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Discrete algebraic estimator design for non-linear Liouvillian systems with sampled output: Application to a class of stirred bioreactor

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Abstract

In this manuscript the state estimator design for a class of continuous bioreactor with Liouvillian system characteristics is addressed. The design procedure take into account the sampled nature of the measured output for this kind of processes, considering the model systems structure, the state equations are transformed in a sampled (discrete) system version, which under the considered assumptions are possible to estimate state variables employing only current and past measured output values and model information, without tuning parameters to yield an exact and immediate state estimation. The corresponding theory results of the proposed estimator are applied, where numerical experiments illustrate a satisfactory performance in comparison with a non-linear Luenberger observer.

Keywords: Liouvillian systems; Sampled output; Discrete algebraic estimator; Biochemical reactor

1. Introduction

As it is well known, the estimation theory deserves an interesting research field, because the estimation methodologies developed are widely employed in on-line monitoring, fault detection, system synchronization and control system and so on. Some of the most important estimation methodologies are related with the observers design, where non-linear Luenberger-type filters, Kalman filters, sliding-mode observers, etc. [1–4] have been presented in the open literature, on the other hand some techniques as neural-networks have been successfully employed too [5,6]. However, the over parameterization presented in this kind of estimators arises several problems as high order systems, problems to generate gains tuning rules and so on. The problem of the observer design for continuous systems with sampled measured outputs has been considered under the above frames [7–9]. For the above mentioned, the design of estimation procedures considering the minimum parameterization looks adequate, to attack this issue the frame of differential algebra offers an important tool for a class of non-linear systems, such that explicit relationships that can be obtained for particular state variables; it is an advantage for a class of observation and control problems. Since the early 1990s some papers have been related with the dynamic characterization of a particular class of non-linear systems named differentially flat [10,13] and Liouvillian systems [11], based on the frame of differential algebra. Some researches have considered the observation problem for non-differentially flat systems based on the characteristics of this kind of equations via the total or partial non-flatness property of the system models with application to monitoring and control purposes [12], but considering in some sense standard observers and continuous outputs availability. In this paper employing the flatness characteristics a discrete algebraic estimator, which only needs model and current and past input–output information, is implemented considering as application example a class of continuous biochemical system. The manuscript is composed by the following sections, Section 2 is related with the main definitions related with Liouvillian systems characteristics, where it is proved that the mathematical model of the continuous bioreactor, corresponds to a Liouvillian system. Section 3 presents the theoretical frame for the estimator design, Section 4 is related with the estimator application for a class of continuous biochemical reactor, where the proposed methodology

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is compared with a standard non-linear Luenberger observer and finally Section 5 presents the concluding remarks of the work.

2. Main definitions

In order to give an introductory background for the understanding of Liouvillian systems, the following definitions are presented:

Definition 1. A dynamics is defined as a finitely generated differentially algebraic extension $H/k\langle u\rangle$ of the differential field $k\langle u\rangle$, where $k\langle u\rangle$ denotes the differential field generated by k and elements of a finite set $u=(u_1,u_2,\ldots,u_n)$ of differential quantities.

Definition 2. A differential transcendence basis $y=(y_1,y_2,\ldots,y_m)$ de H/k such that $H=k\langle y\rangle$ is called linearizing or flat output of the system H/k.

Definition 3. The number of state variables, not permissible in terms of the flat outputs, is known as the defect of the non-flat system, that is to say, the integer number, which does the differential transcendence degree of H/k is minimal, is called algebraic defect of the system.

Definition 4. A system H/k is differentially flat if and only if its defect is zero. If its algebraic defect is non-zero, then the system H/k is said to be differentially non-flat.

Definition 5. Let H/k be a given system and let M be such that $k\subset M\subset H$. Moreover it is assumed that M/k is a flat subsystem of H/k, and then can be said that H/k is Liouvillian if the elements of $H-M$ can be obtained by an adjunction of integrals or exponential of integrals of elements of the flat field M.

For further information of this definitions see Ref. [10].

2.1. Application to continuous bioreactor model

There exists a wide range of models for biological systems; the conceptual and mathematical framework for model's development is largely in place. However, there exist several obstacles standing in the way of using sophisticated biological models for process analysis. These obstacles are related with the qualitative nature of much of the available biological information, the lack of process measurements, mainly. Between the main approaches to develop mathematical models for biological reacting systems are the structured models, which consider in some detail the phenomenology in the cells, the unstructured models, which take into account a global process behavior (for example Monod equation). The segregated models whose take into explicit account of the different physiological states of the cell and other approaches as expert system models, cybernetic model and so on. However, the material mass balance models which are not really biological models at all in that they do not explicit acknowledge of the presence of a biological component, but from the process engineering point of view they are the most commonly employed for optimization, monitoring and control studies.

Following an engineering vision, it is considered a material mass balance model in this work. It is considered a class of continuous bioreactor, whose mathematic model is described by the set of Ode's, for substrate and biomass concentrations for the biological phase, these kinds of reactor models are employed in wastewater process, toxic compound degradation and metabolites production and so on. Obviously more complex models with more state variables could be employed, but the simple model employed for the proposed estimator design would be enough.

The corresponding model is as follows [14]:

substrate mass balance (S):

$$\dot{S}=D(S_e-S)-\frac{\mu(S)}{Y_d}X \tag{1}$$

biomass mass balance (X):

$$\dot{X}=-DX+\mu(S)X \tag{2}$$

where D is the dilution rate; $\mu(S)$ the specific growth rate $=k_1S/k_2+S$; S_e the substrate concentration at reactor input; Y_d the yield coefficient; Y is the output measurement.

In accordance with Definition 1 the following equations define a dynamic system H/k, where $H=k(S, X, u)$, and $k=\Re$.

From Definition 2 the corresponding substrate measured output is the named non-flat output as follows:

$$Y=S(t) \tag{3}$$

Let us show the Liouvillian properties of the considered example. From Eq. (2), the biomass concentration can be obtained as:

$$X=\frac{\dot{X}}{\mu(Y)-D}$$

Substituting it in Eq. (1)

$$\dot{Y}=D(S_e-Y)-\frac{\mu(Y)}{Y_d}\left(\frac{\dot{X}}{\mu(Y)-D}\right)$$

From this equation

$$X=\int\frac{\mu(Y)-D}{\mu(Y)}Y_d\left(u(S_e-Y)-\dot{Y}\right)\,dt$$

with

$$Y=S(t)$$

The algebraic defect according with Definition 3 is related with the state variable X (biomass concentration) therefore the bioreactor model is a non-linear Liouvillian system (Definitions 4 and 5). Note that these explicit relationships for the state variables would be employed to estimate the corresponding states, but this involves output derivatives and complex integrals to be solved, which can be a serious drawback for this approach, however under this frame is presented Section 3.

3. Estimator design

Consider the following continuous Liouvillian system:

$$\begin{aligned} \dot{x} &= f(x) \\ y &= h(x) \end{aligned} \tag{4}$$

Now, for the estimation design purposes, it is considered the sampling time $\pi > 0$, if a solution of the system (4) is denoted by $f(t, x_0)$ and initial condition x_0, the π-sampled system of (4) is:

$$x_{k+1} = f(\pi, x_k); \qquad y_k = h(x_k) \tag{4'}$$

Now, consider the following assumptions:

A1. It is assumed that the system (4′) has observability preservation under output measured sampling conditions, and then the system (4′) obeys the theorem presented in Ammar et al. [15].

A2. It is assumed that the strings of obtained outputs prior to $k = 0$, are known from the times $(1 - n)$ on. In other words, the output values, Y_k for $1 - n < k < 0$ are known or available for use.

3.1. Notation

It is introduced a named delay operator δ to express the following $\delta\varphi_k = \varphi_{k-1}$ and the corresponding advance operator denoted by δ^{-1}, such that the expression stands for the identity $\delta^{-\mu}\varphi_k = \varphi_{k+\mu}$, and similarly $\delta^{\mu}\varphi_k = \varphi_{k-\mu}$, for any $\mu > 0$. Symbol $\hat{\delta}$, as in, $\hat{\delta}^{\mu}$, stands for the collection $\{\varphi_{k-1}, \varphi_{k-2}, \ldots, \varphi_{k-\mu}\}$, i.e. $\hat{\delta}^{\mu}\varphi_k = \{\delta\varphi_k, \ldots, \delta^{\mu}\varphi_k\}$. Evidently, $\delta^0 = \hat{\delta}^0 = Id$ and $\hat{\delta}^1 = \delta$, on the other hand $\hat{\delta}^{-\mu}\varphi_k$ stands for the collection $\{\varphi_k, \varphi_{k+1}, \ldots, \varphi_{k+\mu}\} = \{\varphi_k, \delta^{-1}\varphi_k, \ldots, \delta^{-\mu}\varphi_k\}$.

Note that the system Eq. (4′) is equivalent to $x_k = \delta f(x_k) = f(\delta x_k) = f(x_{k-1})$; $\delta x_{k+1} = x_k = f(x_{k-1})$, then one may write $x_{k-1} = f(x_{k-2}) = f(\delta x_{k-1}) = f(\delta^2 x_k)$ it is clear that $x_k = f(f(\delta^2 x_k))$.

The expression $f^{\mu}(\delta^{\mu}x_k)$ for $\mu > 0$, should be clear from the recursion:

$$\begin{aligned} f^i(\delta^i x_k) &= f(f^{i-1}(\delta^i x_k)) \\ f^1(\delta x_k) &= f(\delta x_k) \end{aligned}$$

Besides the operators δ and $\hat{\delta}$ satisfies the following relation: $\delta^i\hat{\delta}^{-i}\varphi_k = \{\varphi_k, \hat{\delta}^i\varphi_k\}$ since $\delta^i(\varphi_k, \varphi_{k+1}, \ldots, \varphi_{k+\mu}) = \delta^i(\varphi_k, \delta^{-1}, \varphi_k, \ldots, \delta^{-\mu}\varphi_k)$. With it the corresponding expressions for the state advance are defined by:

$$\begin{aligned} x_{k+1} &= \delta^{-1}x_k = f(x_k) \\ x_{k+2} &= \delta^{-2}x_k = f(f(x_k)) \\ &\vdots \\ x_{k+i} &= \delta^{-i}x_k = f(f^{i-1}(x_k)) \end{aligned} \tag{5}$$

Employing the system (5) in an iterative form, the following is obtained:

$$\begin{aligned} x_k\delta f(x_k) &= f(\delta x_k) \\ x_k &= f(\delta(f(\delta x_k))) = f(f(\delta^2 x_k)) \\ &\vdots \\ x_k &= f^{n-1}(\delta^{n-1}x_k) \end{aligned} \tag{6}$$

The elements in a finite sequence of advances of the output signal, y_k, are found to be given by:

$$\begin{aligned} y_k &= h(x_k) = h(f^0(x_k)) \\ y_{k+1} &= \delta^{-1}(h(x_k)) = h(f(x_k)) = hf^{-1}(x_k) \\ y_{k+2} &= \delta^{-1}(hf(x_k)) = (hf^2)(x_k) \\ &\vdots \\ y_{k+(n-1)} &= (hf^{n-1})(x_k) \end{aligned} \tag{7}$$

Proposition 1. *Let the system (4′) under the considered assumptions, suppose that corresponding to the constant value, y_e, there exist a unique state vector equilibrium value x_e. Then, the system is constructible, i.e. there exist a map ζ: $\Re^n \to \Re^n$ such that the system can be exactly reconstructed, from time $k = 0$, on, in terms of the output y_k and a finite string of previously obtained outputs, in the form:*

$$x_k = \zeta(y_k, y_{k-1}, \ldots, y_{k-(n-1)}), \quad k \geq 0$$

Provides the string outputs $\{Y_k\}$ for $-n + 1 < k \leq 0$, is completely known. Moreover, an initialization of the above equation with arbitrary chosen values, y_{-i} with $i = 1, 2, \ldots, n - 1$, an actual y_0, still results in an exact reconstruction of x_k for all $k \geq n - 1$.

Sketch of proof. In accordance with the implicit function theorem and the considered assumptions, it follows that there, locally exists a map $\wp$ such that the set of equations:

$$\begin{bmatrix} y_k \\ y_{k+1} \\ \vdots \\ y_{k+(n-1)} \end{bmatrix} = \begin{bmatrix} h(x_k) \\ (hf^1)(x_k) \\ \vdots \\ (hf^{n-1})(x_k) \end{bmatrix} \tag{8}$$

Has a unique solution for x_k of the form:

$$x_k = \wp(\hat{\delta}^{-(n-1)}y_k) \tag{9}$$

Taking $(n - 1)$ delays in the above equation and using Eq. (4′), the following is obtained:

$$\delta^{n-1}x_k = \wp(\delta^{n-1}\hat{\delta}^{-(n-1)}y_k) = \wp(y_k, \hat{\delta}^{n-1}y_k) \tag{10}$$

Using Eqs. (4) and (10) in Eq. (6):

$$x_k = \begin{cases} x_k = f^{n-1}(\delta^{n-1}x_k) \\ f^{n-1}(\wp(y_k, \hat{\delta}^{n-1}y_k)) \\ \zeta(y_k, \hat{\delta}^{n-1}y_k) \\ \zeta(y_k, y_{k-1}, \ldots, y_{k-(n-1)}) \end{cases} \tag{11}$$

With $k \geq 0$

The result follows. □

4. Application example

One of the major bottlenecks in the application of computer monitoring and control for biological process is the lack of reliable, sterilizable and robust sensors for the on-line measurements of process key variables, such as biomass, precursors and product concentrations. In particular the biomass concentration (or cell activity) is generally measured via optical techniques, electrochemical detection and by viscosity, filtration and fluorescence methods [16], but these approaches frequently do not properly address the most important industrial problems and necessities.

To tackle the problem mentioned above, several state estimation techniques for bioprocess have been developed, these techniques are often named soft-sensors and are based on balancing technique, this approach is adequate for steady-state operation, however it becomes unstable when dynamic and corrupted measured are presented [17,18]; filtering (observing) theory where extended Kalman filters, non-linear Luenberger observers, sliding-mode, high gain and so on [19,20]; observers have been successfully employed, but they present some problems from the application point of view, for example: robustness against modeling errors and noisy measurements, over parameterization, and tuning rules for the corresponding observer's gains.

The mathematical model of a class of continuous bioreactor, obtained from a classical mass balances for biomass and substrate concentrations is considered as an application example (see Eqs. (1) and (2)). The dynamic behavior of this process is highly non-linear and can originate multiplicity of steady states or self-sustained oscillations. It is considered a constant volume vessel with a pure culture is fed with a sterile feed flow. The specific growth rate is giving by Monod's model and the yield coefficient is as follows: $\mu(S)=0.3S/1.75+S$ and $Y_\mathrm{d}=0.01+0.03S$, respectively.

For a dilution rate $D=0.14\,\mathrm{h}^{-1}$ and $S_\mathrm{f}=35$ mg/L the open-loop behavior of the bioreactor presents two steady states and a limit cycle of period one, which is present at the no wash-out steady state of the bioreactor ($X=1.872$ mg/L; $S=1.531$ mg/L), the considered initial conditions for the biomass and substrate concentrations are $X_\mathrm{o}=2$ mg/L and $S_\mathrm{o}=10$ mg/L, respectively.

The main issue of the proposed estimator design is to estimate biomass concentration from sampled (discrete) substrate concentration measurements. To do this, an alternative discrete presentation of Liouvillian system with Eqs. (1) and (2) is considered, via a forward finite differences discretization scheme, such that the corresponding π-sampled system is:

$$S_{k+1}=S_k+\left(D(S_\mathrm{e}-S_k)-\frac{\mu(S_k)}{Y_\mathrm{d}}X_k\right)\pi \tag{12}$$

$$X_{k+1}=(1+(-D+\mu(S_k))\pi)X_k \tag{13}$$

$$Y_k=S_k$$

From Eq. (12)

$$X_k=\left(\left(\frac{Y_k-Y_{k+1}}{\pi}\right)+D(S_\mathrm{e}-Y_k)\right)\frac{Y_\mathrm{d}}{\mu(Y_k)} \tag{14}$$

Substituting in Eq. (13) yields

$$X_{k+1}=(1-D+\mu(S_k))\left(Y_k-Y_{k+1}+D(S_\mathrm{e}-Y_k)\frac{Y_d}{\mu(Y_k)}\pi\right) \tag{15}$$

Now, considering one step delay from Eq. (15), the following is obtained:

$$X_k=(1-D+\mu(S_{k-1}))\times\left(Y_{k-1}-Y_k+D(S_\mathrm{e}-Y_{k-1})\frac{Y_\mathrm{d}}{\mu(Y_{k-1})}\pi\right) \tag{16}$$

Note that Eq. (16) is an algebraic discrete estimator to infer biomass concentration from the sampled substrate measured output; it only depends on the input–output system and the model information, without tuning parameters as the case of standard observers. The parameters employed in the bioreactor model are reported in [14], as can be observed in Fig. 1 the sampled system output (dotted line) the sampling time is taken of 30 min, i.e. $\pi=0.5$ h. In Fig. 2 the proposed estimation methodology performance is presented, as can be noted that the biomass concentration reconstruction looks satisfactory.

For comparison purposes, a non-linear Luenberger observer is implemented too. The observer gain for the substrate observer equation is considered as $k_1=1\,\mathrm{h}^{-1}$ and the corresponding observer gain for the biomass observer equation is $k_2=0.1\,\mathrm{h}^{-1}$ the initial conditions for the Luenberger observer are 0.25 and 16 mg/L for biomass and substrate, respectively. The non-linear Luenberger observer's performance is shown in Figs. 3 and 4 where a satisfactory convergence is reached.

Note that the proposed methodology estimates the biomass concentration immediately and exactly from the measured output information, in comparison the observer presents a learning

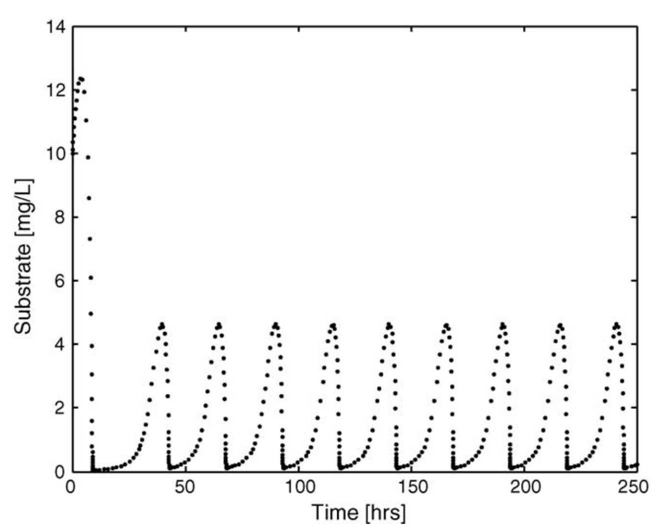

Fig. 1. Substrate concentration measurements.

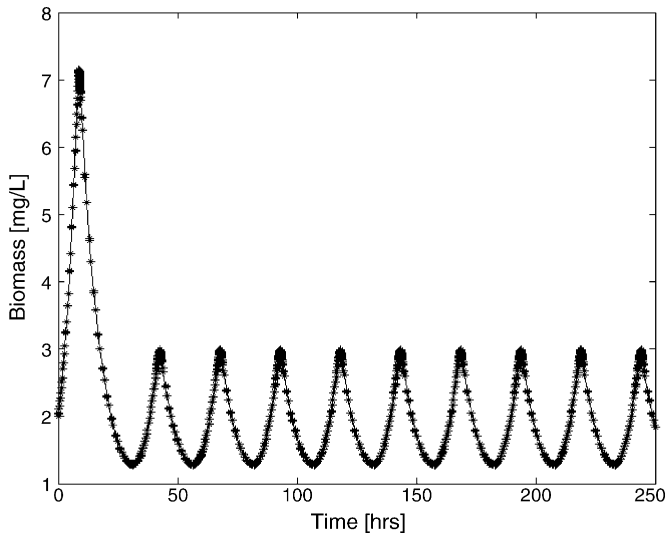

Fig. 2. Biomass concentration reconstruction. Solid line (_) simulation; mark (*) reconstruction.

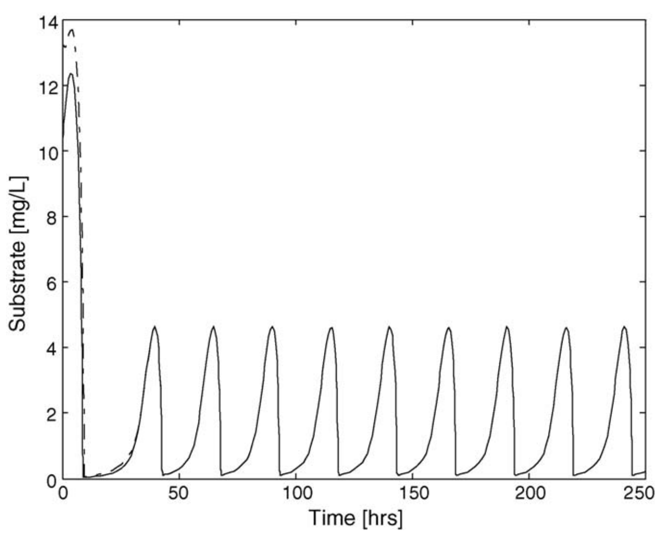

Fig. 3. Substrate concentration filtering using a nonlinear Luenberger observer. Solid line (_) simulation; dashed line (._) filtering.

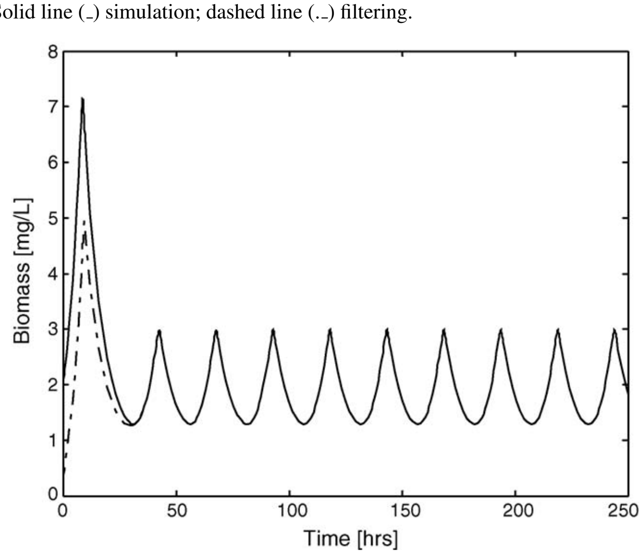

Fig. 4. Biomass concentration estimation using a nonlinear Luenberger observer. Solid line (_) simulation; dashed line (._) estimation.

time period to converge to the *real* value of the biomass concentration. The above is very important when observer based controllers are employed, such that undesirable dynamic effects as the so-named peaking phenomena can be induced, This phenomenon can produce large overshoots which can originate control input saturation, or even worst closed-loop instabilities, because in this situation the feedback is broken and the process behaves as an open-loop with a constant input.

5. Concluding remarks

In this paper a class of non-linear systems named Liouvillian is considered joint with their observability properties. The sampled measurement consideration was tackled for these kinds of systems to design a state estimator. Under the assumptions considered a π-sampled system version is constructed to develop an algebraic state estimator, which only needs for practical implementation current and past output measurements an model information, avoiding the use of tuning parameters as the case of standard state observers. Theoretical properties of the proposed estimator are presented to show the *convergence* characteristics. As a study case a biological continuous reactor is used as an application example, considering as sampled measurement the substrate concentration, as usual, for this kind of systems. Numerical experiments illustrate the adequate performance of the estimator designed in comparison with a non-linear Luenberger observer.

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