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Optimizing manipulated trajectory based on principal time-segmented variables for batch processes

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ABSTRACT

Non-unitized loading cosine similarity A recursive optimization method that updates fewer parameters of the manipulated trajectory determined by principal time-segmented variables (PTVs) for batch processes with multi-stage characteristics is presented. First, the correlation analysis between time-segmented variables and the controlled product quality index variable is carried out in a non-unitized orthogonal latent variable space. Next, the parameters of the manipulated trajectory and the PTVs of each stage are determined according to the correlation and trend characteristics of the trajectory. Then, the parameters of the manipulated trajectory are recursively updated according to the cosine similarity between PTVs and the controlled quality index variable. Finally, performance of the proposed optimization technique is evaluated using the Bisphenol A (BPA) crystallization process to verify the effectiveness and advantages of the methods.

1. Introduction

The batch process is well adapted to rapidly evolving market conditions given its flexible production pattern [1], which renders it suitable for wide applications in food, medicine, chemistry, and other fields [2]. However, batch processes are more complex compared to continuous processes owing to their lack of steady operating states and significant dynamic and non-linear characteristics [3,4]. To control product quality, improve efficiency, and meet the environmental criteria of batch processes, leveraging production data to optimize the manipulated trajectory is a worthwhile avenue for exploration [5,6].

Considering the influence of myriad ambiguous process factors and mismatches between established models and actual processes, it is necessary to improve the optimization performance from batch to batch [7]. Based on mechanism modeling, Mandur et al. [8,9] updated mechanism model parameters by using state measurements to ensure that the gradient of the model matches the actual gradient. Further, considering the difficulty and sensitivity of noise when updating all model parameters, Hille et al. [10] proposed that a particular subset of parameters be updated based on the parametric sensitivity of the model output and of the cost and constraint gradients. In general, the establishment of a mechanism model requires a certain degree of expertise, and the complex characteristics of batch processes make it expensive to devise an accurate mechanism model. By contrast, the empirical model is somewhat easier to establish and is more suitable for batch processes [11].

For a gradient-based optimization strategy, Camacho et al. [12] proposed a self-tuning extremum unfolded partial least squares (u-PLS) model to revise the manipulated variable trajectory, after which they [13] introduced smoothing techniques to accelerate the optimization procedure. Based on the quadratic performance index of the optimization strategy, Flores-Cerrillo et al. [14] established a regression relationship between the latent variables and index variables using PLS and then adjusted the latent variables to make the end-time production quality approach the desired value. Duran-Villalobos et al. [15] extended the approach described in Ref. [14] by creating a cost function between the actual process variables and end-time production quality. Li et al. [16] proposed extending the input matrix with outputs of hidden nodes in a radial basis function (RBF) network to establish a nonlinear PLS model, in which the manipulated trajectory is updated from batch to batch.

In the aforementioned approaches, the manipulated trajectory is discretized using a piecewise constant method; a set of constant parameters can be used to describe the trajectory, after which all parameters are updated to achieve the desired optimization performance. For long-period batch processes, a large set of parameters may increase the computational burden and render the optimization algorithm unstable (e.g., falling into a local optimum or ill-conditioned matrix obtained during the calculation) [17]. To deal with this problem, a new parameterization method describing the manipulated trajectory is presented for

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multi-stage batch processes. Then, the parameters of the manipulated trajectory are optimized based on PTVs from batch to batch. These PTVs are selected from time-segmented variables (each segment of the discretized measurement variable trajectory is defined as a time-segmented variable) according to the rounding function that divides the degree of correlation. The correlation between variables is calculated using non-unitized loading cosine similarity. Considering the influence of data quality on optimization performance, the incremental of the controlled quality index variable between batches is introduced into the optimization algorithm. Finally, the proposed method is applied to maximize the feedstock conversion of the BPA crystallization process.

The remainder of this paper is structured as follows. Section 2 introduces the optimization methodology used in this study. The parameterization method of the manipulated trajectory based on the correlation between time-segmented variables and the controlled product quality index variable is described in Subsection 2.1. Subsection 2.2 outlines a non-unitized loading cosine similarity method for correlation calculation. Subsection 2.3 presents an optimization strategy in which fewer manipulated trajectory parameters are adjusted. The effectiveness of the proposed method is demonstrated via a case simulation of the BPA crystallization process in Section 3. Finally, Section 4 provides closing remarks.

2. Methodology

2.1. Parameterization of manipulated trajectory

To describe and adjust the manipulated trajectory more simply, the trajectory parameterization depends on two factors: trajectory trend and the correlation between each time-segmented variable and controlled quality index variable. Taking Fig. 1 as an example, Fig. 1(a) shows a discretized temperature-manipulated trajectory with two stages using piecewise constant parameterization; Fig. 1(b) shows a discretized measurement variable trajectory. The correlation between time-segmented variables $[x_1, x_2, \cdots, x_{15}] \in R^{k\times 15}$ from the discretized measurement variable trajectory and controlled quality index variable $Y = [y^1, y^2, \cdots, y^k]^{\mathrm{T}} \in R^{k\times 1}$ is calculated as shown in Fig. 1(c), where k is the

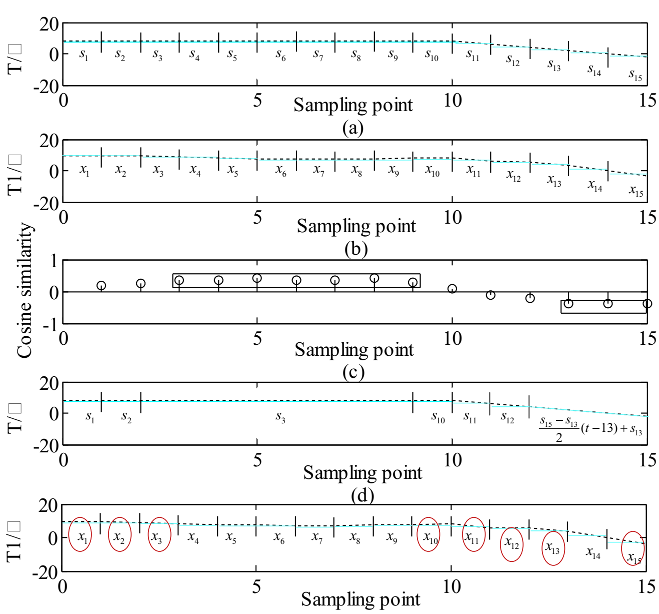

Fig. 1. Manipulated trajectory parameterization.

number of batches. Then we can obtain a new parametric representation of the temperature-manipulated trajectory, displayed in Fig. 1(d). The corresponding mathematical description of trajectory parameterization is as follows:

$$s(t) = \begin{cases} \{s_1, s_2, s_3, s_{10}, s_{11}, s_{12}\} & 0 \le t < 12 \\ \dfrac{s_{15} - s_{13}}{2}(t - 13) + s_{13} & 12 \le t < 15 \end{cases} \tag{1}$$

where $s_1, s_2, \cdots, s_{15}$ are constant parameters from the discretized temperature-manipulated trajectory, and t is the sampling time.

Then, the trajectory can be described by:

$$s = [s_1, s_2, s_3, s_{10}, s_{11}, s_{12}, s_{13}, s_{15}] \tag{2}$$

According to changes in the correlation between each time-segmented variable and controlled quality index variable, the length of the parameterized interval is different. The dividing criteria of parameterized intervals in every stage is given by:

$$\begin{aligned} & f_N \le \phi(|\cos(x, Y)|) < f_{N+1} \\ & s.t. \\ & \Delta t = 1, x \in A_{[f_N, f_{N+1})} \end{aligned} \tag{3}$$

where $x \in R^{k\times 1}$ represents any time-segmented variable, $\phi(\cdot)$ is a custom rounding function to divide the degree of relevance, $\cos(\cdot)$ is cosine similarity, f_N and f_{N+1} are the range of $\phi(\cdot)$, and $A_{[f_N, f_{N+1})}$ represents a set of time-segmented variables with size $\phi(\cdot)$ between f_N and f_{N+1}. To ensure that the time series of all time-segmented variables in $A_{[f_N, f_{N+1})}$ are continuous, the time series difference of the adjacent time-segmented variable in $A_{[f_N, f_{N+1})}$ must be 1; that is, $\Delta t = 1$. Then the set $A_{[f_N, f_{N+1})}$ with the largest number of time-segmented variables is divided into an interval. To select parameters describing this interval, the following process applies: (1) if the trajectory of the interval is a straight line, a parameter may be used to describe the interval, such as s_3 in Fig. 1(c); the parameter can also be obtained by using an appropriate fitting function to fit multiple data points in the interval. (2) If the trajectory of the interval is an oblique line, the parameters at the head and end can be used to describe the interval, as shown in s_{13} and s_{15} in Fig. 1(c); similarly, the parameter can be obtained by using an appropriate fitting function to fit multiple data points in the interval.

The time-segmented variables corresponding to these selected parameters are PTVs used to update the parameters of the manipulated trajectory in the optimization algorithm. The process dynamics are complex in the transitional parts of this stage. Therefore, the piecewise constant parameterization method is still used to describe that part of the trajectory, and each time-segmented variable is considered a PTV. In the above case, the selected PTVs are marked with red in Fig. 1(e).

2.2. Non-unitized loading cosine similarity

To analyze the correlation between the time-segmented and controlled quality index variable, the cosine similarity is calculated by Eq. (4).

$$\cos(Y, x) = \frac{Y^{\mathrm{T}} x}{\|Y\| \|x\|} \tag{4}$$

Information redundancy exists in the original high-dimension data x and Y [18]. To solve this problem and reduce information loss during data processing, a non-unitized loading cosine similarity is presented to calculate the correlation.

Define $X = [x_1, x_2, \cdots, x_c] \in R^{k\times c}$ as a matrix containing c time-segmented variables. Principal component analysis (PCA) is ingeniously adopted to analyze the combined matrix $W = [X \quad Y] \in R^{k\times(c+1)}$: