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CACE-5785; No. of Pages 10

ARTICLE IN PRESS

Computers and Chemical Engineering xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Input estimation as a qualitative trend analysis problem

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ARTICLE INFO

Article history:
Received 25 September 2016
Received in revised form 30 March 2017
Accepted 6 April 2017
Available online xxx

Keywords:
Global optimization
Input estimation
Oxygen uptake rate
Qualitative trend analysis
Wastewater treatment

ABSTRACT

The study of techniques for qualitative trend analysis (QTA) has been a popular approach to address challenges in fault diagnosis of engineered processes. Such challenges include the lack of reliable extrapolation of available models and lack of representative data describing previously unseen circumstances. Many of these challenges appear in biological systems even when normal operation can be assumed. It is for this reason that QTA techniques have also been proposed for the purpose of fault detection, automation, and dynamic modeling. In this work, we adopt a shape-constrained spline function method for the purpose of unknown input estimation. Thanks to data collected at laboratory-scale in a biological reactor for urine nitrification, this novel approach has been demonstrated successfully for the first time.

1. Introduction

Routine execution of on-line process data analysis is a challenging task for many processes. The use of models to extract valuable information from the available data is often known as *soft-sensing* and several such methods for have been developed. Widely-known methods include the Kalman filter and its extensions (e.g., Romanenko and Castro, 2004; Kravaris et al., 2013; Prakash et al., 2014). These techniques provide a systematic approach to the construction of such soft-sensors on the basis of dynamic process models. Factors affecting the success include the completeness of available process understanding, whether or not measured variables include or describe the key process states comprehensively, and whether the process undergoes important changes over time. To obtain a useful model, two modeling approaches are distinguished. The first consists of white-box modeling and is based on models which reflect the mechanistic understanding of the process. Successful application of soft-sensors based on white-box models requires completeness, accuracy, and precision of the applied model. If this is not met, systematic deviations, i.e. bias, should be expected between the extracted estimates and their true values. When a reliable white-box model is not available, one may choose to take the black-box route. In this case, one uses historical data to empirically define the relationships between (i) data that is available cheaply and reliably, and (ii) information that is difficult to obtain directly. Unfortunately, many black-box models (e.g., neural nets, regression trees, support vector machines) lack transparency. As a result, such models may not be trusted to provide information for safety- or quality-critical decisions (e.g., Liu, 2007; Wang et al., 2010). In addition, black-box models often suffer from large estimation errors when extrapolated. Choosing between white-box and black-box approaches often entails a trade-off between these aspects. Quite naturally, several authors have proposed a mixed approach, i.e. grey-box modeling, to represent the process mechanistically in as much as possible while representing the lesser known parts of the process as a black-box model.

In a number of situations, one may simultaneously lack detailed process understanding as well as sufficient data to properly define any of the traditional models described above. This is true for many processes and has led to the development and application of coarse-grained qualitative modeling and simulation techniques (Venkatasubramanian et al., 2003). Such methods are deliberately imprecise which leads to predictions that can be trusted (reliability) despite large uncertainties. Despite this imprecision, this still enables causal reasoning and decision-making (e.g., Kuipers, 1989; Maurya et al., 2003; Bredeweg et al., 2009; Kansou and Bredeweg, 2014). In the process engineering literature, the qualitative approach has been advocated mainly for the purpose of fault diagnosis and is primarily implemented in the form of qual-

Abbreviations: DO, dissolved oxygen; LTI, linear time-invariant; MHE, moving horizon estimation; OUR, oxygen uptake rate; SCS, shape-constrained splines; QTA, qualitative trend analysis.

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http://dx.doi.org/10.1016/j.compchemeng.2017.04.011

itative trend analysis (QTA, Bakshi and Stephanopoulos, 1994; Rengaswamy and Venkatasubramanian, 1995; Dash et al., 2004; Charbonnier et al., 2005; Gamero et al., 2006, 2014; Charbonnier and Gentil, 2007; Maurya et al., 2010; Villez et al., 2012, 2013). The main motivation is that both process understanding and data describing the dynamics of processes subject to rare events are typically extremely limited. The same can often be said even for normal conditions for complex biological processes. When so, qualitative approaches also become valuable outside of the fault diagnosis niche, e.g., for process data mining (Stephanopoulos et al., 1997; Villez et al., 2007). More recent work has pushed the application boundary even further by enabling fault detection (Villez and Habermacher, 2016), image analysis (Derlon et al., 2017), model structure identification (Mašić et al., 2017), data reconciliation (Srinivasan et al., 2017), and process automation (Villez et al., 2008; Thürlimann et al., 2015) on the basis of the QTA philosophy.

Existing methods for QTA are useful to describe the qualitative features (e.g., maxima, minima, inflection points) of a data series. In contrast, we provide a new approach to QTA which describes the qualitative features of a process input signal which cannot be measured directly. To this end, the process itself is represented by a piece-wise linear time-invariant (LTI) model. The analyzed measurement data series is assumed to be univariate, which is typical in the QTA literature apart from a few exceptions (e.g., Flehmig and Marquardt, 2006, 2008). The unknown input signal is represented as a shape constrained spline function. Estimating the parameters of this input signal, i.e. the spline coefficients, by fitting the complete model to process data forms the focus of this study.

The method is applied for estimation of the oxygen uptake rate in an intermittently fed stirred tank reactor for urine nitrification (Udert and Wächter, 2012; Fumasoli et al., 2016). This process has been developed as part of a system to recover resources, in this case a fertilizer, from source-separated wastewater streams. In the urine nitrification process, the oxygen uptake rate (OUR) reflects the respiration rate of the ammonia oxidizing bacteria and the nitrite oxidizing bacteria in the process. One aims to achieve a low respiration rate at the end of each cycle, i.e. right before new untreated urine is fed to the reactor. Estimates of the OUR can thus be used to maximize the efficiency of the process. This is very similar to conventional aerobic sequencing batch reactors for wastewater treatment (e.g., Yoong et al., 2000). Estimates of the OUR are also essential for wastewater characterization (e.g., Spanjers and Vanrolleghem, 1995; Spérandio and Etienne, 2000; Choubert et al., 2013), model identification (e.g., Vanrolleghem and Spanjers, 1998; Petersen et al., 2001; Ferrai et al., 2010), and automation (e.g., Spanjers et al., 1996; Yoong et al., 2000; Gernaey et al., 2001). Most typically, one obtains the OUR at infrequent time points by fitting a linear line to a short series of dissolved oxygen concentration measurements obtained during an unaerated phase. The underlying idea is that the oxygen measurement series are described well by a linear trend, whose slope reflects the respiration rate in the selected time window. This approach means that the OUR is not available continuously and that nonlinear effects of aeration and sensor dynamics are deliberately ignored. With the proposed method, these assumptions are not necessary and the OUR is available as a continuous process input estimate. In addition, the method allows estimating the kinetic parameters of the aeration system and the sensor simultaneously, thus providing additional information regarding the state of the components of the monitored system. We demonstrate the method with data obtained in a single batch cycle and describe the opportunities that lie ahead.

Table 1
Symbol definitions.

Symbol	Description
Θ	Feasible set for $\boldsymbol{\theta}$
Ω	Feasible set for $\boldsymbol{\beta}$
$\boldsymbol{\beta}$	Spline function coefficients
δ_k	Input noise at knot k
ϵ_i	Measurement error at sample i
σ_δ	Input noise standard deviation
σ_ϵ	Measurement error standard deviation
$\boldsymbol{\tau}, \tau_c, \tau_y$	Time constants (for concentration, for measurement)
$\boldsymbol{\theta}$	Transitions
D	Degree of the spline function
E	Number of episodes
I	Total number of samples
K	Number of spline knots
S	Number of process states
$\boldsymbol{S}$	Matrix describing the shape constraints
T	Number of transitions
i	Measurement sample index
k	Spline index
$\boldsymbol{a}_t$	Spline basis function evaluated at t
$\boldsymbol{c}_t$	Convoluted spline basis function evaluated at t
c_{DO}	Dissolved oxygen (state)
$\underline{\boldsymbol{b}}, \underline{b}$	Left-side interval bounds
$\overline{\boldsymbol{b}}, \overline{b}$	Right-side interval bounds
d	derivative index
e	episode index
$\boldsymbol{f}$	Rate of change
$\boldsymbol{g}$	Measurement gains
j	(hyper-)rectangular set
r_{OUR}	oxygen uptake rate (OUR)
$\boldsymbol{s}_0$	Initial state vector
$\boldsymbol{s}$	State vector
t, t_i	Time (at sample i)
$\boldsymbol{u}, u$	Known binary input
$v_0^{(d)}$	Initial values for the unknown process input signal
$v, v^{(d)}$	Unknown process input (dth derivative)
w	Integrand
y	Measurement
y_{DO}	Dissolved oxygen (noise-free measurement)
$\tilde{y}_{DO}$	Dissolved oxygen measurement

2. Materials and methods

All symbol definitions required in this text are given in Table 1.

2.1. Basic model

Data-generating model – Theory. In this work, we aim to describe measurement time series of finite length with the following generative model:

$$\dot{\boldsymbol{s}} = \boldsymbol{f}_t(\boldsymbol{s}, \boldsymbol{u}, v) \tag{1}$$

$$\tilde{y}_i = \boldsymbol{g}^T \boldsymbol{s}(t_i) + \epsilon_i \tag{2}$$

$$\epsilon_i \sim \mathcal{N}(0, \sigma_\epsilon) \tag{3}$$

with $\boldsymbol{s} = \boldsymbol{s}(t)$, $\boldsymbol{u} = \boldsymbol{u}(t)$, $v = v(t)$.

The above model is a continuous-time state-space model composed of a set of ordinary differential equations which generates noisy measurements ($\tilde{y}_i$) at distinct sampling times (t_i, $i = 1, \ldots, I$). We further assume that (i) the ordinary differential equations are piece-wise LTI in the S state variables ($\boldsymbol{s}$) and the uncontrolled input ($v(t)$), and (ii) that the controlled inputs ($\boldsymbol{u}(t)$) are piece-wise constant. In what follows, the parameters of the piece-wise linear LTI system are given as a vector $\boldsymbol{\tau}$.

The univariate input ($v(t)$) is assumed to be described well by a signal consisting of K piece-wise polynomial segments of degree D. Each kth polynomial starts at time t_k and ends at time t_{k+1} ($t_1 = 0$,