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Automatic steady state identification for batch processes by nonparametric signal decomposition and statistical hypothesis test

Bi-Ling Huang, Yuan Yao *

Department of Chemical Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan, R.O.C.

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ABSTRACT

In chemical batch processes, online identification of the batch-to-batch steady state is important for ensuring consistency of final product quality and satisfactory process control. In this paper, an automatic steady state identification (SSID) method is developed for batch processes, which utilizes a nonparametric signal decomposition technique named ensemble empirical mode decomposition (EEMD) to extract related information contained in variable trajectories and then conducts a statistical hypothesis test. In the proposed method, EEMD is combined with a moving window procedure to decompose the signal of each variable trajectory into a finite number of intrinsic mode functions (IMFs) in real-time. Then, the inter-batch trend information is extracted by computing the instantaneous frequencies of each IMF. Using the variance ratio test, batch-to-batch steady state can be identified from the inter-batch trend of each process variable. Since most of the disturbance and noise information have been removed through EEMD, robust SSID result can be expected. To deal with the multiple process variables, a multivariate SSID algorithm is proposed based on the statistical test for the equality of covariance matrices. The effectiveness of the proposed method is demonstrated with an injection molding process.

1. Introduction

In today's chemical industry, batch processing is of great importance due to its flexibility in manufacturing low volume and high value-added products. Generally, a batch process can be divided into two stages: the batch-to-batch start-up stage and the steady-state operation stage. Here, the definition of steady state is different from that in continuous processes. According to Aguado et al. [1], a batch process is considered at the batch-to-batch steady state when the trajectory of each process variable follows a stable pattern with random noise, provided that the process is in normal operation. During the start-up stage, the incoming materials usually have not been sufficiently mixed, and the material properties and the machine conditions have not been stabilized. As a result, the batch operation in such stage is unsteady and cannot guarantee acceptable product quality, while consistent and reliable products are only manufactured in steady-state batch operation. Since the durations of start-up are usually unknown and varied from one process to another, defective products cannot be rejected until a series of laboratory analyses is conducted. Such analyses are time-consuming and may cost a lot of labor, materials as well as financial resources. Therefore, an efficient method is desired for online identification of the batch-to-batch steady state, which indicates the consistency of product quality without laboratory analysis. Meanwhile, as discussed in [1], steady state identification (SSID) is also critical for satisfactory batch process control.

Different types of approaches have been proposed in the research field of automatic SSID, as reviewed by Rhinehart [2]. Among them, the most typical approach is based on Von Neumann's work [3], which estimates the signal variance within a moving window using two different methods and tests the ratio of the estimated variances. If the signal is in steady state, the two estimates should be close to each other. Cao and Rhinehart [4] proposed an alternative approach that uses three exponentially weighted moving filters to estimate the sample mean and the sample variance, so as to avoid the storage of historical data. Then, Ruin et al. [5] proposed to conduct principal component analysis (PCA) before performing SSID. However, in most of these approaches, a signal is defined as in steady state when it is constant with noise. Such definition is obviously different from that in the context of this paper. Due to the inherent nonlinear and non-stationary characteristics of batch processes, the batch process signals are seldom constant. Therefore, these methods cannot be adopted directly in batch process applications. To the best of our knowledge, the SSID problem for batch processes was firstly discussed by Aguado et al. [1]. They use a multiway principal component analysis (MPCA) model [6] to extract the information contained in the trajectories of process variables, and then perform the SSID algorithm developed by Cao and Rhinehart [4] on the principal components (PCs) and the model residuals. The major limitation of such method is that it requires a large number of historical data to build an MPCA model, which limits its online application. To avoid such problem, Yao et al. [7] adopt PCA similarity factor and Mahalanobis distance as the indices to summarize the inter-batch similarity between variable trajectories, and conduct the variance ratio test on both indices for SSID. Such

* Corresponding author. Tel.: +886 3 5713690; fax: +886 3 5715408.
E-mail address: yyao@mx.nthu.edu.tw (Y. Yao).

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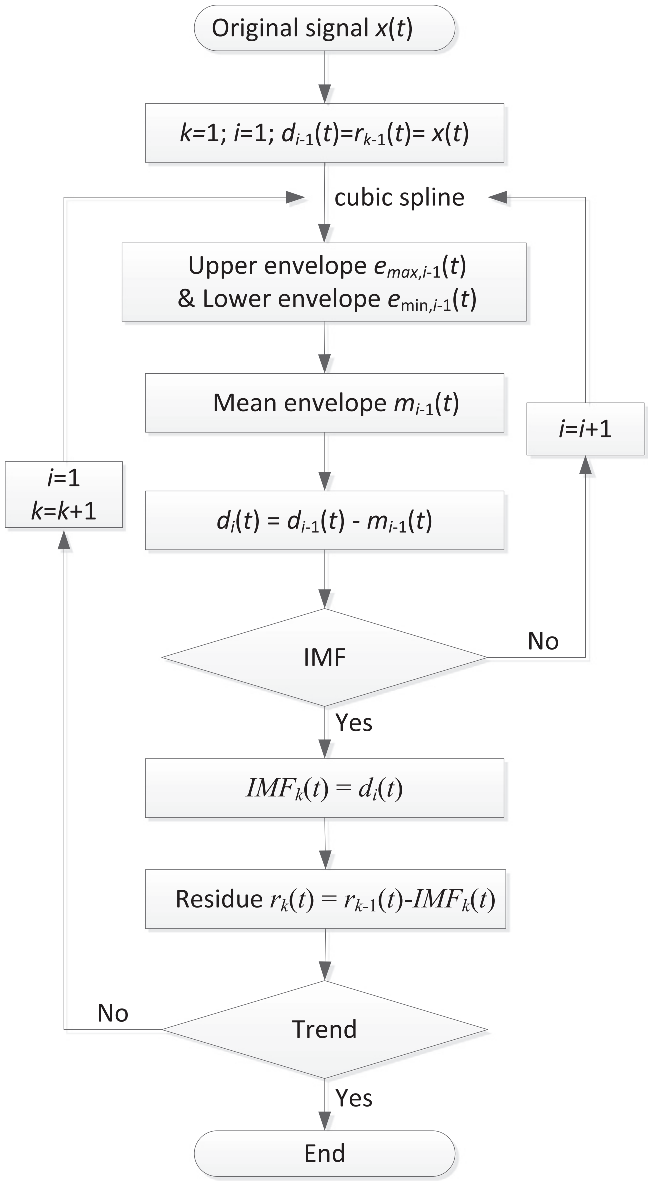

Fig. 1. The sifting process of EMD.

method is more suited to online application. However, the similarity indices tend to be affected by measurement noise and process disturbances, making the method less reliable. In recent years, the two-dimensional dynamic PCA (2D-DPCA) method [8,9] was proposed to model batch process dynamics in both within-batch and batch-to-batch time directions by integrating the PCA technique and the two-dimensional (2D) autoregressive (AR) structure. However, this method assumes that the variable trajectories are stationary 2D time-series, which is not the case in the start-up stage of batch processing. Therefore, 2D-DPCA cannot be applied to batch process SSID.

Typically, the trajectory signal of a batch process variable comprises of high frequency noise, intra-batch variations that include process disturbances with short-term dynamics, and long-term trend from batch to batch. Based on such consideration, this paper proposes to utilize ensemble empirical mode decomposition (EEMD) [10] to decompose the trajectory signals of batch process variables. By doing this, the inter-batch trend can be extracted from each variable trajectory, while the measurement noise and most disturbance information are removed. It is reasonable to expect that more accurate results can be achieved by performing SSID on the inter-batch trend instead of the raw process data. In the first step of the proposed method, EEMD is integrated with the moving window technique to realize online decomposition of batch process signals, i.e. trajectories of process variables. A series of intrinsic mode function (IMF) components can be computed through the decomposition. Then, the generalized zero-crossing (GZC) approach is adopted to calculate the instantaneous frequencies of each IMF, based on which the inter-batch trend is obtained. For each process variable, the SSID result is achieved by conducting the variance ratio test on the inter-batch trend. Furthermore, the SSID algorithm is extended to a multivariate form by testing the equality of covariance matrices.

This paper is organized as follows. The nonparametric decomposition of batch process signals is introduced in Section 2. Then, in Section 3, the GZC approach for the identification of the inter-batch trend is described. Section 4 presents the use of statistical hypothesis tests for SSID. Especially, a multivariate SSID algorithm is developed, and its application to the multiphase batch processes is discussed. In Section 5, the implementation on an injection molding process verifies the effectiveness of the proposed method. Finally, conclusions are drawn in Section 6 to summarize the paper.

2. Decomposition of batch process signals

2.1. EEMD of variable trajectories

In chemical batch processes, variable trajectories are characterized by a variety of nonlinear and non-stationary characteristics that should be taken into consideration during decomposition. Here, EEMD is chosen to decompose the batch process signals, due to its nonparametric nature and capability in handling different types of signals.

The basis of EEMD is empirical mode decomposition (EMD) developed by Huang et al. [11] in 1998. As an adaptive time–frequency data analysis method, EMD separates a time series into a finite number of components corresponding to different frequencies through a sifting process, together with a residue of mean trend. These components are called intrinsic mode functions (IMFs), which should obey the following two requirements. First, the upper and lower envelopes of an IMF are symmetric. Second, the number of zero-crossings and the number of extremes in an IMF are equal or differ at most by one. Thus, the IMFs are approximately monocomponent and orthogonal.

Suppose a batch process signal (i.e. the trajectory signal of a process variable) to decompose is denoted as $x(t)$, where t is the sample index. For the sample collected at the a-th sampling interval in the b-th cycle, $t=(b-1)\times T+a$, where T is the total number of sampling intervals in each cycle. The sifting process finding the IMFs is plotted in Fig. 1, where EMD decomposes the signal from high frequency to

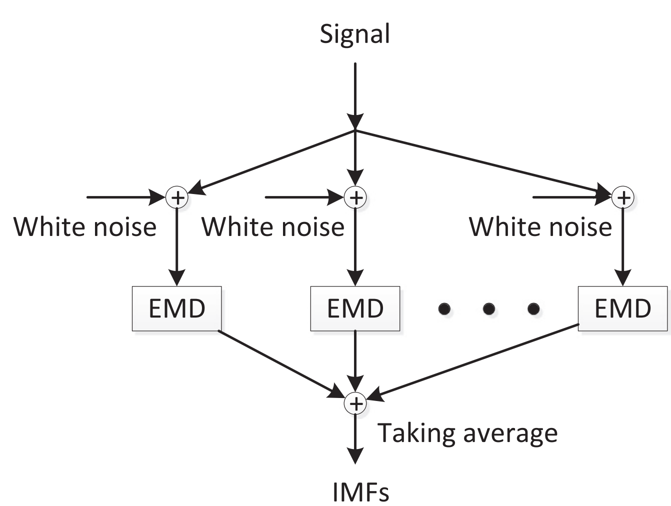

Fig. 2. Illustration of EEMD procedure.