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A Transfer Entropy Method to Quantify Causality in Stochastic Nonlinear Systems ⋆

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Abstract: In modern chemical processes, identification of the process variable connectivity and their topology is vital for maintaining the operational safety. As a general information theoretic method, transfer entropy can analyze the causality between two variables based on estimation of conditional probability density functions. Transfer entropy estimation is typically a data driven method, however, the associated high computational complexity and poor accuracy are not acceptable in real applications. Using a nonlinear stochastic state-space model in conjunction with particle filters, a novel transfer entropy estimation method is proposed. The proposed approach requires less data, is fast and accurate.

Keywords: Causality, transfer entropy, particle filters, state-space models

1. INTRODUCTION

With the ever increasing demand and the tightening stringent quality controls on chemical products, modern chemical processes have become large, complex and highly interconnected. As a consequence, the operation and automation of these processes has also become complex and unwieldy (Noyes (2000)). However, the increased level of automation, and its complexity, often leaves these processes susceptible to unexpected failures (Koutsoukos et al. (2002)). Usually, these failures have significant impact on safety, economy and environment. Therefore, an alarm management system is often deployed to monitor abnormal conditions and faults during everyday production (Yang et al. (2014)).

Alarm management makes it easy for operators and engineers to monitor almost every process variable and its alarm status. However, when some serious failures occur, alarms often start from a single process variable and quickly propagate to other variables resulting in almost continuous appearance of alarms and the monitoring panels will be filled with alarm messages. This condition is often referred to as alarm flooding (Vedam and Venkatasubramanian (1999)).

In order to reduce the number of alarms and avoid alarm flooding, many strategies have been proposed. Causality analysis between different process variables resulting in an extraction of the process variable topology is the central procedure used to trace back to the source alarm in an alarm flood. Transfer entropy is an effective quantity to analyze the causality between two variables in a process. It is a quantitative process - often based on the historical data, the outcome of which is an entropy showing the causal relationships between the variables in a process.

Traditionally, transfer entropy has been estimated using massive historical data sets making it very inefficient computationally and in terms of accuracy. Considering the data are inherently stochastic, any estimation of transfer entropy will only be approximate deviate from the real transfer entropy. In addition, the long time lapse between successive transfer entropy calculations - due to computational inefficiency - will not allow implementation periodical of algorithms that depend on transfer entropy.

These drawbacks can be overcome with more information from a process in the form of a model. While models are difficult to build and often prohibitively expensive, they are required and widely used in designing controllers, monitoring, simulation and fault detection algorithms. The objective of this article is to use the information available from a model in improving the accuracy and speed of calculations of transfer entropy. The approach developed in this article, not only provides qualitative causality relationships but also quantifies the strength of these relationships. In this article, a new transfer entropy

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estimation method is proposed using sequential Monte Carlo methods.

The transfer entropy is a function of probability density functions of relevant process variables. These probability density functions are high dimensional and often are complex enough that any attempts to estimate them using data alone are prone to unacceptable errors and computational inefficiencies. Moreover, methods based on only data often fail with nonstationary, nonGaussian and nonlinear data. In this article, the probability density functions are estimated using a stochastic nonlinear model of the process in conjunction with sequential Monte Carlo methods. In particular, particle filtering algorithms are used to approximate both density functions and integrals.

This paper is organized as follows. In section 2, the general model used in this paper and definition of transfer entropy are introduced. In section 3, a particle approximation of the transfer entropy is presented. In section 4, two case studies are provided to illustrate the effectiveness of the proposed algorithm. Finally, some conclusions are outlined in section 5.

2. MODEL REPRESENTATION

Let's assume we have a chemical process (e.g, continuous-stirred tank reactor system) described by the following discrete-time stochastic nonlinear state-space model:

$$X_{t+1} = f(X_t, U_t) + V_t, \tag{1}$$

where $X_t \in \mathcal{X} \subset \mathbb{R}^{n_x}$ is a Markov state process defined the initial density $X_0 \sim p(x_0)$ and transition density $X_t|(X_{t-1}, U_{t-1}) \sim p(x_t|x_{t-1}, u_{t-1})$. In (1), $U_t \in \mathcal{U} \subset \mathbb{R}^{n_u}$ is a nonlinear state feedback control law given by

$$U_t = g(X_t) + W_t, \tag{2}$$

where $W_t \in \mathbb{R}^{n_u}$ is random noise sequence assumed to be known in its distribution. Further, we assume that all the model parameters of the system are known a priori. A graphical model for the system (1) with control law (2) is given in Figure 1.

2.1 Transfer Entropy

Given a control law (2), it is clear that there is a causal relationship between the inputs and the states in (1). See Figure 1 for illustration. In this paper, we are interested in quantifying the degree of causality between the inputs and the states. There are different metrics available to quantify the causal relationship between variables. A popular approach to measure causality is through the use of differential transfer entropy (TE), which is mathematically defined as follows

$$\begin{aligned} T_{u\to x} &\equiv \mathbb{E}_{p(x_{t+1},x_t,u_t)}\left[\log\left[\frac{p(x_{t+1}|x_t,u_t)}{p(x_{t+1}|x_t)}\right]\right], \\ &= \int \log\left[\frac{p(x_{t+1}|x_t,u_t)}{p(x_{t+1}|x_t)}\right] p(dx_{t+1}, dx_t, du_t), \end{aligned} \tag{3}$$

where $p(dx_{t+1}, dx_t, du_t) \equiv p(x_{t+1}, x_t, u_t)dx_{t+1}dx_t du_t$. Despite the unwieldy definition of TE in (3), it has a simple interpretation – TE from U to X can be understood as the information gained when using the past information of both U and X to predict the future of X compared to only using the past information of X. Note that in Definition (3), we use integrals since X and U are both continuous random variables; however, for discrete random variables we replace integral with summation over the sample space.

The above expression for transfer entropy can also be written using an equivalent discrete form (Schreiber (2000)) using a unit sample time:

$$T_{u\to x} = \sum p(x_{k+1}, x_k, u_k)\log\frac{p(x_{k+1}|x_k,u_k)}{p(x_{k+1}|x_k)} \tag{4}$$

where the summation is over the states x_{k+1}, x_k and the inputs u_k.

2.2 Data-Based Transfer Entropy Calculation

It is standard practice to calculate transfer entropy using only the routine operating data. This is a rather challenging task as no assumptions are made about the process model and the routine measured data is often nonstationary, noisy and has unknown correlations. The above discrete transfer entropy expression (4) simplified as shown below (Duan et al. (2013)):

$$T_{u\to x} = \sum p(x_{t+1}, x_t, u_t)\log\frac{p(x_{t+1},x_t,u_t)}{p(x_{t+1},x_t)}\cdot\frac{p(x_t)}{p(x_t,u_t)} \tag{5}$$

Hence the main challenge in estimating the transfer entropy is in approximating the joint probability density functions purely from data. According to (Silverman (1986)), for a q dimensional vector x, the probability density function (pdf) can be estimated by the following function:

$$p(x) = \frac{(\det(S))^{-1/2}}{N\Gamma^q}\sum_{i=1}^{N} K\left\{\Gamma^{-2}(\boldsymbol{x}-X_i)^T S^{-1}(\boldsymbol{x}-X_i)\right\} \tag{6}$$

Γ is the bandwidth chosen to minimize the mean integrated squared error of the joint pdf estimation and calculated by $\Gamma = 1.06N^{-1/(4+q)}$. S is the covariance matrix of the sampled data. $K\left\{\Gamma^{-2}(x-X_i)^T S^{-1}(x-X_i)\right\}$ is a kernel estimation - using Gaussian kernel function

$$K(u) = (2\pi)^{-q/2}\mathrm{e}^{-\frac{1}{2}u}.$$

The above calculation procedure is often not very accurate. Γ is often chosen by trial and error and the Gaussian kernel function can have many forms. To improve the accuracy of the density approximation large data are needed and according to (Bauer et al. (2007)) more than 2000 observations should typically be considered. In addition, large data sets increase the computational complexity significantly and thus slow down the calculation process.

3. PARTICLE APPROXIMATION OF TRANSFER ENTROPY

As discussed in Section 2, for the model and control law considered in (1) and (2) there is no closed-form solution to the TE in (3). In this section, we use particle methods to approximate the TE in (3).