal of Process Control 66 (2018) 98–107

Contents lists available at ScienceDirect

Journal of Process Control

journal homepage: www.elsevier.com/locate/jprocont

Novel common and special features extraction for monitoring multi-grade processes

Jingxiang Liu [a], Tao Liu [a,*], Junghui Chen [b,*], Pan Qin [a]

[a] Institute of Advanced Control Technology, Dalian University of Technology, Dalian, 116024, P.R. China
[b] Department of Chemical Engineering, Chung-Yuan Christian University, Chung-Li District, Taoyuan, 32023, Taiwan

ARTICLE INFO

Article history:
Received 24 May 2017
Received in revised form 11 January 2018
Accepted 1 March 2018

Keywords:
Multi-grade processes
Process monitoring
Limited samples
Common feature extraction
Subspace division

ABSTRACT

Since industrial plants manufacture different specifications of products in the same production line by simply changing the recipes or operations to meet with diversified market demands, it often happens that very limited samples could be measured for each grade of products, thus inadequate to establish a model for monitoring the corresponding process. To cope with the difficulty for monitoring such multi-grade processes, a novel feature extraction method is proposed in this paper to establish process models based on the available data for each grade, respectively. Firstly, a common feature extraction algorithm is proposed to determine the common directions shared by different grades of these processes. Based on the extracted common features, the principal component analysis is then used to extract the special directions for each grade, respectively. Consequently, each grade of these processes is divided into three parts, namely common part, special part, and residual part. Three indices are correspondingly introduced for on-line monitoring of each part, respectively. A numerical case and an industrial polyethylene process are used to demonstrate the effectiveness of the proposed method.

1. Introduction

In many industrial process operations, it is a common practice that different grades or specifications of one type product (e.g., a high-molecular polymer) are produced by simply changing the operating conditions and/or the ratio of ingredients in the feed to a process [1,2]. In other words, although these processes have different operating conditions, duration time, and product sizes etc., they inherently belong to the same chemical or physical principles for production [3,4]. For example, in the industrial polyethylene process, different product grades are produced with different kinds of plastic materials and quality requirements (such as the melt index) [5], for which the corresponding processes having the same mechanism but with different operating conditions or product specifications were defined as multi-grade processes [6]. Owing to wide applications of multi-grade processes for a lot of industrial manufacturing systems [7–9], it has been increasingly appealed to develop advanced on-line monitoring methods for these processes. However, it often happens that very limited samples could be measured for each grade of these processes, therefore insufficient for establishing reliable models for process monitoring. Note that even if sufficient samples could be measured to establish a detailed model for each grade of these processes, such exercise may require a longer time that is not cost-effective or even impractical for application. Moreover, for operating multi-grade processes, grade changeover is usually conducted by operator in engineering applications, which may result in a large settling time, overshoot, and off-grade products.

In the past three decades, multivariate statistical process modeling (MSPM) methods, such as principal component analysis (PCA) [10], partial least squares (PLS) [11], and Fisher discriminant analysis (FDA) [12,13] have been widely explored for process analysis and monitoring [14]. These modeling methods utilize measured process data rather than a prior process knowledge. However, the traditional MSPM methods were mainly developed based on single-population samples and therefore, may be invalid for the presence of multiple data sets with different properties. To tackle the problem, a number of specific approaches under the heading of 'multi-mode' have been proposed [15–20]. For instance, Gaussian mixture methods (GMMs) were explored to determine different modes and then to establish separate or mixture models [19,20]. By using the principal angle based algorithms for multiple-product data to extract the most relevant directions corresponding to the minimized angles, the references [21,22] developed alternative modeling methods for monitoring processes with multiple

* Corresponding authors.
E-mail addresses: liurouter@ieee.org (T. Liu), jason@wavenet.cycu.edu.tw (J. Chen).

https://doi.org/10.1016/j.jprocont.2018.03.001
0959-1524/

Nomenclature

$\boldsymbol{x}_{i,k}^{T}$	the kth sample in the ith grade
$\mathbf{X}_i$	measured data of the ith grade
$\mathbf{X}$	measured data of all grades
J	the number of variables
M	the number of grades
N_i	the number of measured samples of the ith grade
N	the number of measured samples of all grades
$\mathbf{S}_{\mathrm{t}}$	the total-scatter matrix
$\mathbf{S}_{\mathrm{w}}$	the within-class-scatter matrix
$\mathbf{S}_{\mathrm{b}}$	the between-class-scatter matrix
$\bar{\boldsymbol{x}}$	the mean vector of all measured samples
$\bar{\boldsymbol{x}}_i$	the mean vector of the samples measured from the ith process
$\boldsymbol{p}^{\mathrm{C}}$	the common directions
$\boldsymbol{p}_k^{\mathrm{C}}$	the kth common directions
$\mathbf{P}^{\mathrm{C}}$	the common direction matrix
λ	the eigenvalue
$\boldsymbol{\Lambda}$	diagonal matrix consists of eigenvalue
R^{C}	the number of retained common directions
$\mathbf{X}_i^{\mathrm{C}}$	the common subspace for the ith grade
$\mathbf{E}_i^{\mathrm{C}}$	the residual subspace by subtracting the common part for the ith grade
$\boldsymbol{e}_{i,k}^{\mathrm{C}}$	the kth column of $\mathbf{E}_i^{\mathrm{C}}$
$\boldsymbol{p}_i^{\mathrm{S}}$	the special direction for the ith grade
$p_{i,k}^{\mathrm{S}}$	the kth special direction for the ith grade
$\mathbf{P}_i^{\mathrm{S}}$	the special direction matrix for the ith grade
R_i^{S}	the number of retained special directions for the ith grade
$\mathbf{X}_i^{\mathrm{S}}$	the special subspace for the ith grade
$\mathbf{E}_i$	the overall residual subspace for the ith grade
$\boldsymbol{e}_{i,k}^{T}$	the kth row vector of the residual matrix $\mathbf{E}_i$
$\mathbf{A}$	a non-singular constant matrix
$\boldsymbol{t}_{i,k}^{\mathrm{C}}/\boldsymbol{t}_{i,k}^{\mathrm{S}}$	common/special score vector of the kth sample in the ith grade
$\bar{\boldsymbol{t}}_i^{\mathrm{C}}/\bar{\boldsymbol{t}}_i^{\mathrm{S}}$	the mean common/special score vector of all samples in the ith grade
$\boldsymbol{\Sigma}_i^{\mathrm{C}}/\boldsymbol{\Sigma}_i^{\mathrm{S}}$	covariance matrix of common/special score vectors in the ith grade
$T_{i,k}^{\mathrm{C}}/T_{i,k}^{\mathrm{S}}$	statistical magnitude of common/special score of the kth sample in the ith grade
$(T_i^{\mathrm{C}})^2/(T_i^{\mathrm{S}})^2$	threshold of statistical magnitude $(T_{i,k}^{\mathrm{C}})^2/(T_{i,k}^{\mathrm{S}})^2$
$\boldsymbol{\theta}$	parameter vector
α	the probability value of retained components
$SPE_{i,k}$	squared prediction error of the kth sample in the ith grade
SPE_i	threshold of $SPE_{i,k}$ in ith grade
a/b	the estimated mean/variance of $SPE_{i,k}$
g_i/h_i	intermediate variables with respect to a and b
$\boldsymbol{x}_{i,\mathrm{new}}$	new sample from the ith grade
$\boldsymbol{t}_{i,new}^{\mathrm{C}}/\boldsymbol{t}_{i,new}^{\mathrm{S}}$	common/special score of the new sample
$\boldsymbol{e}_{i,new}^{\mathrm{C}}$	the residual by subtracting the common part of the new sample
$\boldsymbol{e}_{i,new}$	the overall residual of the new sample
$T_{i,\mathrm{new}}^{\mathrm{C}}/T_{i,\mathrm{new}}^{\mathrm{S}}$	statistical magnitude of common/special score of the new sample
$SPE_{i,\mathrm{new}}$	squared prediction error of the new sample
$W_{k,j}^{\mathrm{C}}$	the weight of the jth variable of the kth common direction
$W_{i,k,j}^{\mathrm{S}}$	the weight of the jth variable of the kth special direction in the ith grade

operating modes. By comparison, clustering-based modeling methods were presented for monitoring multi-mode processes [23,24] where individual models were established for each mode and then specific indices were defined for monitoring each mode. Note that sufficient samples are needed to apply the above methods for effectively modeling each mode or grade of these processes.

In fact, a lot of multi-grade processes like the above-mentioned polyethylene processes have the same or similar operating conditions but with different ratios of ingredients or else for production. It is therefore desirable to establish a comprehensive model for monitoring all of these processes with different products belonging to the same category. A natural idea is to extract the common features from all data sets of different products for building up an integrated monitoring model [25]. The existing methods such as the three-way factor analysis [26], generalized Procrustes analysis [27], generalized canonical analysis [28], and common PCA (CPCA) [29] may be adopted for this purpose, constructing a common loading matrix which represents the common features for multiple-source data. For instance, the CPCA approach may be used to find out the common principal axes for the covariance matrices of all data, such that these covariance matrices could be simultaneously reduced to a diagonal form by the same orthogonal rotations. A structured overview of simultaneous component methods for dealing with coupled data could be found in the reference [30]. However, it may be somewhat restrictive by using CPCA to assume that the orthogonal principal axes are the same for all data sets, because the underlying distribution of each data set may differ from process to process. Moreover, the common features of different processes are extracted for model building, but the individual features of each process are neglected. To better extract the common features, a two-step multi-set basis vector extraction algorithm (MsVCA) was proposed [31], where basis vectors were constructed to describe the cross-set correlations. However, due to a rank-deficient problem involved with such computation [32], the sampled data were modified by combination coefficients in the first step, which could degrade the monitoring performance. It should be noted that sufficient samples of each data set for different processes are still needed to determine the common features for model building in the above methods. It remains challengeable if there are no sufficient samples for such modeling.

In this paper, a novel feature extraction method is proposed to establish the common and special features of multi-grade processes for simultaneous modeling of all grades and on-line monitoring, based on limited samples that are insufficient for separately modeling individual grades. Firstly, a common feature extraction algorithm is proposed to compute the common directions shared by all grades of these processes, by minimizing the scatter between classes while maximizing the scatter within classes of these processes simultaneously. By subtracting the determined common parts, the special features of each grade are subsequently determined by using PCA, respectively. Thus, each grade of these processes is divided into common part, special part, and residual part. Both common and special features are taken into account for modeling each grade. For on-line monitoring, three indices are defined for the above parts of each grade, respectively, to facilitate practical applications. Meanwhile, the common and special variables can be determined by the proposed method, which can facilitate better understanding of these processes and on-line monitoring.

For clarity, the paper is organized as follows. Firstly, the research background of multi-grade processes is briefly introduced in Section 2. The proposed method for common and special feature extraction are detailed in Section 3. Subsequently, three indices are defined for establishing an on-line monitoring method in Section 4. Two illustrative examples are shown to demonstrate the effec-