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Quality prediction for multi-grade processes by just-in-time latent variable modeling with integration of common and special features

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HIGHLIGHTS

- Novel common feature extraction for multi-grade processes with complex nonlinearity.
- Each grade is divided into common, special and residual parts for model building.
- Just-in-time learning strategy to tackle the nonlinearity for on-line monitoring.
- Efficient quality prediction based on the integration of common and special features.

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ABSTRACT

To cope with the difficulty of on-line quality prediction for multi-grade processes widely operated in process industries, a just-in-time latent variable modeling method is proposed based on extracting the common and special features of multi-grade processes. Considering the complicated nonlinear characteristics of multi-grade processes encountered in engineering applications, a just-in-time learning (JITL) strategy is developed to choose the relevant samples from different grades with respect to the query sample. A novel common feature extraction algorithm is proposed to determine the common directions shared by different grades of processes. After extracting the common features, a partial least-squares modeling algorithm is used to extract the special directions for each grade, respectively. Hence, product quality prediction can be simply conducted by integrating the common and special parts of each grade for model building in terms of a JITL strategy. A numerical case and an industrial polyethylene process are used to demonstrate the effectiveness and advantage of the proposed method.

1. Introduction

To meet with various market demands, multi-grade processes have been widely operated to yield multiple products with different specifications in process industries (Liu, 2007; Liu and Chen, 2013). These processes inherently belong to the same chemical or physical principles, but have different product sizes, operating conditions, and duration time etc (Jaeckle and MacGregor, 1998; Lu et al., 2009). Take the industrial polyethylene process for example, different grades of products are produced with different proportions of plastic materials and quality requirements (e.g., melt index (MI)) (Liu and Chen, 2013). Owing to wide applications of multi-grade processes, it has been increasingly appealed to develop advanced quality prediction methods for these processes (Sharmin et al., 2006). For multi-grade processes, grade changeover is often conducted in operating these processes, which could result in a large settling time, overshoot, and off-grade products. Establishing a detailed principle model for each grade of these processes may require a long time, and could be troublesome or even impractical for engineering application (Kim et al., 2005). To deal with this problem, process operation data have been increasingly explored to develop data-driven methods for multi-grade processes. However, it is often encountered in practical applications that there is no sufficient data to establish data-driven models for each grade of these processes, respectively. Integrated modeling methods were therefore proposed for using multiple data sets, mainly including the 3-way factor analysis methods (Kroonenberg and Leeuw, 1980), generalized Procrustes analysis (Tenberge, 1977), generalized canonical analysis (Dahl and Naes, 2006), and the common PCA (CPCA) approach (Flury, 1984). A structured overview of simultaneous component integration methods was provided for analysis of coupled data sets (Van Deun et al., 2009). By using

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the principal angle based algorithms for multiple-product data to extract the most relevant directions in terms of the minimized angles, the references (Zhao et al. 2004, 2006) developed a multiple PCA model building method for manufacturing processes with multiple operating modes. A common feature of the above methods lies with extending the existing methods for single-population samples to the multiple-populations samples, with an aim to construct a 'consensus' type of matrix to reflect the common information for all data sets.

In the past two decades, soft sensors have been intensively explored to predict product qualities owing to the difficulties involved with on-line measurement of process quality properties (Yuan et al., 2014; Yao and Gao, 2009; Kadlec et al., 2009). Data-driven soft sensors for quality prediction have been mainly developed by using the statistical analysis methods including the partial least-squares (PLS) (Li et al., 2005; Burnham et al., 1996), support vector regression (SVR) (Lee et al., 2005) and least-squares support vector regression (LSSVR) (Shi and Liu, 2006), and Gaussian process regression (GPR) (Ge et al., 2011; Yu, 2012). Although no prior knowledge of the process is needed, these methods require a sufficient number of sample data for quality modeling. For multi-grade processes, it is desired to develop a unified soft sensor model to predict product quality for each grade of these processes. In fact, the underlying data distribution of each grade may differ from each other. In the published papers, PLS was applied to predict the MI in the chemical processes (Sharmin et al., 2006), which would lose validity for the complicated nonlinear processes. Fuzzy c-means (Liu, 2007) and clustering-based methods (Kim et al., 2005) were suggested to assign the sample data to different clusters to establish model prediction for each grade, respectively. However, the clustering-based methods may not be applied if the sample data are very limited for any grade of these processes. To analyze the common feature of multi-set data for multi-grade processes, a two-step basis vector extraction algorithm multi-set regression analysis (MsRA) (Zhao and Gao, 2012) is designed, which focuses on matching the pure variable correlations from one set to another. The extracted basis vectors focus on maximizing their cross-set linear correlations. These basis vectors are regarded to be common ones and can be employed to explain the variable similarity over sets. However, due to a rank-deficient problem involved with such computation, the combination coefficients of the initial measured data were used instead for model building, which in fact had no physical meaning and might degrade the overall prediction performance (Zhao et al., 2010). Owing to grade changeover is frequently operated in engineering applications, the above PLS and MsRA methods were extended to model the process transitions (Duchesne et al., 2002; Zhao et al., 2013). It should be noted that most of the existing methods including the aforementioned had been devoted to establishing linear models for quality prediction.

To cope with nonlinear properties of many industrial processes, just-in-time learning (JITL) modeling methods were proposed in the literature (Atkeson et al., 1997; Cheng and Chiu, 2005; Fujiwara et al., 2009; Ge and Song, 2010; Liu et al., 2012). In the JITL model structure, a local model is built up by using the most relevant samples from the historical data set with respect to a query sample. JITL based modeling methods are different from the traditional off-line or recursive soft sensors that need to establish global models. Generally, a JITL model is built up on-line in a "lazy learning" manner to track the current state of the process. In this way, a JITL model could provide effective description of nonlinear process characteristics with respect to the time evolution.

In this paper, a just-in-time common and special feature extraction (JCSFE) method is proposed to establish on-line quality prediction models for multi-grade processes. There are three steps in the proposed JCSFE method. The first step is to develop a JITL strategy to select the most relevant samples from historical data of each process grade with respect to a query sample. The second step is to extract the commonly shared features based on all the selected samples, by maximizing the correlation between process variables and quality variables while minimizing the scatter between different process grades. The third step is to identify the special features of each process grade, after subtracting the determined common parts from the correspondingly selected samples. Thus, each grade is divided into common, special and residual parts in the proposed method. On-line quality prediction is conducted based on the common and special features of each process grade. For practical applications with limited samples of each process grade, the proposed JCSFE method could show obvious advantage over the existing methods where each process grade was modelled separately.

For clarity, the paper is organized as follows. Firstly, the problem of quality prediction for multi-grade processes is briefly introduced. A novel JCSFE method is therefore proposed for on-line quality prediction in the following section. A numerical case and an industrial polyethylene process are then used to demonstrate the effectiveness and advantage of the proposed method. Finally, some conclusions are drawn.

2. Problem description

It is common in industrial applications that a manufacturing system produces different grades of products by simply changing material types and operating conditions, while complying with the sample principle for production. The corresponding processes are called multi-grade processes. Suppose there are M grades in these processes, the process data and quality data are denoted by $\mathbf{X}_i = [\boldsymbol{x}_{i,1}, \ldots, \boldsymbol{x}_{i,N_i}]^{\mathrm{T}} \in \Re^{N_i \times J_x}$ and $\mathbf{Y}_i = [\boldsymbol{y}_{i,1}, \ldots, \boldsymbol{y}_{i,N_i}]^{\mathrm{T}} \in \Re^{N_i \times J_y}$, where, $\boldsymbol{x}_{i,n} \in \Re^{J_x}$, $\boldsymbol{y}_{i,n} \in \Re^{J_y}$, J_x and J_y are the numbers of process variables and quality variables, respectively, $n = 1, \ldots, N_i$, $i = 1, \ldots, M$. For the convenience of modeling and on-line quality prediction, J_x and J_y are specified to be the same for all grades. Denote by N_i the number of measured samples for the ith grade, and by $N = \sum_{i=1}^{M} N_i$ the total samples of all grades. Owing to that grade changeover is generally associated with multi-grade process operation for yielding products with different specifications, it is of paramount important to establish on-line prediction of product qualities for control design and system operation, in order to reduce the amount of off-grade products.

It should be recognized that if there are sufficient samples measured for each process grade, they should be used to build up the corresponding quality prediction models, respectively. However, it is often encountered in engineering applications that the samples measured in each grade of these processes are very limited, bring difficulties to separate model building for each grade. Moreover, nonlinear characteristics are usually involved with multi-grade processes in industrial applications, thus hindering the application of linear modeling methods mainly developed in the literature. There are two typical characteristics associated with multi-grade processes: (1) The samples measured in different process grades share some common features; (2) Each process grade has its own features, named special features, different from other process grades. As far as we know, it remains open to extract the shared common features for building up quality prediction model (s) with limited data for multi-grade processes. The main difficulties to establish an efficient prediction model for multi-grade processes lie with: (1) how to tackle nonlinear characteristics involved with multi-grade processes; (2) how to distinguish the common and special features of each grade.

To effectively use the limited data sampled for each process grade, a novel common and special feature extraction method is proposed in this paper to build up a unified quality prediction model for on-line application. To deal with nonlinear