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Unmeasured Concentrations and Reaction Rates Estimation in CSTRs

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Abstract: In this paper, we focus on continuously stirred tank reactors. For such plants we present a dynamical system capable of estimating i) unmeasured concentrations exponentially fast and ii) completely unknown reaction rates exactly and in finite-time. Towards this end, this observer requires the (partial) knowledge of the mathematical model, along with the inputs and outputs to the system; furthermore, we require that the number of measured concentrations equals the number of unknown reaction rates.

Keywords: Observers; reaction rate estimation; state estimation; uncertain systems; uncertain bioprocess models; discontinuous observers; biotechnology

1. INTRODUCTION

The intricate nature of biochemical networks hinders the implementation of sensors that provide online measurements of the variables involved in these kind of processes. However, the knowledge of such underpinning, unmeasurable processes are important for the analysis and control of such kind of systems.

Typically the functional form of the reaction rates are unknown; hence, expensive, daunting experimental procedures must be engaged to estimate their functional form, along with the parameters that characterise them.

In the following, we focus on continuously stirred tank reactors (CSTRs) (Bastin and Dochain, 2013; Dochain, 2013) with constant, controlled temperature. Thus, presenting spatial homogeneity in the concentrations, along with constant kinetic parameters.

To tackle these estimation problems, dynamical systems capable of estimating the unmeasured variables have been developed, given the (partial) knowledge of the mathematical model of the reaction network, along with its inputs and outputs. This class of systems is denoted as software sensors or observers (Besançon, 2007; Dochain, 2003).

The classical observation problem is the online estimation of unmeasured states. For surveys and classification of observers applied to reaction networks, we refer the interested reader to (Dochain, 2003; Bastin and Dochain, 2013; Ali et al., 2015), for instance.

There exist some approaches capable of estimating the *unknown* reaction rates in (bio)chemical reaction networks: Farza et al. (1998) avails of a nonlinear observer for estimating the reaction rates of a class or reaction networks. Oliveira et al. (2002) present an observer capable of estimating unknown parameters in the reaction kinetics, given the measurement of the concentrations; in turn, Nuñez et al. (2013) present a second order, quasi-continuous sliding mode algorithm for estimating multiple consumption and or production kinetic. Whereas, Moreno and Mendoza (2014); Vargas et al. (2014) avail of the generalised super-twisting algorithm (Moreno, 2012) to estimate the unmeasured concentrations along with the *unknown* reaction kinetics.

Surveys of sliding mode approaches, such as the super-twisting algorithm, may be found in (Fridman, 2012; Fridman et al., 2015); whereas particular application to observation are described, e.g., in (Spurgeon, 2008; Shtessel et al., 2014).

In this paper, we present an observer capable of i) estimating the unmeasured states exponentially fast and ii) providing the multiple, *unknown*, time-dependent reaction rates in finite-time.

The unmeasured concentrations are estimated via an asymptotic observer (Dochain et al., 1992). In turn, the estimation of the reaction rates avails of a particular case of the Generalised Multivariable Super-Twisting Algorithm (López-Caamal and Moreno, 2016); thereby, providing such an estimate exactly and finite-time. This approach requires as many online concentrations measurements as unknown reaction rates.

We choose a particular version of the Generalised Super-Twisting Algorithm that is easily tunable, as it only requires four tuning parameters regardless of the number of states and reaction rates to estimate; and that allows convergence to the true estimates exactly at the same time (López-Caamal and Moreno, 2015).

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To demonstrate applicability, we analyse a simple reaction network whose dynamics is based on the Law of Mass Action.

1.1 Notation

We use $\overline{\lambda}(\circ)$ (resp. $\underline{\lambda}(\circ)$) to denote the largest (smallest, resp.) eigenvalue of the argument. The definition of $\overline{\sigma}(\circ)$ and $\underline{\sigma}(\circ)$, follows accordingly but referring to the singular value. In turn $\otimes$ denotes the matrix Kronecker product.

Moreover, we use superindexes to distinguish different vectors and matrices. For instance, the scalar x_2^1 denotes the second element of the vector $\mathbf{x}^1$.

2. BACKGROUND

Let us consider a continuously stirred tank reactor (CSTR), described by the following mathematical model

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\xi}(t) = \mathbf{K}\boldsymbol{\psi}(t,\boldsymbol{\xi}) - d\boldsymbol{\xi}(t) - \mathbf{q}(\boldsymbol{\xi}) + \mathbf{f}(t), \tag{1}$$

which represents a reaction network, whose species concentrations compose the vector $\boldsymbol{\xi}(t) \in \mathbb{R}^n$ and the stoichiometric matrix is $\mathbf{K} \in \mathbb{R}^{n\times q}$. Thus, the vector $\boldsymbol{\psi}(t,\boldsymbol{\xi}) : \mathbb{R}_{\geq 0}\times\mathbb{R}^n \to \mathbb{R}^q$ comprises the reaction rates. This reaction network is also subject to an equal, constant influx and efflux, characterised by the dilution rate $d \in \mathbb{R}_{>0}$. In turn, the vector $\mathbf{q}(\boldsymbol{\xi}) : \mathbb{R}^n_{\geq 0} \to \mathbb{R}^n_{\geq 0}$ gathers the instantaneous gaseous outflow rate; whereas $\mathbf{f}(t) : \mathbb{R}_{\geq 0} \to \mathbb{R}^n_{\geq 0}$ describes the known feedrate.

Assumption 1. In the rest of the paper we adopt the following assumptions:

(1) The number of states is larger than the number of independent reaction rates; that is to say, $n > q$.
(2) The number of measured components, $\mathbf{y}(t)$, is equal to the number of independent reaction rates.
(3) The functional forms of the reaction rates in $\boldsymbol{\psi}(t,\boldsymbol{\xi})$ are *unknown*, yet their time-derivative is bounded independently of the state.
(4) $\mathbf{K}, d, \mathbf{f}(t)$, and the functional form of $\mathbf{q}(\circ)$ are known.

By splitting the concentration vector in measured $\boldsymbol{\xi}^a(t) : \mathbb{R}_{>0} \to \mathbb{R}^q$ and unmeasured components $\boldsymbol{\xi}^b(t) : \mathbb{R}_{>0} \to \mathbb{R}^{n-q}$ we may rewrite the reaction network in (1) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\xi}^a(t) = \mathbf{K}^a\boldsymbol{\psi}(t,\boldsymbol{\xi}) - d\boldsymbol{\xi}^a(t) - \mathbf{q}^a(\boldsymbol{\xi}) + \mathbf{f}^a(t) \tag{2a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\xi}^b(t) = \mathbf{K}^b\boldsymbol{\psi}(t,\boldsymbol{\xi}) - d\boldsymbol{\xi}^b(t) - \mathbf{q}^b(\boldsymbol{\xi}) + \mathbf{f}^b(t) \tag{2b}$$

$$\mathbf{y}(t) := \boldsymbol{\xi}^a(t), \tag{2c}$$

where $\mathbf{K}^i, \mathbf{q}^i, \mathbf{f}^i$, $i = \{a, b\}$ have appropriate dimensions according to the partition of the state.

Within this framework, we address the problem of estimating the unmeasured states $\boldsymbol{\xi}^b(t)$ along with the reaction rates $\boldsymbol{\psi}(t,\boldsymbol{\xi})$ exactly and in finite-time. As described in the following section, the states in $\boldsymbol{\xi}^b(t)$ will be estimated via an asymptotic observer (Dochain et al., 1992) and the reaction rates, via a Generalised Multivariable Super-Twisting Algorithm (López-Caamal and Moreno, 2016).

This strategy was originally proposed in (Moreno and Mendoza, 2014); here, however, we prefer a multivariable sliding mode approach, thereby enhancing the applicability of such a methodology to a richer class of reaction networks.

3. UNMEASURED STATES AND UNKNOWN REACTION RATES ESTIMATION

In order to achieve an estimate of the states in $\boldsymbol{\xi}^b(t)$ and the reaction rates $\boldsymbol{\psi}(t,\boldsymbol{\xi})$, let us consider the following state transformation

$$\begin{pmatrix}\boldsymbol{\xi}^a(t)\\ \boldsymbol{\xi}^b(t)\end{pmatrix} = \begin{pmatrix}\mathbf{0}_{q\times n-q} & \mathbf{K}^a\\ \mathbf{I}_{n-q} & \mathbf{K}^b\end{pmatrix}\begin{pmatrix}\mathbf{x}^1(t)\\ \mathbf{x}^2(t)\end{pmatrix}, \tag{3a}$$

$$\begin{pmatrix}\mathbf{x}^1(t)\\ \mathbf{x}^2(t)\end{pmatrix} = \begin{pmatrix}-\mathbf{K}^b(\mathbf{K}^a)^{-1} & \mathbf{I}_{n-q}\\ (\mathbf{K}^a)^{-1} & \mathbf{0}_{q\times n-q.}\end{pmatrix}\begin{pmatrix}\boldsymbol{\xi}^a(t)\\ \boldsymbol{\xi}^b(t)\end{pmatrix}. \tag{3b}$$

Moreover, let $\mathbf{x}^3(t) := \boldsymbol{\psi}(t,\boldsymbol{\xi})$. In the $\mathbf{x}^i$ coordinates, the model in (2) is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}^1(t) = -d\mathbf{x}^1(t) + \mathbf{K}^b(\mathbf{K}^a)^{-1}[\mathbf{q}^a(\boldsymbol{\xi}) - \mathbf{f}^a] - [\mathbf{q}^b(\boldsymbol{\xi}) - \mathbf{f}^b] \tag{4a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}^2(t) = -d\mathbf{x}^2(t) - (\mathbf{K}^a)^{-1}[\mathbf{q}^a(\boldsymbol{\xi}) - \mathbf{f}^a] + \mathbf{x}^3(t) \tag{4b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}^3(t) = \boldsymbol{\delta}(t) \tag{4c}$$

$$\mathbf{y}(t) = \mathbf{K}^a\mathbf{x}^2(t). \tag{4d}$$

Here $\boldsymbol{\delta}(t)$ is an unknown, element-wise bounded vector which arises from Assumption 1.3). Please notice that the states in $\mathbf{x}^1(t)$ i) are a linear combination of the measured and unmeasured states; and ii) present dynamics *independent* of the reaction rates.

In turn, the vector $\mathbf{x}^2(t)$ is a linear combination of the measured states and its dynamics depend on the (unknown) reaction rates. The following proposition summarises the design of the observer for system (4).

Proposition 3.1. Consider Assumptions 1. By denoting the estimate of $\mathbf{x}^i$ with $\hat{\mathbf{x}}^i$, consider the following observer.

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{x}}^1(t) = -d\hat{\mathbf{x}}^1(t) + \mathbf{K}^b(\mathbf{K}^a)^{-1}[\mathbf{q}^a(\mathbf{y},\hat{\mathbf{x}}^1) - \mathbf{f}^a] - [\mathbf{q}^b(\mathbf{y},\hat{\mathbf{x}}^1) - \mathbf{f}^b] \tag{5a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{x}}^2(t) = -d\mathbf{x}^2(t) - (\mathbf{K}^a)^{-1}[\mathbf{q}^a(\mathbf{y},\hat{\mathbf{x}}^1) - \mathbf{f}^a] + \hat{\mathbf{x}}^3(t) - k_1\boldsymbol{\phi}^1\left((\mathbf{K}^a)^{-1}[\hat{\mathbf{y}} - \mathbf{y}]\right) \tag{5b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{x}}^3(t) = -k_2\boldsymbol{\phi}^2\left((\mathbf{K}^a)^{-1}[\hat{\mathbf{y}} - \mathbf{y}]\right) \tag{5c}$$

$$\hat{\mathbf{y}}(t) := \mathbf{K}^a\hat{\mathbf{x}}^2(t). \tag{5d}$$

Here $k_1, k_2 > 0$ and the nonlinearities $\boldsymbol{\phi}(\circ) : \mathbb{R}^q \to \mathbb{R}^q$, $i = \{1, 2\}$, and are

$$\boldsymbol{\phi}^1(\mathbf{w}) := \left(\alpha\,||\mathbf{w}||_2^{-1/2} + \beta\right)\mathbf{w},$$

$$\boldsymbol{\phi}^2(\mathbf{w}) := \left(\frac{\alpha}{2}\,||\mathbf{w}||_2^{-1/2} + \beta\right)\boldsymbol{\phi}^1(\mathbf{w}),$$

where $\alpha, \beta > 0$.

Then observer (5) estimates the unmeasured $\mathbf{x}^1$ exponentially and the reaction rates $\mathbf{x}^3(t)$ in (4) in finite-time, provided that the vectors $\mathbf{q}^a$ and $\mathbf{q}^b$ are globally Lipschitz in $\mathbf{x}^1(t)$ uniformly in $\mathbf{y}(t)$, that is to say:

$$\left|\left|\mathbf{q}^i(\mathbf{y},\mathbf{z}^1) - \mathbf{q}^i(\mathbf{y},\mathbf{z}^2)\right|\right| \leq \ell^i\left|\left|\mathbf{z}^1 - \mathbf{z}^2\right|\right|, \quad \ell^i > 0. \tag{6a}$$