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Real-time product quality control for batch processes based on stacked least-squares support vector regression models

Shuning Zhang[a], Fuli Wang[a,b,*], Dakuo He[a,b], Runda Jia[a]

[a] College of Information Science and Engineering, Northeastern University, Shenyang 110004, Liaoning Province, PR China

[b] Key Laboratory of Integrated Automation of Process Industry, Northeastern University, Ministry of Education, Shenyang 110004, PR China

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ABSTRACT

A novel real-time final product quality control method for batch operations based on stacked least-squares support vector regression models (stacked LSSVR) is proposed. It combines midcourse correction (MCC) and batch-to-batch control. To enhance the model prediction accuracy and generalization capability, a stacked LSSVR approach is presented. Quality control is achieved by predicting the final product quality using stacked LSSVR models and adjusting process variables at some pre-specified decision points. Then a decision is made on whether or not control action is taken at every decision point. Once the control action is expected, the manipulated variable values are calculated and the control action is taken to bring the off-spec product quality back to the target. Then a batch-to-batch control is used to overcome the model plant mismatches and unmeasured disturbances. At last, the proposed modeling and quality control strategy is illustrated on a simulated batch reactor.

1. Introduction

Batch and semi-batch processes play an important role in the manufacturing of many high-value-added products such as specialty chemicals, pharmaceuticals, polymers, and biology industries. In these processes, it is necessary to achieve tight final quality specifications. Quality control of batch process is therefore of great importance. However, the success of the quality control approach depends on the accurate process model. Developing first principle models requires physical insight into the batch processes and a large amount of time and may not be suitable for agile responsive manufacturing. Data based empirical models, such as neural network models (Ahmad & Zhang, 2006), partial least square models (Qin & McAvoy, 1992), and support vector regression models (Vapnik, 1995) can be a very useful alternative in this case. Least-squares support vector regression (LSSVR) as an alternate formulation of SVR, has been applied to data-driven process modeling applications and several system identification problems.

However, most of these LSSVR models for quality prediction using historical data are single model, which is strongly influenced by the availability of training data. To build an accurate and robust LSSVR model, ideally a large amount of training data should be made available. However, in practice in many industrial plants the collection of sufficient, appropriate good quality data is still a real problem. In addition, data for off-line measured quality variables are usually limited. Due to the cost in laboratory analysis, off-line quality measurements are generally taken at large time intervals. Limited process data is a serious problem in development of accurate and robust LSSVR models.

In order to address the problem of limited process data, stacked neural networks, also known as aggregated neural networks, have been shown to possess better generalization capability than single neural networks (Sridhar, Seagrave, & Bartlett, 1996; Zhang, Morris, Martin, & Kiparissides, 1997). In the approach, a set of neural network models is developed on a bootstrap re-sampling replication of the original training data. Then the trained individual neural networks are combined. However, the selection of the design parameters for neural network models is usually difficult. Furthermore, the structure determination of neural network models is still unsolved completely. LSSVR can obtain the global solution without the above-mentioned issues. Hence, a stacked LSSVR is presented to model batch processes in this paper.

Despite the large amount of work devoted to improving the model accuracy, model plant mismatches are unavoidable because data for building stacked LSSVR model are usually not abundant in batch processes. Furthermore, the effort of batch process control is often hampered by unknown disturbances. Within-batch control for improving product quality has generated a challenging area of research. Bonvin and co-workers (Bonvin, Srinivasan, & Ruppen, 2002; Srinivasan, Bonvin, Visser, & Palanki, 2003; Srinivasan, Palanki, & Bonvin, 2003) introduced a novel strategy based on

* Corresponding author at: College of Information Science and Engineering, Northeastern University, 3 Lane 11, Wenhua Road, Heping District, Shenyang 110004, Liaoning Province, PR China. Tel.: +86 024 83687434; fax: +86 024 23890912.
E-mail address: flwang@mail.neu.edu.cn (F. Wang).

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characterizing nominal solutions using a simplified theoretical model. However, the central assumptions of the approach are the set of active constraints and the structure of the optimal solution for the manipulated variable trajectories is known a priori. Yabuki and MacGregor (Yabuki & MacGregor, 1997; Yabuki, Nagasawa, & MacGregor, 2002) proposed a practical approach to the control of final product quality in semi-batch reactors using midcourse correction (MCC) policies. In their approach, on-line measurements (e.g. temperatures, flows) are assumed to be available. And off-line laboratory analyses (e.g. residual monomer concentrations, volume-average particle size in the semibatch emulsion polymerization of styrene–butadiene rubber) are assumed to be available for use at one or more times during the progress of the batch. Hence simple and readily available on-line measurements plus some off-line measurements at some midcourse points are used to predict the final product quantities. If the predictions fall outside of a defined in-control region, then a midcourse correction is made to bring the product quality closer to target. Control in MCC approaches which is based on models for quality prediction require the online measurements that form the basis for quality prediction. However, all the data necessary for predicting the end of batch quality becomes available only when the batch has finished. The conundrum from the absence of future data is usually solved by using data imputation methods. Wang and Srinivasan (2009) presented a multi-model based real-time final product quality control strategy for batch operation. However, since the rest information of the batch is not used for modeling, it is hard to ensure the model prediction accuracy. Moreover, the batch-to-batch optimization was not developed in the paper.

Although within-batch control can be able to respond to control errors in real time, it cannot handle those disturbances that persist over a number of batches. Batch-to-batch control can improve the performance of future batch runs using results from previous batches. Various batch-to-batch control strategies have been proposed in the literatures. Lee, Lee, and Kim (2000) propose the quadratic criterion based ILC approach for tracking control for temperature of batch processes based on a linear time-varying error transition model. Clarke-Pringle and MacGregor (1998) used batch-to-batch manipulated variable trajectories adjustments to control MW distribution in linear polymers. The operating policy can be optimized by batch-to-batch control to address the problem of model plant mismatch and/or unknown disturbances in batch processes (Filippi-Bossy, Border, Villermaux, Marchal-Brasselya, & Georgakis, 1989; Rastogi, Fotopoulos, Georgakis, & Stenger, 1992; Zhang, 2008). However, the approach may not always produce on-spec products at the end of the batch, even with perfect tracking control of process variables (Russell, Kesavan, Lee, & Ogunnaike, 1998; Russell, Robertson, Lee, & Ogunnaike, 1998). This is because the regulatory model is hard to capture disturbances' subtle effects on final product quality sufficiently. Hence, the implementation of an off-line calculated trajectory does not guarantee optimal batch performance.

Under batch-to-batch control, the product quality of the current batch run will depend completely on the recipe decided off-line. Real-time feedback control should be integrated into batch-to-batch control in some appropriate manner (Zhang, 2005). Flores-Cerrillo and MacGregor (2003) presented an inferential control strategy that combines within-batch information from process variable trajectories with information from prior batches to control multivariate product quality properties in semi-batch reactors. The approach used the batch-to-batch information to update the PLS model. And the approach assumes that the deviations from the mean trajectories at each one of the time instances along the batch are linear. However, linear approaches are not viable for describing nonlinear processes. An integrated batch-to-batch iterative learning control and on-line shrinking horizon model predictive control strategy for the tracking control of product quality in batch processes was proposed by Xiong, Zhang, Wang, and Xu (2005). However, control actions were taken at every sample, which will increase the computational complexity.

The purpose of this paper is to present an integrated strategy for quality control in batch processes by combining the MCC strategy within a batch with batch-to-batch control strategy. The integrated control strategy can complement both methods to obtain good performance because the MCC strategy can respond to disturbances immediately and batch-to-batch control can correct bias left uncorrected by the MCC strategy. However, the core of the control strategy is an accurate process model. Therefore in order to enhance the model prediction accuracy and generalization capability, a stacked LSSVR model is built on historical data including all measured variables for end-point quality prediction and control calculations. While in the procedure to control a new batch, estimate of the future trajectories is accomplished using a missing data imputation method, i.e. all past data up to the current point in time and the future data which is estimated by the nominal values in our paper are used to predict the final product quality. When the predicted quality deviates beyond a statistically defined in-control zone, MCC are used during the batch's evolution to reduce variations in final quality. At the end of a batch, batch-to-batch control for final product quality is used to bring the new batch's final quality closer to the desired target. The contributions of the paper are as follows: a stacked LSSVR model is proposed to model batch processes for the optimal control purpose, and the optimal manipulated variables are computed within the current batch run and for the next batch run based on stacked LSSVR model.

The rest of this paper is structured as follows. A new modeling method based on stacked LSSVR is introduced in Section 2. Section 3 presents a quality control strategy which combines the MCC strategy and batch-to-batch control strategy based on stacked LSSVR. Application of this control strategy to a simulated batch process is given in Section 4. Finally, Section 5 draws some concluding remarks.

2. Stacked LSSVR

2.1. Least-squares support vector regression

Least-squares support vector regression (LSSVR) proposed by Suykens is an alternate formulation of SVR (Suykens & Vandewalle, 1999; Suykens, Vandewalle, & De Moor, 2001). Consider first a model in the primal weight space of the following form:

$$f(\mathbf{x}) = \boldsymbol{\omega}^{\mathrm{T}}\varphi(\mathbf{x}) + b \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^m$, $\varphi(\cdot)$: $\mathbb{R}^m \to \mathbb{R}^d$ is the mapping to the high dimensional and potentially infinite dimensional feature space, $\boldsymbol{\omega}$ is weight vector, and b is bias term. Given a training set of n points $\{\mathbf{x}_k, y_k\}_{k=1}^n$ with input data $\mathbf{x}_k \in \mathbb{R}^m$ and output data $y_k \in \mathbb{R}$, e_k is the deviate between the output data y_k and the model prediction $f(\mathbf{x}_k)$, i.e. $y_k = f(\mathbf{x}_k) + e_k$. Hence we can formulate the following optimization problem in the primal weight space

$$\begin{aligned} &\min_{\boldsymbol{\omega},b,\mathbf{e}} \quad J_p(\boldsymbol{\omega}, \mathbf{e}) = \frac{1}{2}\boldsymbol{\omega}^{\mathrm{T}}\boldsymbol{\omega} + \frac{\gamma}{2}\sum_{k=1}^{n} e_k^2 \\ &\text{s.t.} \quad y_k = \boldsymbol{\omega}^{\mathrm{T}}\varphi(\mathbf{x}_k) + b + e_k, \quad k = 1, \ldots, n \end{aligned} \tag{2}$$

where γ is penalty parameter and e_k is error variable.

However, the primal problem is difficult to solve as $\boldsymbol{\omega}$ is high dimensional. Therefore, let us proceed by constructing the