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Refined convergent cross-mapping for disturbance propagation analysis of chemical processes

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ABSTRACT

In chemical processes, determining the root causes of faults and disturbances is important for improving process safety and economic profit. Recently proposed convergent cross-mapping (CCM) is suitable for both linear and nonlinear systems. However, it cannot be directly applied to chemical processes. This is because chemical processes possess characteristics, such as nonlinearity, high dimensions, continuity, and time delay, that are significantly different from ecosystems, where CCM is applicable. In this paper, we propose refined CCM (RCCM), which integrates fast embedding dimension determinations with a modified procedure to improve the speed of the calculation and accuracy of the analysis. Examples show that RCCM fits chemical processes with the above characteristics. In addition, it shows better performance than other methods in finding the propagation paths of disturbances.

1. Introduction

In chemical processes, disturbance propagation paths describe ways in which disturbance signals consisting of stream flows and control paths travel through the process. Root-cause identification of plant-wide faults and disturbances is important for safe and efficient operation of chemical processes. However, because of the process complexity and existence of control loops and time delays, it is still difficult to determine the correct propagation paths. Several methods have been proposed to solve this problem. Most of these methods originate from cause-and-effect analysis approaches and are then utilized to identify the time-delay relationships between the variables. Among the approaches to determine the correct propagation paths, the simplest approach is called cross-correlation analysis (Bauer and Thornhill, 2008). In this method, different values of the cross-correlation function (CCF) are obtained at different time delays. The best estimated time delay and its corresponding cross-correlation are determined by the maximum absolute value of the CCF. Although this method is practical and computationally efficient, it is too simple to identify nonlinear causal relationships existing in the system. For example, Yang et al. (2010) found that if $y = x^2$ with a time delay of one sample, where x is a superposition of a sine signal and white noise, then the CCF cannot determine this causality because all of the values are too small compared with the detecting threshold. In fact, the true correlation is zero, which means that the CCF cannot find the result. In another method called the Granger causality (GC) test, variable x "Granger causes" y if the prediction ability for y decreases when x is removed from all possible causative variables of y. However, the GC test is not suitable for coupled systems because it requires that the two variables for the test should be mutually independent, so the influence of one variable, such as x, on the other variable, such as y, could be eliminated by simply removing x from the original system. This is impossible in a coupled system and the result is trustless when the separability cannot be satisfied (Sugihara et al., 2012). Schreiber (2000) proposed the transfer entropy based on the concept of information entropy, aiming to pairwise measure the interactions of variables in a system. The transfer entropy is model-free and it is widely used in cause-and-effect analysis of chemical processes, atmospheric science, civil engineering, neuroscience, and other fields (Bauer et al., 2007; Vicente et al., 2011; Xie et al., 2012; Zhang et al., 2013). However, because this method is a probability-based method, the result accuracy is based on estimation of probability density functions and the whole computational burden is very high. Furthermore, the transfer entropy cannot always ensure the correct time-delay relationships between variables, so the arc sign in signed directed graphs cannot be obtained (Yang et al., 2010). The k-nearest neighbor (KNN) method proposed by Stockmann and Haber (2010) uses information about the nearest points that are close to

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input sample points to predict the actual outputs of those input samples, and it then finds the time-delay peaks by comparing the predicted and actual values along the time axis. This method is thought to be faster than the transfer entropy and applicable for nonlinear systems. However, in the KNN method, the important imputation number k_{imp} is chosen to be 2, 4, or 6. This subjective selection cannot always ensure accurate results and it is difficult to apply in automatic detection. In addition, the KNN method cannot avoid the false-nearest-neighbor problem in high-dimensional situations because of the absence of phase-space reconstruction.

For the above methods, the result accuracy and calculation efficiency are two crucial aspects for evaluating their performance. Most of these methods have shortcomings such as high computational burden or limited performance for linear or weak nonlinear systems. These methods cannot ensure correct results for causality identification of coupled variables in strong nonlinear systems, while recently proposed convergent cross-mapping (CCM) can overcome this problem (Sugihara et al., 2012). CCM uses the diffeomorphic features of coupled systems and converts the original causality detecting problem into comparisons between the mutual prediction effects of embedding manifolds. Recently, Ye et al. (2015) found that CCM is also capable of distinguishing time-delayed interactions between different process variables. In their method, if a time delay exists in the effect of an upstream variable y on a downstream variable x then $x_t = f(y_{t-\Delta t})$. CCM should have the best detecting performance when two variable series are matched in accordance with Δt. However, in our previous study (Luo et al., 2016), we found that because of significant differences in the embedding parameters between variables of continuous chemical processes, directly applying CCM usually cannot obtain as accurate results as when CCM is applied to ecosystems, especially when the process is high-dimensional with complicated dynamic behaviors.

In this paper, we refine the original CCM procedure and apply it to a chemical process to determine the propagation paths and root causes of process faults and disturbances. In Section 2, we introduce the original CCM and its refinement for chemical processes (RCCM). Compared with CCM, RCCM includes two modifications. First, it refines the manifold reconstructing process by using the time lag of the predicted variable to build both of the reconstructed manifolds, which enables it to be more suitable for variables with significant differences in time lags, like the situation in chemical processes where the data is usually from the distributed control system and each variable fluctuates at different frequencies. In addition, it integrates fast and accurate parametric determinations for τ and E in the flowchart. This step is important because there are tens to hundreds of variables in a chemical process, so efficient and automatic parameter determination procedures will greatly facilitate the analysis. At the end of Section 2, we compare RCCM with original CCM and provide the program flowchart of RCCM. In Section 3, we test RCCM on three examples to show its applicability for chemical processes and its advantages over other well-known methods. In example 1, we apply RCCM to a continuous stirred tank reactor to show its applicability for chemical processes. In examples 2 and 3, we test RCCM for four different linear and nonlinear single-input-single-output (SISO) systems and a benchmark model with nonlinear subprocesses. In Section 4, we test RCCM on a benchmark process: the Tennessee Eastman process.

2. CCM and RCCM

CCM was proposed by Sugihara et al. (2012) to determine the interaction strengths between different variables in a nonlinear ecosystem. This method is based on diffeomorphism theory and uses the characteristics of the interactions between coupled variables of nonlinear systems to provide reliable detection of causal relationships.

According to the Takens embedding theorem, if two variables are causally linked in a dynamic system, their corresponding shadow manifolds $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$ would be diffeomorphic to the manifold of the original system $\boldsymbol{M}$. Here, $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$ are reconstructed using lagged-coordinate embedding of time series x and y with embedding dimension E and time lags τ_x and τ_y. The elements of $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$ are denoted as x_t and y_t. Therefore, there is a consecutive one-to-one mapping relationship between the points in $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$. For some specific points $x_{t,1}, x_{t,2}, \ldots, x_{t,i}$ in $\boldsymbol{M_x}$, there must be corresponding $y_{t,1}, y_{t,2}, \ldots, y_{t,i}$ points in $\boldsymbol{M_y}$. If $x_{t,1}$ converges to a specific point x_{t0}, $y_{t,i}$ would also converge to the corresponding point y_{t0} in $\boldsymbol{M_y}$. Thus, once the process data is available, CCM attempts to find the nearest points for each $x_{t,i}$ in $\boldsymbol{M_x}$ and their mapping points in $\boldsymbol{M_y}$ to predict the corresponding value of $y_{t,i}$, which is denoted as $\hat{y}_{t,i}$. The cross-mapping ability of x for y can be evaluated by the correlation coefficient $\rho_{x\to y}$ between $\{y_t\}$ and $\left\{\hat{y}_t\right\}$. As the sample number L increases, $\hat{y}_{t,i}$ converges, and so does ρ_y. Thus, x can be used to estimate y, and vice versa. However, if x and y are not coupled, the accuracy of the prediction decreases owing to asymmetric information exchange between the two observed variables. Note that the unilateral causality in CCM is counterintuitive compared with other methods, such as the transfer entropy. A higher value of $\rho_{x\to y}$ means that the variable x is more affected by y, so y tends to be a cause of x.

Here, we describe the mathematical mechanism of CCM. The variables are produced by an n-dimensional dynamic system:

$$\frac{d\boldsymbol{X}}{dt} = f(\boldsymbol{X}, \boldsymbol{U}) \tag{1}$$

Here, $\boldsymbol{X}$ and $\boldsymbol{U}$ are vectors of the variables and parameters: $\boldsymbol{X} = [x_1, x_2, \ldots, x_n]^{\mathrm{T}}$ and $\boldsymbol{U} = [u_1, u_2, \ldots, u_l]^{\mathrm{T}}$. For example, taking the two variables x and y of $\boldsymbol{X}$, each element of the corresponding shadow manifolds of x and y are constructed according to

$$\boldsymbol{M_{x,t}} = \left[x_t, x_{t-\tau_x}, x_{t-2\tau_x}, \ldots, x_{t-(E-1)\tau_x}\right] \tag{2}$$

$$\boldsymbol{M_{y,t}} = \left[y_t, y_{t-\tau_y}, y_{t-2\tau_y}, \ldots, y_{t-(E-1)\tau_y}\right] \tag{3}$$

First, $\boldsymbol{M_x}$ is used to predict $\boldsymbol{M_y}$ and evaluate the influence of y on x. If parameter u is stable according to the Takens embedding theorem, $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$ would be stable and they are diffeomorphic to the manifold of the original system $\boldsymbol{M}$. This will lead to a consecutive one-to-one mapping relationship between the points on in $\boldsymbol{M_x}$ and $\boldsymbol{M_y}$:

$$\lim_{\boldsymbol{M_{x,i}}\to\boldsymbol{M_{x,k0}}} \boldsymbol{M_{y,i}} \to \boldsymbol{M_{y,k0}} = 0 \tag{4}$$

Thus, if we determine $E+1$ points in $\boldsymbol{M_x}$ then

$$\{\boldsymbol{M_{x,ki}}\} = \{\boldsymbol{M_{x,k1}}, \boldsymbol{M_{x,k2}}, \ldots, \boldsymbol{M_{x,k(E+1)}}\} \tag{5}$$

which are close to $\boldsymbol{M_{x,k0}}$. The value of $\boldsymbol{M_{y,k0}}$ can then be estimated by $\{\boldsymbol{M_{y,ki}}\}$:

$$d(\boldsymbol{M_{x,ki}}, \boldsymbol{M_{x,k0}}) = \exp\left(-\frac{\boldsymbol{M_{x,ki}} - \boldsymbol{M_{x,k0}}}{\boldsymbol{M_{x,k1}} - \boldsymbol{M_{x,k0}}}\right) \tag{6}$$

$$\hat{\boldsymbol{M}}_{\boldsymbol{y,k0}}|\boldsymbol{M_x} = \sum_{i=1}^{E+1} \frac{d(\boldsymbol{M_{x,ki}}, \boldsymbol{M_{x,k0}})}{\sum_{j=1}^{E+1} d(\boldsymbol{M_{x,kj}}, \boldsymbol{M_{x,k0}})} \boldsymbol{M_{y,ki}} \tag{7}$$

If L is sufficiently large to ensure that $\{\boldsymbol{M_{x,ki}}\}$ is sufficiently close to $\boldsymbol{M_{y,k0}}$, the predicting ability of $\boldsymbol{M_x}$ for $\boldsymbol{M_y}$ will converge to a positive constant between 0 and 1:

$$\lim_{L\to+\infty} cov\left(\boldsymbol{M_y}, \hat{\boldsymbol{M}}_{\boldsymbol{y}}|\boldsymbol{M_x}\right) = \rho_{x\to y} \tag{8}$$