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Self-tuning final product quality control of batch processes using kernel latent variable model

Runda Jia[a,b,*], *Zhizhong Mao*[a,b], *Fuli Wang*[a,b], *Dakuo He*[a,b]

[a] *School of Information Science & Engineering, Northeastern University, Shenyang 110004, China*
[b] *State Key Laboratory of Synthetical Automation for Process Industries, Northeastern University, Shenyang 110004, China*

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ABSTRACT

A mid-course correction (MCC) strategy based self-tuning final product quality control of batch processes is presented. The method employs KPLS model developed using batch-wise unfolding data set to capture the relationship between the process variables and final quality. The estimators for the future unknown trajectories are accomplished using statistical latent variable missing data imputation method based on multi-PCA models. Then the optimal control problem is formulated such that the solution is constrained to lie in the kernel latent variable space of the model defined by historical batch data set, and heuristic rule is used for weighting factor to balance the control objective and score magnitude. Finally, SQP is implemented to solve the constraint optimization problem. Application to a simulated cobalt oxalate synthesis process demonstrates that the proposed modeling and quality control strategy can improve process performance.

1. Introduction

Batch/semi-batch processes are commonly used for manufacturing of many high-value-added products such as pharmaceuticals, specialty chemicals, foods and metals. They possess a number of features that lead to interesting control problems, some of which are: the control objective is to obtain a desired product by the end of the batch; the product quality is only available by offline assay after the finish of the batch. In batch/semi-batch processes, it is usually necessary to achieve tight final quality specifications (Flores-Cerrillo and MacGregor, 2003; Albazzaz and Wang, 2004). However, such quality control problems are not easily solved due to the nonlinear behavior of the chemical reactors, and constant changes in raw material properties (Wang and Srinivasan, 2009; Yacoub and MacGregor, 2004).

Theoretical approaches to the control of batch product quality are often based on the use of first principle models (Kozub and MacGregor, 1992; Kravaris and Soroush, 1990). The difficulty in practice is the need for physical insight into the batch processes and a large amount of computational effort that may not be suitable for agile responsive manufacturing. Numerous simpler approaches have been proposed to reduce the variation in product quality based on the idea of mid-course correction (MCC) and empirical models such as partial least squares (PLS) models (Wan et al., 2012; Wang and Srinivasan, 2009; Kano and Nakagawa, 2008; MacGregor et al., 2005; Flores-Cerrillo and MacGregor, 2003; Kesavan et al., 2000; Russell et al., 1998). In these approaches, simple and easily available online measurements with some offline measurements at some mid-course points (decision points) are used to predict the final product quality. If the final quality predicted by empirical models fall out of a statistically defined acceptable region, the mid-course correction should be employed to get the product quality back to this desired region. The central assumption of these approaches is that process conditions during the batch will tend to dominate systematic batch-to-batch variation (Wang and Srinivasan, 2009), thus the riddle for the absence of future data is usually solved by utilizing data imputation methods (Arteaga and Ferrer, 2002; Nelson et al., 1996).

* *Corresponding author at*: School of Information Science & Engineering, Northeastern University, Shenyang 110004, China. Tel.: +86 24 83689525; fax: +86 24 83687434.
E-mail address: jiarunda@ise.neu.edu.cn (R. Jia).
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However, in some industrial applications, nonlinear models are more appropriate than linear ones to capture the behavior of the batch processes (Zhang, 2009). In order to deal with the nonlinear issue of the batch quality control, an artificial neural network (ANN) was employed to generate model of batch process relating product quality to process input variables and processing conditions (Joseph and Hanratty, 1993). Yacoub and MacGregor (2004) used nonlinear PLS model and sequential quadratic programming (SQP) to solve several important product development and batch process control objectives. Zhang et al. (2011) used stacked least squares support vector regression (LS-SVM) model to perform the first order Taylor series expansion that linearizes the nonlinear kernel based model and then obtained the solution by solving quadratic programming (QP) problem. Nonetheless, for MCC approaches based on nonlinear data-driven models, the success of the quality control approach depends on the single global model (Golshan et al., 2010), thus a nonlinear modeling method with high prediction accuracy and generalization capability ought to be utilized. And since the nonlinear data-driven model only provides causal information in the region where the model is valid, constraints are necessary to constrain the optimization solution in this region.

Recently, kernel based algorithms are often used to improve the product quality of nonlinear batch process (Zhang and Qin, 2007, 2008; Yan et al., 2004). The proper method to kernel based algorithms for batch process involves the use of kernel partial least squares (KPLS). KPLS can efficiently compute latent variables in the feature space by means of nonlinear kernel functions (Jia et al., 2010; Kim et al., 2005). Compared to other nonlinear modeling methods, the main advantage of the kernel based algorithm is that it does not involve nonlinear optimization, which makes it as simple as the conventional linear PLS. In addition, because of its ability to use different kernel functions, KPLS can handle a wide range of nonlinearities (Rosipal, 2003; Rosipal and Trejo, 2001). This paper considers an alternative MCC based approach for nonlinear problem of the batch product quality control. In this approach, a KPLS model based on historical batch data is built to capture the relationship between the process variables and final product quality. As in most MCC methods, one or more decision points are specified firstly, and then the prediction of final quality based on KPLS model is used to determinate whether or not to take control action at each decision point. If the prediction of the final quality falls out of an acceptable region, the control action is calculated by utilizing optimization technique. The three formulations proposed in this paper are: (i) the unknown future trajectories are estimated using multi-PCA models; (ii) the soft constraint on the score magnitude is used to constrain the solution in the kernel latent variable space of KPLS model; (iii) heuristic rule is used for weighting factor to balance the control objective and score magnitude.

The remainder of this paper is organized as follows. A brief review of the theory of PLS and KPLS is described in Section 2. Section 3 presents the MCC strategy for quality control based on KPLS model. Application of the proposed MCC strategy to a simulated cobalt oxalate synthesis process and some discussions are given in Section 4. Finally, Section 5 draws some concluding remarks.

2. Preliminary materials

2.1. Partial least squares (PLS)

The PLS model aims to describe the linear relationship between input and output variable sets. The observations for each set of variables are stored in matrices, that is the input matrix $\mathbf{X} \in \mathbb{R}^{I\times N}$ and the output matrix $\mathbf{Y} \in \mathbb{R}^{I\times M}$, and possess the model structure

$$\mathbf{Y} = \mathbf{XB} + \mathbf{V} \tag{1}$$

where $\mathbf{B} \in \mathbb{R}^{N\times M}$ is the regression coefficient matrix and $\mathbf{V} \in \mathbb{R}^{I\times M}$ is the residual matrix.

In its basic form, nonlinear iterative partial least squares (NIPALS) algorithm (Wold et al., 2001; Geladi and Kowalski, 1986) is used to sequentially extract the latent variables $\mathbf{t} \in \mathbb{R}^I$, $\mathbf{u} \in \mathbb{R}^I$ and the weight vectors $\mathbf{w} \in \mathbb{R}^N$, $\mathbf{c} \in \mathbb{R}^M$ from the $\mathbf{X}$ and $\mathbf{Y}$ matrices in decreasing order of their corresponding singular values. As a result, PLS algorithm decomposes $\mathbf{X}$ and $\mathbf{Y}$ matrices with mean zero into the form

$$\mathbf{X} = \mathbf{TP}^{\mathrm{T}} + \mathbf{E} \tag{2}$$

$$\mathbf{Y} = \mathbf{UQ}^{\mathrm{T}} + \mathbf{F} \tag{3}$$

where $\mathbf{T} \in \mathbb{R}^{I\times A}$ and $\mathbf{U} \in \mathbb{R}^{I\times A}$ are matrices of the A latent variables, $\mathbf{P} \in \mathbb{R}^{N\times A}$ and $\mathbf{Q} \in \mathbb{R}^{M\times A}$ are matrices of loading vectors, $\mathbf{E} \in \mathbb{R}^{I\times N}$ and $\mathbf{F} \in \mathbb{R}^{I\times M}$ represent matrices of residuals.

When A latent variables are obtained, using the following equalities (Rosipal and Trejo, 2001)

$$\mathbf{W} = \mathbf{X}^{\mathrm{T}}\mathbf{U} \tag{4}$$

$$\mathbf{P} = \mathbf{X}^{\mathrm{T}}\mathbf{T}(\mathbf{T}^{\mathrm{T}}\mathbf{T})^{-1} \tag{5}$$

$$\mathbf{C} = \mathbf{Y}^{\mathrm{T}}\mathbf{T}(\mathbf{T}^{\mathrm{T}}\mathbf{T})^{-1} \tag{6}$$

and the orthogonality of the matrix $\mathbf{T}$ columns, we can write the final regression coefficient matrix $\mathbf{B}$ in the following form

$$\mathbf{B} = \mathbf{X}^{\mathrm{T}}\mathbf{U}(\mathbf{T}^{\mathrm{T}}\mathbf{X}\mathbf{X}^{\mathrm{T}}\mathbf{U})^{-1}\mathbf{T}^{\mathrm{T}}\mathbf{Y} \tag{7}$$

which will be used to make predictions in PLS regression.

2.2. Kernel partial least squares (KPLS)

Since PLS regression is essentially a linear regression method, it can only perform on batch historical data that vary linearly. When the variations are nonlinear, the data can be mapped into a higher dimension space in which they vary linearly. According to Cover's theorem (Shawe-Taylor and Cristianini, 2004), the nonlinear data structure in the input space is more likely to be linear after high-dimensional nonlinear mapping. This higher dimensional linear space is referred to as the feature space $\mathfrak{I}$. KPLS is formulated in this feature space to extend linear PLS to its nonlinear kernel form.

Consider a nonlinear transformation of the input variables $\mathbf{x}_i \in \mathbb{R}^N (i = 1, 2, \ldots, I)$ into the feature space $\mathfrak{I}$

$$\mathbf{x}_i \in \mathbb{R}^N \rightarrow \Phi(\mathbf{x}_i) \in \mathfrak{I} \tag{8}$$

where $\Phi(\mathbf{x}_i)$ is a nonlinear mapping function that projects the input vectors from the input space to the feature space $\mathfrak{I}$. Note that the dimensionality of the feature space is arbitrarily large and can even be infinite. Denote $\mathbf{\Phi}$ as the $I \times S$ matrix whose ith row is the vector $\Phi(\mathbf{x}_i)$ in an S-dimensional feature space $\mathfrak{I}$. A KPLS algorithm can be derived from a sequence of NIPALS steps (Rosipal, 2003). Through the introduction of the kernel trick (Cristianini and Shawe-Taylor, 2000), one can avoid performing explicit nonlinear mapping. Note that $\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}$ represents the $I \times I$ *kernel Gram matrix* $\mathbf{K}$ of the cross dot products between all mapped input data points $\Phi(\mathbf{x}_i)$.

The deflations of the $\mathbf{K}$ and $\mathbf{Y}$ matrices using a new latent variable $\mathbf{t}$ are

$$\mathbf{K} \leftarrow (\mathbf{I} - \mathbf{t}\mathbf{t}^{\mathrm{T}})\mathbf{K}(\mathbf{I} - \mathbf{t}\mathbf{t}^{\mathrm{T}}) \tag{9}$$