Engineering Applications of Artificial Intelligence 55 (2016) 219–230

Contents lists available at ScienceDirect

Engineering Applications of Artificial Intelligence

journal homepage: www.elsevier.com/locate/engappai

Estimating the unknown time delay in chemical processes

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ARTICLE INFO

Article history:
Received 24 September 2015
Received in revised form
16 February 2016
Accepted 20 June 2016

Keywords:
Input-delay system
Least squares support vector machines
Continuous stirred tank
Open and closed-loop identification

ABSTRACT

Although time delay is an important element in both system identification and control performance assessment, its computation remains elusive. This paper proposes the application of a least squares support vector machines driven approach to the problem of determining constant time delay for a chemical process. The approach consists of two steps, where in the first step the state of the system and its derivative are approximated based on the LS-SVM model. The second step consists of modeling the delay term and estimating the unknown model parameters as well as the time delay of the system. Therefore the proposed approach avoids integrating the given differential equation that can be computationally expensive. This time delay estimation method is applied to both simulation and experimental data obtained from a continuous, stirred, heated tank. The results show that the proposed method can provide accurate estimates even if significant noise or unmeasured additive disturbances are present.

1. Introduction

The rapid growth and development of new chemical processes involves a need for effective, safe, and efficient methods for understanding and assessing their performance. The general framework for understanding the process, often called system identification, is a well-developed field (Ljung, 1999; Söderström and Stoica, 1988). Similarly, performance assessment of the process has been well developed (Shardt et al., 2012; Jelali, 2006; MacGregor and Kourti, 1995). However, one area within these two frameworks that still requires further research is that of effective time delay determination. In system identification, a time delay is often assumed to be known *a priori* or determined using auxiliary methods, such as a step test or the cross-correlation method (Seborg et al., 2006). Similarly, many performance assessment methods, such as the Harris index, require the time delay to be known beforehand in order to effectively implement the assessment. This need for the time delay means that such a method can only rarely be implemented in industry due to the inability to obtain the relevant information (Shardt et al., 2012). This problem is especially acute in closed-loop process operation, that is, when a chemical process is being actively controlled by a controller. In such cases, many of the previously developed methods do not apply due to the correlation between the input and outputs signals, introduced by the controller.

Time delay estimation can be divided into four broad categories (Björklund, 2003): time-delay approximation methods, explicit time-delay parameter methods, area and moment methods, and finally, higher-order statistics methods. Time-delay approximation methods convert or project the given input and output signals into another basis from which a process model can be estimated. Using the estimated process model, the time delay can be back calculated. Of the available methods, the most common methods are the various Laguerre-domain based approximation methods. The explicit time-delay parameter methods seek to estimate the time delay directly with all the other parameters in the model. The most common approach is to assume a high-order autoregressive model with exogenous input (ARMAX) with varying time delays and select the time delay that provides the best overall fit as the time delay for the model. This approach is implemented in MATLAB's DELAYEST function and hence is often used in practical cases. However, although it can provide decent results for both open- and closed-loop cases, it does require the user to know at least approximately the range over which the time delays could vary. Furthermore, selecting an appropriate higher order model can be an issue as it can slow down the brute force search tremendously. The area and moment methods seek to determine the delay by examining either step or impulse response characteristics of the observed input and output signals and fitting an appropriate signal. It can be noted that in this approach there are two main steps: first, the desired response coefficients must be estimated and then the time delay extracted. Often the extraction of the time delay is

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http://dx.doi.org/10.1016/j.engappai.2016.06.014
0952-1976/

performed visually since only a small data set is being used. The most common such methods are the various methods which seek to determine the cross-correlation or impulse coefficients between the input and output signals to determine the estimated time delay (Seborg et al., 2006; Björklund, 2003). The time delay is inferred by determining which of the computed cross-correlation lags is nonzero. Although this approach can provide very accurate results, it does require that the error be uncorrelated with the inputs and outputs and that the input be a white noise signal. In practice, this implies that this method only applies for open-loop processes driven by white noise or pseudorandom binary signals, which have properties similar to white noise (Huang and Kadali, 2008). Time delay methods based on higher order statistics are rarely used for industrial data since it can be complicated to compute the required values.

An active area of research is the development of methods to extend the explicit time delay estimation methods to handle more complex situation that involve solving the exact differential equations given all the available information and, thus, relatively easily obtain the optimal time delay. However, at each iteration, it is necessary to integrate the differential equation, which can be a computationally intensive task. Recently, with the expansion and development of new methods for rapid computation and implementation of the various time-delay optimization methods, a potentially new approach to time delay estimation has been proposed. Mehrkanoon et al. (2014a) proposed an approach based on least squares support vector machines (LS-SVM) for estimating the time delay given the observational data. Support Vector Machines (SVMs) are a powerful methodology for solving pattern recognition and function estimation problems (Vapnik, 1998), which solves the dual quadratic programming problem. LS-SVMs have been applied to function estimation, classification, problems in unsupervised learning and others (Suykens et al., 2002). The LS-SVM problem formulation involves equality, instead of inequality constraints and employs a quadratic loss function. Training of the model in the dual is then done by solving a set of linear equations. The method converts the parameter estimation problem into an algebraic optimization problem and, thus, does not require repeated numerical integration of the system. The ability of LS-SVM to produce a continuous output is used to estimate the state and its derivative. This information is then cast into an optimization problem that seeks to determine the time delay.

Therefore, given the potential suitability of this approach to chemical engineering application, the objectives of this paper are to develop and understand the least squares support vector machine approach for time delay estimation in the context of chemical engineering examples; to investigate the behavior and properties of this method using simulations of a heated tank; and to apply the method to experimental data obtained from running a pilot scale heated tank. In both cases, open- and closed-loop cases will be considered and the results compared. For the closed-loop case, two further subcases will be considered depending on whether or not the reference signal changes its value during the course of operation.

2. Overview of LS-SVM regression

Consider a given training set $\{t_i, y_i\}_{i=1}^N$ with input data $t_i \in \mathbb{R}^d$ and output data $y_i \in \mathbb{R}$. In the LS-SVM framework, one assumes that the underlying function describing the relation between input and output of the system has the following form:

$$y(t) = w^T\varphi(t) + b. \tag{1}$$

where $\varphi(\cdot)$: $\mathbb{R}^d \to \mathbb{R}^h$ is the feature map and h is the dimension of the feature space. Due to the nonlinear feature map, the data are embedded into a feature space and the optimal solution is sought in that space by minimizing the residual between the model outputs and the measurements. To this end, one formulates the following optimization problem known as primal LS-SVM formulation (Suykens et al., 2002):

$$\begin{aligned} &\underset{w,b,e}{\text{minimize}} \quad \frac{1}{2}w^Tw + \frac{\gamma}{2}e^Te \\ &\text{subject to} \quad y_i = w^T\varphi(t_i) + b + e_i, \quad i = 1, \ldots, N, \end{aligned} \tag{2}$$

where $\gamma \in \mathbb{R}^+$, $b \in \mathbb{R}$, $w \in \mathbb{R}^h$. Given the first regularization term in the objective function, the complexity of the model is controlled and therefore overfitting problem is avoided (Suykens et al., 2002). In the LS-SVM approach the feature map φ is not explicitly known in general and can be infinite dimensional. Therefore the kernel trick is used and the problem is solved in the dual (Suykens et al., 2002). The Lagrangian of the constrained optimization problem (2) becomes:

$$\mathcal{L}(w, b, e_i, \alpha_i) = \frac{1}{2}w^Tw + \frac{\gamma}{2}e^Te - \sum_{i=1}^{N}\alpha_i\left[w^T\varphi(t_i) + b + e_i - y_i\right] \tag{3}$$

where $\{\alpha_i\}_{i=1}^N$ are Lagrange multipliers. Then the Karush–Kuhn–Tucker (KKT) optimality conditions are,

$$\begin{aligned} &\frac{\partial\mathcal{L}}{\partial w} = 0 \to w = \sum_{i=1}^{N}\alpha_i\varphi(t_i), \\ &\frac{\partial\mathcal{L}}{\partial e_i} = 0 \to \alpha_i = \gamma e_i, \\ &\frac{\partial\mathcal{L}}{\partial b} = 0 \to \sum_{i=1}^{N}\alpha_i = 0, \\ &\frac{\partial\mathcal{L}}{\partial \alpha_i} = 0 \to w^T\varphi(t_i) + b + e_i = y_i. \end{aligned} \tag{4}$$

Eliminating the primal variables e_i and w leads to the following linear system in the dual problem:

$$\left[\begin{array}{c|c} \Omega + I_N/\gamma & 1_N \\ \hline 1_N^T & 0 \end{array}\right]\left[\begin{array}{c} \alpha \\ \hline b \end{array}\right] = \left[\begin{array}{c} y \\ \hline 0 \end{array}\right] \text{ where } \Omega_{ij} = K(t_i, t_j) = \varphi(t_i)^T\varphi(t_j)$$

is the ijth entry of the positive definite kernel matrix. $1_N = [1, \ldots, 1]^T \in \mathbb{R}^N$, $\alpha = [\alpha_1, \ldots, \alpha_N]^T$, $y = [y_1, \ldots, y_N]^T$ and I_N is the identity matrix. The model in the dual form becomes:

$$y(t) = w^T\varphi(t) + b = \sum_{i=1}^{N}\alpha_iK(t, t_i) + b. \tag{6}$$

3. Time delay estimation in a system with input delay

3.1. Problem statement

Systems with input delays are ubiquitous and widely used in modeling of real phenomena such as in control theory, population dynamics (Mahaffy et al., 1998) and engine cooling systems (Hansen et al., 2011). The delay can be constant, time varying or state dependent. For instance in milling processes, speed-dependent delays arise due to the deformation of the cutting tool (Altıntas et al., 1999).

A typical first order single input delay model may be expressed as:

$$\dot{x}(t) = f(t, x(t), u(t-\theta), p(t)), \quad t \geq t_0, \tag{7}$$

where $p(t)$ is the parameter vector, u is the input to the system and θ is the time delay or lag which is nonnegative and can be either constant or depend on time or state, that is, $\theta = \theta(t, x(t))$. The initial time is denoted by t_0.