Operation Profile Optimization for Batch Process through Wavelet Analysis and Multivariate Analysis

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Abstract

In the present work, a new regression method based on wavelet analysis and multivariate analysis is proposed. Referred to as wavelet coefficient regression (WCR), the proposed method can build a statistical model that relates operation profiles with product quality in a batch process. In WCR, selected wavelet coefficients of operation profiles are used as input variables of a statistical model, and thus time-related information such as timing of manipulation can be successfully modeled. In addition, by integrating multivariate analysis and wavelet analysis, WCR can cope with correlation of input variables. As a result, WCR enables us to build a accurate statistical model of a batch process. On the basis of WCR, a data-driven method for improving product quality in a batch process is also proposed. The proposed method can determine operation profiles that can achieve the desired product quality and optimize the operation profiles under a given performance index and various constraints. The usefulness of the proposed WCR and profile optimization method is demonstrated through a case study of lysine production based on a semi-batch fermentation process.

Introduction

More than ever, it becomes crucial in various industries to improve product quality and yield in a brief period of time, as product life cycles are getting shorter and international competition is getting keener. Especially, batch processes play an important role to produce specialty or high value-added products. Since batch processes are operated by following predetermined operation profiles, operation profile optimization is a key technology to offer strong competition to others.

To improve product quality and yield and to optimize operation profile, it is necessary to relate product quality with operating condition. In the last decade or so, statistical approaches for building models and optimizing operating conditions have been proposed [1, 2]. In most statistical approaches, partial least squares (PLS) or principal component regression (PCR) has been used. However, it is difficult in general to build a good model of a batch process through conventional multivariate analysis methods. Although multiway methods such as multiway PCA (MPCA) and multiway PLS (MPLS) are available to build batch process models [3, 4], such methods tremendously increase the number of input variables to cope with non-stationary operation profiles. The explosion of input variables would deteriorate the prediction performance of derived models.

In the present research, to realize operation profile optimization of batch processes through a statistical approach, a new regression method based on wavelet analysis and multivariate analysis is proposed. In addition, a data-driven method for improving product quality and optimizing operation profile in a batch process is proposed. The usefulness of the proposed methods is demonstrated through a case study of lysine production based on a semi-batch fermentation process.

Wavelet Coefficient Regression (WCR)

In the present work, to realize operation profile optimization of batch processes, a new regression method based on wavelet analysis and multivariate analysis is proposed. The proposed method uses selected wavelet coefficients of operation profiles as input variables. Therefore, it is referred to as wavelet coefficient regression (WCR).

Consider a batch process, which has I input variables with non-stationary operation profiles, L input variables with constant values, and Q output variables including product quality. These variables are described as $\boldsymbol{u}_i$ $(i = 1, 2, \cdots, I)$, $\boldsymbol{s} \in \Re^L$, and $\boldsymbol{y} \in \Re^Q$, respectively.

First, wavelet decomposition of level J_i is applied to operation profiles $\boldsymbol{u}_i$, and wavelet coefficients $\boldsymbol{a}_{J_i,i}, \boldsymbol{d}_{j,i}$ $(i = 1, 2, \cdots, I;\ j = 1, 2, \cdots, J_i)$ are calculated. Here, $\boldsymbol{a}$ and $\boldsymbol{d}$ are approximation coefficients and detail coefficients, respectively.

The wavelet coefficients are arranged in the form of

$$\boldsymbol{c}_i = \left[\begin{array}{cccc} \boldsymbol{a}_{J_i,i}^T & \boldsymbol{d}_{1,i}^T & \cdots & \boldsymbol{d}_{J_i,i}^T \end{array} \right]^T \tag{1}$$

and then

$$\boldsymbol{c} = \left[\begin{array}{cccc} \boldsymbol{c}_1^T & \boldsymbol{c}_2^T & \cdots & \boldsymbol{c}_I^T \end{array} \right]^T \quad . \tag{2}$$

In addition, matrices $\boldsymbol{S} \in \Re^{N \times L}, \boldsymbol{C} \in \Re^{N \times P}, and \boldsymbol{Y} \in \Re^{N \times Q}$ are generated from the vectors $\boldsymbol{s}$, $\boldsymbol{c}$, and $\boldsymbol{y}$. Here, N denotes the number of batches.

Second, unimportant columns are removed from the wavelet coefficient matrix $\boldsymbol{C}$, and the resultant matrix is denoted by $\boldsymbol{C} \in \Re^{N \times M}$ again. For example, wavelet coefficients or columns of $\boldsymbol{C}$ are judged to be unimportant when the wavelet coefficients are not useful for reconstructing original signals and estimating outputs.

Finally, a statistical model is built by using an arbitrary modeling method after columns of the input data matrices $\boldsymbol{S}$ and $\boldsymbol{C}$ and the output data matrix $\boldsymbol{Y}$ are mean-centered and scaled if necessary.

Profile Optimization

The authors have developed the DDQI (Data-Driven Quality Improvement) method [2]. In this section, a new method for improving product quality and optimizing operation profile in a batch process is proposed by integrating WCR and DDQI.

A statistical model of a batch process can be built through WCR, and it is described as

$$\boldsymbol{y} = \boldsymbol{K}^T \boldsymbol{t} = \boldsymbol{K}^T \boldsymbol{V}_R^T \boldsymbol{z} \tag{3}$$

where $\boldsymbol{z} = [\boldsymbol{s}^T \ \boldsymbol{c}^T]^T$. Each variable in $\boldsymbol{y}$ and $\boldsymbol{z}$ are assumed to be autoscaled. In addition, $\boldsymbol{K}$ denotes a regression coefficient matrix of PCR, $\boldsymbol{t}$ principal component scores, $\boldsymbol{V}_R$ a loading matrix, and R is the number of principal components retained in the PCR model.

Given the desired product quality $\tilde{\boldsymbol{y}}$, the scores $\tilde{\boldsymbol{t}}$ that can achieve $\tilde{\boldsymbol{y}}$ is given by the following equation when $R > Q$.

$$\tilde{\boldsymbol{t}} = (\boldsymbol{K}^T)^+ \tilde{\boldsymbol{y}} + \mathrm{null}(\boldsymbol{K}^T) \tag{4}$$

where $\boldsymbol{A}^+$ denotes the pseudo-inverse matrix of $\boldsymbol{A}$, $\mathrm{null}(\boldsymbol{A})$ the kernel of $\boldsymbol{A}$, and $\dim(\mathrm{null}(\boldsymbol{K}^T)) = R - Q$. The solution $\tilde{\boldsymbol{t}}$ can not be determined uniquely from Eq. (4), but it can be optimized under a given objective function and constraints. The optimal solution $\tilde{\boldsymbol{t}}$ is projected back onto the space spanned by $\boldsymbol{z}$.

$$\tilde{\boldsymbol{z}} = \boldsymbol{V}_R \tilde{\boldsymbol{t}} \tag{5}$$

The derived $\tilde{\boldsymbol{z}}$ is inversely autoscaled, and consequently $\tilde{\boldsymbol{s}}$ and $\tilde{\boldsymbol{c}}$ are derived. Since $P - M$ wavelet coefficients of $\tilde{\boldsymbol{c}}$ were removed when the WCR model was built, such wavelet coefficients are complemented with zero. The wavelet coefficients $\tilde{\boldsymbol{c}}_i$ representing the i-th operation profile are extracted from the reconstructed vector $\tilde{\boldsymbol{c}}$. Finally, the optimal operation profile $\tilde{\boldsymbol{u}}_i$ can be derived by applying inverse wavelet transformation to $\tilde{\boldsymbol{c}}_i$.

Case Study

The usefulness of WCR and the profile optimization method is demonstrated through a case study of lysine production based on a semi-batch fermentation process [5]. In this process, substrate flow rate is manipulated by following the predefined profile.

The lysine production process is operated with various operation profiles of substrate flow rate, and lysine production y at the batch end $T_f = 40$ h is measured. The substrate flow rate is measured every 20 min, and its time-series is denoted by $\boldsymbol{u}$. WCR and multiway PCR (MPCR) are used to build linear regression models. The dimension of inputs, i.e., the number of selected approximation coefficients, is only 18 while the dimension of the operation profile $\boldsymbol{u}$

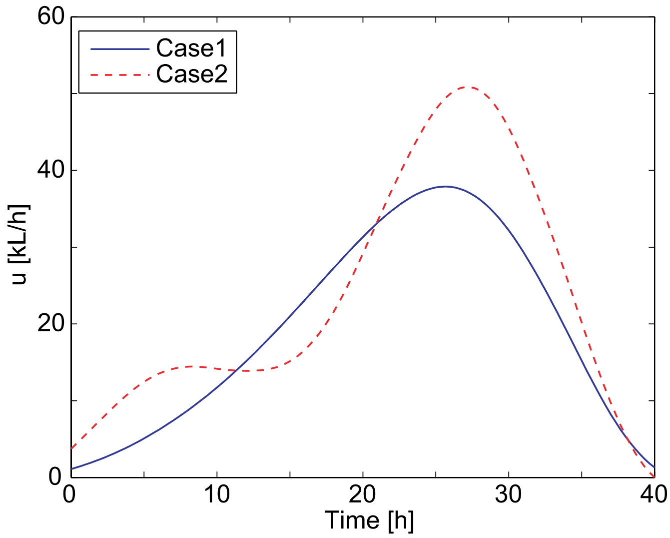

Figure 1: Optimal operation profiles for realizing $\tilde{y} = 30$ with minimum operation cost (Case 1) and for maximizing y (Case 2).

is 121. Furthermore, the input dimension is reduced to 5 through PCA. The model construction results clearly show that WCR is greatly superior to MPCR in prediction performance.

On the basis of the developed WCR model, operation profile optimization is executed for minimization of substrate consumption (Case 1) and for maximization of lysine production (Case 2). The constraints are 1) liquid holdup is below $V_{max} = 1000$ kL, 2) substrate flow rate is not negative, and 3) the solution is interpolated. To satisfy the third constraint, Hotelling's T^2 statistic must be below its threshold. The optimization results are shown in Fig. 1. In Case 1, substrate consumption is reduced from 892 to 782, and lysine production of 30.2 agrees with its desired value of 30. In Case 2, lysine production is 35.7, and liquid holdup at the batch end is its maximum V_{max}.

Conclusions

A new regression method, WCR, is proposed by integrating wavelet analysis and multivariate analysis. In addition, a data-driven method for and optimizing operation profile in a batch process is proposed. The usefulness of the proposed methods is demonstrated through a case study of lysine production process.

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