

State Estimation for Bioprocesses

Olivier Bernard* and Jean-Luc Gouzé

COMORE, INRIA, France

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LNS0280013

*obernard@sophia.inria.fr

Abstract

In these lecture notes we explain how to build an observer for a biological system. We review the existing linear and nonlinear observers and we propose criteria to define which is the best observer with respect to the available information. Depending on the model reliability and on the level of noise, we can develop observers which use the full model description (high gain observers) or asymptotic observers which use only a mass balance model where the biological kinetics are considered as unknown inputs. If the bounds on the uncertainties can be characterised, interval observers can be designed. Each observer is illustrated with an example performed on a biological system.

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1 Introduction

One of the main limitations to the improvement of monitoring and optimisation of bioreactors is probably due to the difficulty to measure chemical and biological variables. Indeed there are very few sensors which are at the same time cheap and reliable and that can be on-line used. The measurement of some biological variables (biomass, cellular quota, etc.) is sometimes very difficult and can necessitate complicated and sophisticated operations.

The question is to estimate the internal state of a bioreactor when only a few measurements are available. In this lecture we propose methods to build observers which will use the available measurements to estimate non measured state variables (or at least some of them). The principle of this so called “software sensor” is to use the process model to reconstruct asymptotically the state on the basis of the outputs. As it will be detailed in this chapter, the system must be observable, or at least detectable, in order to estimate the internal state.

There are numerous methods to design an observer. They rely on ideas that can be very different. Thus the best observer must be chosen with respect to the type of problem. The choice will then be strongly connected to the quality and the uncertainties of the model and of the data. If the biological kinetics are not precisely known, the mass balance will be the core of the asymptotic observers. If there are bounded uncertainties on the inputs and/or on the parameters, then we will estimate intervals in which the state of the system should lie. If the model has been correctly identified and validated, then we can fully exploit it and -if the output are not corrupted with a high level of noise- we can develop a high gain observer.

The type of observer to be developed must not be based only on the model quality: it must also take into account the objectives to be achieved. Indeed, an observer can have other purposes than monitoring a bioreactor: it can be developed to apply a control action which need an estimate of the internal state. It can also be used to determine if a failure did not happen in the process.

2 Notions on system observability

We will only recall the main useful notions, we will give references for the more technical parts (see [1, 2]).

The observability notion is fundamental in automatic control. Intuitively,

one tries to estimate the state variables from the available measurements. If this is possible from a theoretical point of view, the system is said to be observable. Then the next question is how to derive an observer which is another dynamical system providing a state estimate. Let us mention that the question of observability and of observer design are very different: the observability property does not give any clue on how to build an observer.

The theory is extensively developed in the linear case (see next section) and, in the nonlinear case, has been strongly developed during the last years but for particular classes of models.

2.1 System observability: definitions

We will consider the general continuous time system:

$$(\mathcal{S}) \begin{cases} \frac{dx}{dt}(t) = f(x(t), u(t)) & ; \quad x(t_0) = x_0 \\ y(t) = h(x(t)) \end{cases} \quad (1)$$

where $x \in \mathbb{R}^n$ is the state vector, $u \in \mathbb{R}^m$ is the input vector, $y \in \mathbb{R}^p$ is the output vector, x_0 is the initial condition for initial time t_0 , $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $h : \mathbb{R}^n \rightarrow \mathbb{R}^p$. The functions are assumed to be sufficiently smooth in order to avoid problems of existence and uniqueness of the solutions.

Example: For the bioreactors described by a mass balance model, we have:

$$f(x(t), u(t)) = Kr(x(t)) + D(x_{in}(t) - x(t)) - Q(x(t))$$

Here D and x_{in} stands for the input vector.

We assume therefore that, for system (\mathcal{S}) ,

- the input $u(t)$ is known
- the output $y(t)$ is known
- functions f and h , are known, *i.e.* the model is known (for a bioreactor it means that $r(\cdot)$ is known in the mass balance based modelling).

We want to estimate $x(t)$; the observability is a theoretical notion that states if it is possible.

Definition 1 *Two states x_0 and x'_0 are said indiscernible if for any input time function $u(t)$ and for any $t \geq 0$, the outputs $h(x(t, x_0))$ and $h(x(t, x'_0))$ that result are equal.*

Definition 2 *The system is said to be observable if it do not have any distinct couple of initial state x_0, x'_0 that are indiscernible.*

This means that for any input the initial condition can be uniquely estimated from the output. It can be noticed that generally for nonlinear system the observability depends on the input; a system can be observable for some inputs and not observable for others.

Definition 3 *An input is said to be universal if it can distinguish any couple of initial conditions.*

Definition 4 *A non universal input is said to be singular.*

Even in the case where all the inputs are universal (the system is said to be uniformly observable and can be rewritten under a specific shape, see section 4), this can be insufficient in practice. We impose then that the universal property persists with time, and we obtain (at least for some systems) the notion of regularly persisting input (see Hypothesis 5, paragraph 5.3).

For the linear systems things are much simpler (see next section).

2.2 General definition of an observer

Once the system has been proven to be observable, the next step is the observer building in order to estimate the state variable x from the inputs, the outputs and the model.

The observer principle is presented on Figure 1. It is a second dynamical system that will be coupled to the first one thanks to the measured output.

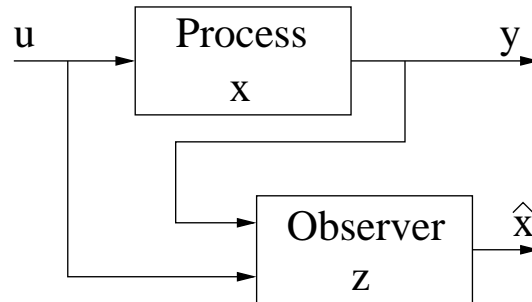


Figure 1: Observer principle

Definition 5 *An observer is an auxiliary system coupled with the original system:*

$$(\mathcal{O}) \begin{cases} \frac{dz}{dt}(t) = \hat{f} : (z(t), u(t), y(t)) ; z(t_0) = z_0 \\ \hat{x}(t) = \hat{h} : (z(t), u(t), y(t)) \end{cases} \quad (2)$$

with $z \in \mathbb{R}^q$, $\hat{f} : \mathbb{R}^q \times \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}^q$ and $\hat{h} : \mathbb{R}^q \times \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}^n$ such that

$$\lim_{t \rightarrow \infty} \|x(t) - \hat{x}(t)\| = 0 \quad (3)$$

It is the classical definition which may be insufficient in some cases. It is stated that the estimation error tends asymptotically toward zero. Indeed one tries to tune the error decreasing rate (convergence rate). Let us explain this with a simple linear example: let us consider the linear system $\frac{dx}{dt} = Ax + Bu$ where $x \in \mathbb{R}^n$ and let us assume that matrix A is stable. A trivial observer can be obtained with a copy of the system: $\frac{d\hat{x}}{dt} = A\hat{x} + Bu$. Indeed, the error $e = x - \hat{x}$ follows the same dynamics $\frac{de}{dt} = Ae$ and therefore converges toward zero. Let us remark that this observer does not necessitate any output. This example shows that the stable internal dynamics is sufficient to estimate the final state. This example highlights a property which will be called detectability for linear systems and which will be the basis of asymptotic observer (section 4) in a different framework. As a consequence, an additional requested property is to be able to tune the convergence rate of the observer in order to be able to reconstruct the state variables more rapidly than the dynamics of the system. Let us remark that the observer variable (z in \mathcal{O}) can be of greater dimension than the state variable to be estimated x .

Another property that we wish is that if the observer is properly initiated, *i.e.* with the true value $x(0)$, then its estimation remains equal to $x(t)$ for all t . This suggests a peculiar structure for the observer

Definition 6 *Often, the following observer is taken:*

$$(\mathcal{O}) \begin{cases} \frac{d\hat{x}}{dt}(t) = f(\hat{x}(t), u(t)) + k[z(t), h(\hat{x}(t)) - y(t)] \\ \frac{dz}{dt}(t) = \hat{f}(z(t), u(t), y(t)) \quad \text{with} \quad k(z(t), 0) = 0 \end{cases}$$

This is a copy of the system with a correcting term depending on the discrepancy between the true measured outputs and the value of the output computed from the observer. The correction amplitude is tuned thanks to the function k that can be seen as a gain (it is an internal tuning of the

observer).

In the ideal case, the gain k can be tuned in order to have a converging rate as large as requested.

Definition 7 *System (O) is said to be an exponential observer if, for any positive λ , the gain k can be tuned such that*

$$\forall(x_0, \hat{x}(0), z_0) \quad \forall t > 0, \quad \|\hat{x}(t) - x(t)\| \leq e^{-\lambda t} \|\hat{x}(0) - x(0)\|.$$

2.3 How to manage the uncertainties in the model or in the output

In real life- and especially in the biological field- one often considers that there are noises either in the output (measurement noise) or in the state equation (model noise). In general the model noise is assumed to be additive (see section 3.5), which is a strong hypothesis (it could be e.g. multiplicative).

Another important case which often appears in the bioprocesses is when the model integrates some unknown parts. For example the biological kinetics in the mass balance models for bioreactors are generally not precisely known [3].

How to manage these two problems which have some related aspects ?

- Linear filtering, and more specifically Kalman filtering. It is the most popular method. It assumes that the noises are additive and white; it minimises the error variance (see next section).
- The approach L^2 , H^2 or H^∞ . It consists in assuming that the noises or perturbations $w(t)$ belong to a given class of functions (L^2) and to try to minimise their impact on the output using the transfer function. In the H^2 approach, one tries to minimise the norm of this transfer function. in the approach H^∞ , one tries to minimise the input effect in the worst case (see [4]). For example, for a $\gamma > 0$ and R a positive definite matrix, one wants the observer \hat{x} to verify:

$$\sup_{w(\cdot)} \int_0^\infty |\hat{x}(t) - x(t)|_R^2 - \gamma^2 |w(t)|^2 dt \leq 0.$$

- Disturbance rejection. One tries to build observers independent from the unknown perturbation. The disturbance is cancelled for example thanks to linear combinations of variables [5, 6].

The asymptotic observers are among this class of systems (see section 5).

- Bounds on the perturbations and on the uncertainties. One assumes that uncertainties are bounded, and one tries to design interval observers which provide the best possible bounds for the variables to be estimated. For some cases, one tries to minimise this bounding (section 6).
- One can also use these bounds to design sliding mode observers which have a correcting term of the type $\text{sign}(x - \hat{x})$. Note that the way these observers take the uncertainties into account generates a discontinuous dynamics on the sliding manifolds [7].

Remark: it is possible to construct examples where a system is observable when the model is known and becomes unobservable when a part of the model is unknown. For such cases the requirement for a classical observer may be relaxed. In particular, we will not assume anymore that

$$\lim_{t \rightarrow \infty} \|x(t) - \hat{x}(t)\| = 0 \quad (4)$$

but that the discrepancy tends toward a reasonable value for practical applications.

3 Observers for linear systems

For single output linear stationary systems we have:

$$(\mathcal{S}_L) : \begin{cases} \frac{dx}{dt}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) \end{cases} \quad (5)$$

with $A \in \mathcal{M}^{n \times n}(\mathbb{R})$ ($n \geq 2$), $C \in \mathcal{M}^{1 \times n}(\mathbb{R})$.

The well known observability criterion is formulated as follows:

$$(\mathcal{S}_L) \text{ observable} \Leftrightarrow \text{rank} \begin{pmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{pmatrix} = n.$$

which relies on the fact that the observability space is generated by the vectors (C, CA, \dots, CA^{n-1}) .

The canonical observability forms, that can be obtained after a linear change of coordinates, highlight the observation structure. They will reappear in the nonlinear case for the high gain observer (section 6).

Theorem 1 *If the pair (A, C) is observable, then there exists an invertible matrix P such that:*

$$A_0 = P^{-1}AP, \quad C_0 = CP$$

with

$$A_0 = \begin{pmatrix} -a_n & 1 & 0 & \dots & 0 \\ -a_{n-1} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -a_2 & 0 & 0 & \dots & 1 \\ -a_1 & 0 & 0 & \dots & 0 \end{pmatrix} \quad C_0 = (1 \quad 0 \dots 0)$$

What happens if the system is not observable? One can rewrite it in two parts, as it is shown in the following theorem. Here A_1 and A_3 are two square matrices with dimensions corresponding to x_1 and x_2 . The canonical form shows clearly that x_1 can not be estimated from x_2 .

Theorem 2 *General canonical form:*

$$\begin{aligned} \frac{dx_1}{dt} &= A_1x_1 + A_2x_2 + B_1u \\ \frac{dx_2}{dt} &= A_3x_2 + B_2u \\ y &= C_2x_2 \end{aligned}$$

Matrix A_1 imposes the dynamics of the unobservable part; if it is stable, then the dynamics of the total error will be stable, but the unobservable part will tend toward zero with its own dynamics (given by A_1); the system is said to be detectable.

3.1 Luenberger observer

If system (5) is observable, a Luenberger observer [8] can be derived:

$$\frac{d\hat{x}(t)}{dt} = A\hat{x}(t) + Bu(t) + K(C\hat{x}(t) - y(t))$$

where K is a dimension n gain vector, which allows to tune the convergence rate of the observer.

Indeed, the dynamics of the observation error $e = x - \hat{x}$ is:

$$\frac{de}{dt} = (A + KC)e$$

Let us note that this dynamics do not depend on the input. The pole placement theorem states that the error dynamics can be arbitrarily chosen.

Theorem 3 *If (A, C) is observable, the vector K can be chosen to have an arbitrary linear dynamics of the observation error.*

In particular, the gain vector K can be chosen in order that the error converges rapidly toward zero. But then the observer will be very sensitive to perturbations (measurement noise for example). A good compromise must be chosen between stability and precision. The Kalman filter is a way to manage this compromise.

3.2 The linear case up to an output injection

There is a very simple case for which a linear observer can be designed for a nonlinear system, it is the case where the nonlinearity depends only on the output y .

$$(\mathcal{S}) : \begin{cases} \frac{dx}{dt}(t) &= Ax(t) + \phi(t, y(t)) + Bu(t) \\ y(t) &= Cx(t) \end{cases} \quad (6)$$

ϕ is a nonlinear (known) function which takes its values in \mathbb{R}^n . The following “Luenberger like” observer generates a linear observation error equation:

$$\frac{d\hat{x}(t)}{dt} = A\hat{x}(t) + \phi(t, y(t)) + Bu(t) + K(C\hat{x}(t) - y(t))$$

The dynamics can be arbitrarily chosen if the pair (A, C) is observable.

3.3 Local observation of a nonlinear system around an equilibrium point

Let us consider the general system (1), and let us assume that it admits a single equilibrium point (working point) at (x_e, u_e) . The system can then be linearised around this point:

Theorem 4 *The linearised system of (1) around (x_e, u_e) is*

$$(\mathcal{S}) \begin{cases} \frac{dX}{dt}(t) = AX + BU \\ Y(t) = CX \end{cases} \quad (7)$$

with

$$A = \frac{\partial f(x, u)}{\partial x} \quad B = \frac{\partial f(x, u)}{\partial u} \quad C = \frac{\partial h(x)}{\partial x}$$

Matrices A, B, C are estimated at x_e, u_e . Variables X, U, Y are deviations toward equilibrium:

$$X = x - x_e, \quad U = u - u_e, \quad Y = y - Cx_e$$

If the pair (A, C) is observable, the nonlinear system is locally observable around the equilibrium.

3.4 PI observer

The Luenberger observer is based on a correction of the estimations with a term related to the difference between the measured outputs and the predicted outputs.

The idea behind the proportional integral observer is to use the integral of this error term. We consider the auxiliary variable \hat{w} :

$$\hat{w} = \int_0^t (C\hat{x}(\tau) - y(\tau))d\tau.$$

The PI observer for system (8) will then be rewritten:

$$\begin{cases} \frac{d\hat{x}}{dt}(t) &= Ax(t) + Bu(t) + K_I(C\hat{x}(t) - y) + K_P\hat{w} \\ \frac{d\hat{w}}{dt}(t) &= C\hat{x} - y \end{cases} \quad (8)$$

The error equation ($e_x = \hat{x} - x$ and $e_w = \hat{w}$) is then:

$$\begin{pmatrix} \frac{de_x}{dt}(t) \\ \frac{de_w}{dt}(t) \end{pmatrix} = \begin{pmatrix} A + K_I C & K_P \\ C & 0 \end{pmatrix} \begin{pmatrix} e_x(t) \\ e_w(t) \end{pmatrix} \quad (9)$$

The gains K_I and K_P can be chosen such as to ensure stable error dynamics [9]. The integrator addition provides more robustness to the observer to deal with measurement noise or modelling uncertainties.

3.5 Kalman filter

The Kalman filter (see [10]) is very famous in the framework of linear systems; it can be seen as Luenberger observer with a time varying gain; this allows to minimise the error estimate variance.

A stochastic representation can be given by the observable system:

$$\begin{cases} \frac{dx}{dt}(t) = A x(t) + Bu(t) + w(t) & ; & x(t_0) = x_0 \\ y(t) = C x(t) + v(t) \end{cases} \quad (10)$$

where $w(t)$ and $v(t)$ are independent centred white noises (Gaussian perturbations), with respective covariances $Q(t)$ and $R(t)$. Let us also assume that the initial distribution is Gaussian, such that:

$$E[x_0] = \hat{x}_0 & ; & E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] = P_0 \quad (11)$$

where E represents the expected value and P_0 is the initial covariance matrix of the error. The filter is written in several steps:

1. Initialisation:

$$E[x_0] = \hat{x}_0 & ; & E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] = P_0 \quad (12)$$

2. Estimation of the state vector:

$$\frac{d\hat{x}}{dt}(t) = A \hat{x}(t) + Bu(t) + K(t) [y(t) - C \hat{x}(t)] & ; & \hat{x}(t_0) = \hat{x}_0 \quad (13)$$

3. Error covariance propagation (Riccati equation):

$$\frac{dP}{dt}(t) = A P(t) + P(t) A^T - P(t) C^T R(t)^{-1} C P(t) + Q(t) \quad (14)$$

4. Gain computation:

$$K(t) = P(t) C^T R(t)^{-1} \quad (15)$$

Some points can be emphasised:

- This filter can still be applied when matrices A and C depend on time (the observability must nevertheless be proven).
- The estimation of the positive definite matrices R, Q, P_0 is often very delicate, especially when the noise properties are not known.
- A deterministic interpretation of this observer can be given: it consists in minimising the integral from 0 to t of the square of the error.
- This observer can be extended by adding a term $-\theta P(t)$ in the Riccati equation. This exponential forgetting factor allows to consider the cases where $Q = 0$.

3.6 The extended Kalman filter

The idea consists in linearising a nonlinear system around its estimated trajectory. Then the problem is equivalent to build a Kalman filter for non stationary system. Let us consider the system

$$\begin{cases} \frac{dx}{dt}(t) = f(x(t)) + w(t) ; & x(t_0) = x_0 \\ y(t) = h(x(t)) + v(t) \end{cases} \quad (16)$$

and the observer is designed as above, with a change in the second step:

2. Estimation of the state vector:

$$\frac{d\hat{x}}{dt}(t) = f(\hat{x}(t)) + K(t) [y(t) - h(\hat{x}(t))] ; \hat{x}(t_0) = \hat{x}_0 \quad (17)$$

and using the matrices of the tangent linearised:

$$A(t) = \left. \frac{\partial f(x(t))}{\partial x(t)} \right|_{x(t)=\hat{x}(t)} \quad C(t) = \left. \frac{\partial h(x(t))}{\partial x(t)} \right|_{x(t)=\hat{x}(t)} \quad (18)$$

This extended filter is often used, even if only few theoretical results guarantee its convergence (see Section 4.4).

4 High gain observers

4.1 Definitions, hypotheses

In this chapter, we will assume that a simulation model of the process is available, (*i.e.* with modelling of the biological kinetics). We also assume that the model has been deeply validated: the high gain observers are dedicated to the nonlinear systems and require a high quality modelling.

We will consider now the systems which are affine with respect to the input, that are described as follows:

$$\frac{d\xi}{dt} = f(\xi) + ug(\xi) \quad (19)$$

We consider here the case where $u \in \mathbb{R}$. For bioreactors, the input corresponds generally to the dilution rate $u = D$. In this case $f(\xi) = Kr(\xi) - Q(\xi)$ and $g(\xi) = \xi_{in} - \xi$.

Moreover, we assume that the output is a function of the state: $y = h(\xi) \in \mathbb{R}$.

Hypothesis 1 We will state the two following hypotheses:

- [i] the system (19) is observable for any input.
- [ii] there exists a positively invariant compact \mathcal{K} , such that for any time t , $\xi(t) \in \mathcal{K}$.

We will denote $L_f h(\xi) = \frac{Dh}{D\xi} f(\xi)$, which is the Lie derivative of h along the vector field f . By convention, we will write $L_f^p h(\xi) = L_f L_f^{p-1} h(\xi)$.

4.2 Change of variable

Let us consider the following change of coordinates, defined on the compact set \mathcal{K} :

$$\phi : \xi \longrightarrow \zeta = \left[h(\xi), L_f h(\xi), \dots, L_f^{(n-1)} h(\xi) \right]^T \quad (20)$$

This change of variable consists in considering (in the autonomous case) the output y and its $n - 1$ first derivatives as new coordinates.

Hypothesis 2 The mapping ϕ is a global diffeomorphism.

One can verify [11] that under Hypothesis 2 ϕ transforms (19) into:

$$\frac{d\zeta}{dt} = A\zeta + \tilde{\psi}(\zeta) + \bar{\psi}(\zeta)u \quad (21)$$

$$y = C\zeta \quad (22)$$

with:

$$A = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \quad C = [1, 0, \dots, 0]$$

$$\tilde{\psi}(\zeta) = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ L_f^p h(\phi^{-1}(\zeta)) \end{pmatrix}, \quad \bar{\psi}(\zeta) = \begin{pmatrix} \bar{\psi}_1(\zeta_1) \\ \bar{\psi}_2(\zeta_1, \zeta_2) \\ \vdots \\ \bar{\psi}_2(\zeta_1, \zeta_2, \dots, \zeta_n) \end{pmatrix}$$

where

$$\bar{\psi}_i(z) = \bar{\psi}_i(\zeta_1, \dots, \zeta_i) = L_g L_f^{(i-1)} h[\phi^{-1}(\zeta)] \quad (23)$$

In this canonical form, all the system nonlinearities have been concentrated in the terms $\tilde{\psi}(\zeta)$ and $\bar{\psi}(\zeta)$. We will present the various observers using this canonical form (let us note that this canonical form is very close to the one in section 3 for the observer pole assignment).

Let us remark that an observer in the new basis will provide an estimate $\hat{\zeta}$ which will estimate ζ , *i.e.* the successive output derivatives. The idea consists in writing the observer in this canonical basis *i.e.* a numerical differentiator of the output. Then, going back to the initial coordinates (applying $\phi^{-1}(\zeta)$), the observer will be expressed in the original basis.

To design a high gain observer, we need an additional technical hypothesis:

Hypothesis 3 *The mappings $\tilde{\psi}$ and $\bar{\psi}$ defined in (21) are global Lipschitz on \mathcal{K} .*

Intuitively, this hypothesis will allow us to dominate the non-linear part, imposing that the dynamics of the observer can be faster than the system ones (this explains the idea of the “high gain”).

4.3 Fixed gain observer

Property 1 [12] *For a sufficiently high gain θ , and under Hypotheses 1, 2 and 3 the following differential system is an exponential observer of (19):*

$$\frac{d\hat{x}}{dt} = f(\hat{x}) + u g(\hat{x}) - \left[\frac{\partial \phi}{\partial x} \right]_{x=\hat{x}}^{-1} S_{\theta}^{-1} C^t (h(\hat{x}) - y) \quad (24)$$

where S_{θ} , is the solution of the equation $\theta S_{\theta} + A^t S_{\theta} + S_{\theta} A = C^t C$
 S_{θ} can be computed as follows:

$$S_{\theta}(i, j) = \frac{(-1)^{i+j}}{\theta^{i+j-1}} \frac{(i+j-2)!}{(i-1)!(j-1)!} \quad (25)$$

For the convergence proof and other details we refer to [12].

4.4 Variable gain observers (Kalman like observer)

The extended Kalman filter is often used in a framework where its convergence is not guaranteed (see section 3.5). We show here how to build a high gain observer very close to the Kalman filter (after change of variable), whose convergence is guaranteed.

Property 2 [13] *For a gain θ sufficiently high, and under hypotheses 1, 2 and 3 the following differential system is an exponential observer of (19):*

$$\begin{cases} \frac{d\hat{x}}{dt} = f(\hat{x}) + u g(\hat{x}) - \frac{1}{r} \left[\frac{\partial \phi}{\partial x} \right]_{x=\hat{x}}^{-1} S^{-1} C^t (h(\hat{x}) - y) \\ \frac{dS}{dt} = -SQ_{\theta}S - A^{*t}(\hat{x}, u)S - SA^{*}(\hat{x}, u) + \frac{1}{r}C^t C \end{cases} \quad (26)$$

with $r > 0$, Q_θ is computed from the two positive definite symmetric matrices Δ_θ and Q :

$$\Delta_\theta = \text{diag}(\theta, \theta^2, \dots, \theta^n) \quad (27)$$

$$Q_\theta = \Delta_\theta Q \Delta_\theta \quad (28)$$

Matrix A^* can be computed from the diffeomorphism ϕ :

$$A^*(\hat{\xi}, u) = A + \left[\frac{\partial \phi}{\partial \zeta} \right]_{\zeta=\phi(\hat{\xi})} + u \left[\frac{\partial \psi}{\partial \zeta} \right]_{\zeta=\phi(\hat{\xi})} \quad (29)$$

We refer to [13] for the proof of the convergence of this observer and for more details, especially for the choice of r and of matrix Q .

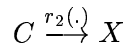
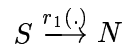
It is worth noting that, even if the filtering and noise attenuation performances of this extend Kalman filter are *a priori* better, this observer is above all a high gain observer; it will therefore present the same generic high sensitivity with respect to the measurement noises and modelling errors.

The advantages of the Kalman like high gain observer have a price: this observer is heavier to implement. $\frac{n(n+3)}{2}$ differential equations must be integrated instead of n equations for the simple high gain observer.

4.5 Example: growth of micro-algae

We will consider the growth of micro algae in a continuous photobioreactor. The algal development is limited by a nitrogen source (NO_3) denoted S , and uses principally the inorganic dissolved carbon (C), mainly under the form of CO_2 . The algal biomass (X) will then correspond to an amount of particulate nitrogen (N).

In order to simultaneously describe the cellular carbon and nitrogen uptake, we will consider the following reaction scheme



Setting $\xi = (X, N, S, C)^t$, the mass balance based model (33) can be written with:

$$K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \\ -1 & 0 \\ 0 & -k_1 \end{pmatrix}, \quad \xi_{in} = \begin{pmatrix} 0 \\ 0 \\ S_{in} \\ C_{in} \end{pmatrix}, \quad Q(\xi) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ Q_c(\xi) \end{pmatrix}$$

The units for carbon and nitrogen are the same for biomass and substrate, and moreover the nitrogen uptake yield is assume to be unitary. The nutrient uptake rate is assumed to follow a Michaelis-Menten law [14]:

$$r_1(\xi) = \rho_{max} \frac{S}{S + k_S} X$$

The algal growth from carbon is $r_2(\xi) = \mu(\xi)X$, where the growth rate $\mu(\xi)$ is described by the Droop law [15]:

$$\mu(\xi) = \mu(q) = \bar{\mu} \left(1 - \frac{k_q}{q}\right) \tag{30}$$

Variable q represents the internal nitrogen quota defined by the amount of nitrogen per biomass unit: $q = \frac{N}{X}$.

We assume that biomass is measured (it is estimated by its total biovolume), and will be used to design a high gain observer to determine S and q .

In this case, the nitrate concentration in the renewal medium (S_{in}) can be controlled. More precisely, S_{in} can vary as follows:

$$S_{in} = s_{in}(1 + u)$$

where u is the control, and s_{in} the nominal concentration, corresponding to $u = 0$.

In the sequel, we will consider only the 3 first equations of this system, and we will consider the following change of variables:

- $x_1 = \frac{\rho_m X}{s_{in}}$; $x_2 = \frac{N}{X k_q}$; $x_3 = \frac{S}{s_{in}}$
- $a_1 = \frac{k_s}{s_{in}}$; $a_2 = \bar{\mu}$; $a_3 = \frac{\rho_m}{k_q}$

that leads to the following system:

$$\begin{cases} \frac{dx}{dt} = f(x) + ug(x) \\ y = h(x_1) \end{cases} \tag{31}$$

with:

$$x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, f(x) = \begin{pmatrix} a_2 \left(1 - \frac{1}{x_2}\right) x_1 - D x_1 \\ a_3 \frac{x_3}{a_1 + x_3} - a_2 (x_2 - 1) \\ D(1 - x_3) - \frac{x_1 x_3}{a_1 + x_3} \end{pmatrix}, \tag{32}$$

$$g(x) = \begin{pmatrix} 0 \\ 0 \\ D \end{pmatrix}, h(x_1) = x_1$$

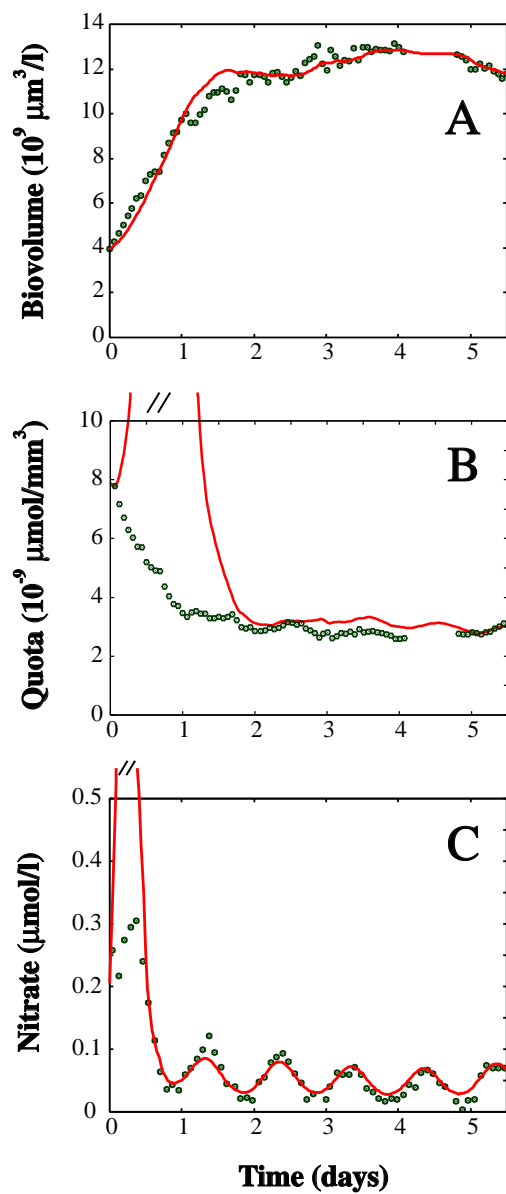


Figure 2: Comparison between direct measurements (\bullet) and observer predictions ($—$) for model (31): (A) Biomass estimated from total algal biovolume. (B) internal quota. (C) Nitrate concentration

The high gain observer for model (31) is then given by:

$$G(\hat{x}) = \begin{pmatrix} 3\theta \\ \left[3\theta \frac{\hat{x}_2}{\hat{x}_1} \left[1 - \left(1 - \frac{D}{a_2} \right) \hat{x}_2 \right] + 3\theta^2 \frac{\hat{x}_2^2}{a_2 \hat{x}_1} \right] \\ \left[3\theta \hat{B}_{31} + 3\theta^2 \hat{B}_{32} + \theta^3 \frac{\hat{x}_2^2 (a_1 + \hat{x}_3)^2}{a_1 a_2 a_3 \hat{x}_1} \right] \end{pmatrix}$$

with:

$$\begin{aligned} \hat{B}_{31} &= \frac{1}{a_1 a_3 \hat{x}_1} \left[\frac{a_3 \hat{x}_3}{a_1 + \hat{x}_3} + 2a_2 + \hat{x}_2^2 \left(2a_2 - 3D - \frac{D^2}{a_2} \right) \right. \\ &\quad \left. - \hat{x}_2 \left(2 \frac{a_3 \hat{x}_3}{a_1 + \hat{x}_3} \left(1 - \frac{D}{a_2} \right) + 4a_2 - 4D \right) \right] \\ \hat{B}_{32} &= \frac{\hat{x}_2 (a_1 + \hat{x}_3)^2}{a_1 a_2 a_3 \hat{x}_1} \left[\hat{x}_2 (2D - 3a_2) + 4a_2 + 2 \frac{a_3 \hat{x}_3}{a_1 + \hat{x}_3} \right] \end{aligned}$$

An experiment where u fluctuates sinusoidally was used to validate the observer. Figure 2 proves the observer efficiency when the model is well known. The observer predictions are in agreement with the experimental measurements. For more details on this example, see [16, 17].

5 Observers for mass balance based systems

5.1 Introduction

In the previous sections we have considered the case where the uncertainties were due to noise on the outputs and, in some cases were due to modelling noise. We have seen Chapter 2 that the bioprocess models are often badly known. In particular when the model is written on the basis of a mass balance analysis, a term representing the reaction rates appears. This term which represents the biological kinetics with respect to the model state variable is often speculative. Often the modelling of the reaction rate is not reliable enough to base an observer on it. In this section we will use the results for the observers with unknown inputs [6, 18, 5], whose principle relies on a cancellation of the unknown part after a change of variable in order to build the observer.

We will show how to build an observer for a system represented by a mass balance and for which the kinetics would not have been expressed. We

will see that the main condition to design such an observer is that enough variables are measured. In particular we will not assume any observability property. This is not so surprising since the observability property relies on its full description (including the kinetics) which is not used to build the mass balance observer. In fact it is not really an observer *stricto sensu*, but more precisely a detector, relying on hypothesis that the non observable part is stable.

5.2 Definitions, hypotheses

In this chapter we will consider the biotechnological processes that are modelled with a mass balance model:

$$\frac{d\xi}{dt} = Kr(\xi) - D(t)\xi + D(t)\xi_{in}(t) - Q(\xi) \quad (33)$$

with

$$\xi \in \mathbb{R}^n \quad r \in \mathbb{R}^p \quad (34)$$

We assume that the set of available measurements y can be decomposed into three vectors:

$$y = [y_1 \ y_2 \ y_3]^T \quad (35)$$

where:

- y_1 is a set of q measured state variables. To simplify the notations, we will order the components of the state so that, y_1 corresponds to the q first components of ξ .
- y_2 represents the measured gaseous flow rates: $y_2 = Q(\xi)$
- y_3 represents the other available measurements (pH, conductivity,...) that are related to the state through the following relationship: $y_3 = h(\xi)$

Let us rewrite system (33) after splitting the measured part ($\xi_1 = y_1$) from the other part of the state (ξ_2).

$$\frac{d\xi_1}{dt} = K_1 r(\xi) - D\xi_1 + D\xi_{in1} - Q_1(\xi) \quad (36)$$

$$\frac{d\xi_2}{dt} = K_2 r(\xi) - D\xi_2 + D\xi_{in2} - Q_2(\xi) \quad (37)$$

Matrices K_1 and K_2 , vectors ξ_{in1} , ξ_{in2} , Q_1 and Q_2 are such that

$$K = \begin{pmatrix} K_1 \\ K_2 \end{pmatrix}, \quad \xi_{in} = \begin{pmatrix} \xi_{in1} \\ \xi_{in2} \end{pmatrix}, \quad Q = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}$$

5.3 The asymptotic observer

In order to build the asymptotic observers we need the two following technical hypotheses:

Hypothesis 4 (i) *There are more measured quantities than reactions: $q \geq p$.* (ii) *Matrix K_1 is of full rank.*

Hypothesis 4(ii) means that a non zero r cannot cancel $K_1 r$ (a reaction can not compensate the other ones with respect to the measured variables).

Consequences: under Hypothesis 4, the $q \times p$ matrix K_1 admits a left inverse; there exists a $p \times q$ matrix G such that:

$$GK_1 = I_{p \times p} \quad (38)$$

Let us set: $A = -K_2 G$, and let us consider the following linear change of coordinates:

$$\zeta_1 = \xi_1 \quad (39)$$

$$\zeta_2 = A\xi_1 + \xi_2 \quad (40)$$

this change of variable transforms (36) and (37) into:

$$\frac{d\zeta_1}{dt} = K_1 r(T\zeta) - D\zeta_1 + D\xi_{in1} - Q_1(T\zeta) \quad (41)$$

$$\frac{d\zeta_2}{dt} = -D(\zeta_2 - \zeta_{in2}) - (AQ_1(T\zeta) + Q_2(T\zeta)) \quad (42)$$

with

$$T = \begin{pmatrix} I_p & 0_{p,n-p} \\ -A & I_{n-p} \end{pmatrix}, \quad M = \begin{pmatrix} A & I_{n-p} \end{pmatrix} \quad (43)$$

and

$$\zeta_{in2} = M\xi_{in} \quad (44)$$

The equation of ζ_2 can be rewritten using the output y_2 :

$$\frac{d\zeta_2}{dt} = -D(\zeta_2 - \zeta_{in2}) - My_2 \quad (45)$$

Remark: System (45) is a linear system up to an output injection (cf. Section 3.2).

We can now design an observer for this system, simply after copying equations (45). But we must first state an hypothesis to guarantee the observer convergence:

Hypothesis 5 *The positive scalar variable D is a regularly persisting input i.e. there exists positive constants c_1 and c_2 such that, for all time instant t :*

$$0 < c_1 \leq \int_t^{t+c_2} D(\tau) d\tau$$

In practice, c_2 must be low with respect to the time constant of the system. Moreover $\frac{c_1}{c_2}$ must be high because it determines the minimal converging rate of the observer.

Lemma 1 (see [3]) *Under Hypothesis ??, the solution $\hat{\xi}_2$ of the following asymptotic observer:*

$$\begin{aligned} \frac{d\hat{\zeta}_2}{dt} &= -D(\hat{\zeta}_2 - \zeta_{in2}) - My_2 \\ \hat{\xi}_2 &= \hat{\zeta}_2 - Ay_1 \end{aligned} \quad (46)$$

converges asymptotically toward the solution ξ_2 of the reduced system (37).

Proof: it can be easily verified that the estimation error $e_2 = \hat{\xi}_2 - \xi_2 = \hat{\zeta}_2 - \zeta_2$ satisfies:

$$\frac{de_2}{dt} = -De_2. \quad (47)$$

and converges asymptotically toward ξ_2 if Hypothesis ?? is fulfilled. [3].

5.4 Example

We will consider as example the growth of the filamentous fungi *Pycnoporus cinnabarinus* (X) [19]. The fungi uses two substrates to grow: glucose as carbon source (C) and ammonium as nitrogen source (N). The reaction scheme is assumed to be composed by one reaction:



The model is then of the type (33), with:

$$\xi = [N \ C \ X]^T, \ K = [-k_1 \ -k_2 \ 1]^T, \ \xi_{in} = [N_{in}, C_{in}, 0]^T$$

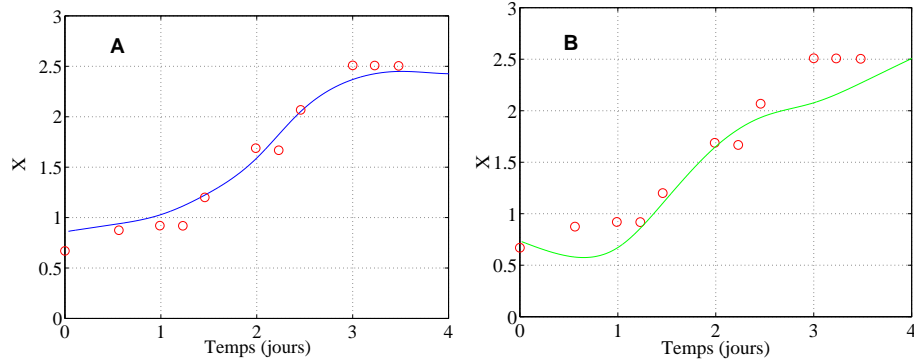


Figure 3: Comparison between direct biomass measurements of *Pycnoporus cinnabarinus* (o) and observer predictions based on the nitrogen measurement (A) or on the carbon measurement (B)

The following measurements are available: $y_1 = [N \ C]^T$.

The state partition will then be the following:

$$\xi_1 = [N \ C]^T, \ \xi_2 = X$$

associated with:

$$K_1 = [-k_1 \ -k_2]^T, \ K_2 = 1$$

Matrix K_1 has an infinite number of left inverses. We will consider two of them: $G_1 = [-\frac{1}{k_1}, 0]$ and $G_2 = [0, -\frac{1}{k_2}]$. These two matrices will naturally lead to two observers. The first one based on the nitrogen measurements:

$$\begin{aligned} \frac{d\hat{\zeta}_2^1}{dt} &= -D(\hat{\zeta}_2^1 - \frac{N_{in}}{k_1}) \\ \hat{X}^1 &= \hat{\zeta}_2^1 - \frac{N}{k_1} \end{aligned} \tag{48}$$

and the other one based on carbon:

$$\begin{aligned} \frac{d\hat{\zeta}_2^2}{dt} &= -D(\hat{\zeta}_2^2 - \frac{C_{in}}{k_2}) \\ \hat{X}^2 &= \hat{\zeta}_2^2 - \frac{C}{k_2} \end{aligned} \tag{49}$$

The results of these observers obtained with experimental data are presented in Figure 5.4. In this case, the observer based on the nitrogen measurements is more reliable.

5.5 Improvements

The asymptotic observers work in open loop. Indeed, their estimate relies on the mass balances and are not corrected by a discrepancy between measured and estimated quantities. It assumes that the mass balance model is ideal. Nevertheless, the yield parameters are difficult to estimate properly, and in some cases (wastewater treatment) the mass inputs in the system are not precisely known. In this case it can be dangerous to base the observer only on the mass balance model without taking into account some measurements on the system that reflect its actual state. It can be possible to on-line estimate these unknown parameters, but we will see here another method aiming at improving the observer robustness with respect to some uncertainties.

In this paragraph, we will see how to exploit the available measurements y_3 to improve the asymptotic observer performances.

We assume here that $y_3 \in \mathbb{R}$. We define the mapping h :

$$h : (\xi_1, \xi_2) \in (\mathbb{R}^p \times \mathbb{R}^{n-p}) \longrightarrow y_3 = h(\xi_1, \xi_2) \in \mathbb{R}$$

We suppose that h satisfies the following hypothesis:

Hypothesis 6 *the mapping h is monotonous with respect to ξ_2 , i.e.: $\frac{Dh}{D\xi_2}$ is of fixed sign on the considered domain Ω .*

Example: in the example detailed hereafter, $h(\xi_1, \xi_2) = \alpha S + \beta P$, and thus:

$$\frac{Dh}{D\xi_2} = [\alpha \ \beta] \quad (50)$$

which is of fixed sign. Of course, h can be nonlinear.

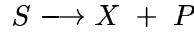
Proposition 1 *Let $\lambda \in \mathbb{R}^p$ be a unitary constant vector ($\|\lambda\| = 1$), whose signs are chosen such that $\text{sign}(\lambda) = \text{sign}(\frac{Dh}{D\xi_2})$, θ is a positive scalar (which can depend on time) and $z_{in} = M\xi_{in}$. The following system:*

$$\frac{d\hat{z}}{dt} = -D(\hat{z} - z_{in}) - M y_2 - \theta \lambda (h(y_1, \hat{z} - Ay_1) - y_3) \quad (51)$$

is an asymptotic observer of the reduced system (45).

For the proof of this property, and for more details, we invite the reader to refer to [20].

Example: we will consider a bacterial biomass (X) growing in a bioreactor. The micro-organisms uptake the substrate S and metabolise a product P :



The associated model is then:

$$\begin{cases} \frac{dX}{dt} = r(\xi) - DX \\ \frac{dS}{dt} = -c_1 r(\xi) + D(S_{in} - S) \\ \frac{dP}{dt} = c_2 r(\xi) - DP \end{cases} \quad (52)$$

where S_{in} is the influent substrate, c_1 and c_2 are the yield coefficients.

We assume that the bacterial biomass and the conductivity of the solution can be measured. The conductivity is related to a positive linear combination of the ions in the liquid i.e. S and P . We have therefore:

$$y_1 = X \quad (53)$$

$$y_2 = (0, 0, 0)^t \quad (54)$$

$$y_3 = \alpha S + \beta P \quad (55)$$

We suppose that the substrate concentration in the influent S_{in} is not precisely known, and we will use an estimate denoted \hat{S}_{in} .

Thanks to Proposition 1 we can design the following observer (for sake of clarity we choose $\lambda = [1 \ 0]$ which satisfies the right hypotheses).

$$\begin{cases} \frac{d\hat{z}_1}{dt} = D(\hat{z}_{in1} - \hat{z}_1) - \theta(\alpha\hat{S} + \beta\hat{P} - y_3) \\ \frac{d\hat{z}_2}{dt} = -D\hat{z}_2 \\ \hat{S} = \hat{z}_1 - \frac{y_1}{c_1} \\ \hat{P} = \hat{z}_2 + \frac{y_1}{c_2} \end{cases} \quad (56)$$

with $\hat{z}_{in1} = \hat{S}_{in}$.

let us show now the robustness properties when the estimate S_{in} is false. If S^* and P^* represent equilibrium values of S and P , we denote \hat{S}^* and \hat{P}^* the equilibrium values for the closed loop observer. If the observer is in open loop ($\theta = 0$), using \hat{S}_{in} , a direct computation provides:

$$\hat{S}^* = S^* + \hat{S}_{in} - S_{in} \quad (57)$$

The prediction error is thus exactly the error on S_{in} . With the closed loop observer, the steady state is:

$$\hat{S}^* = S^* + \frac{D}{\theta\alpha + D}(\hat{S}_{in} - S_{in}) \quad (58)$$

If the gain θ is high, it is easy to see that $\hat{S}^* \simeq S^*$: the bias is reduced by the closed loop observer.

6 interval observers

The usual observers implicitly assume that the model is a good approximation of the real system. Nevertheless, we have seen that a model of a bioprocess is often poorly known. In this case, the observation principle must be revisited: generally it will no more be possible to build an exact observer (which would guaranty: $\|e(t)\| = \|\hat{x}(t) - x(t)\| \rightarrow 0$ when $t \rightarrow \infty$) whose convergence rate could be tuned (as for example an exponential observer). Therefore, in this case the result must be weakened.

We present here a possible way (among others) consisting in bounding the uncertainty on the model. The bound on the variable to be estimated is deduced. To simplify, we will first present the linear (or close to linear) case (see [21, 22]).

6.1 Principle

The idea is to use the known dynamical bounds of the uncertainties:

The dynamical bounds on the model uncertainties allow to derive (in the good cases) the dynamical bounds on the state variable to be estimated.

Figure 4 summarises the philosophy of the interval estimation.

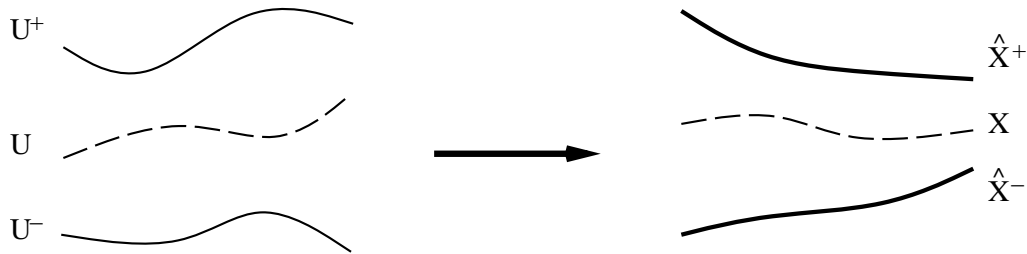


Figure 4: Principle of interval estimation for bounded uncertainties: *a priori* bounds on the uncertainties U provide bounds on the non measured state X

Let us consider the general system:

$$(\mathcal{S}_0) \begin{cases} \frac{dx}{dt}(t) = f(x(t), u(t), w(t)) & ; \quad x(t_0) = x_0 \\ y(t) = h(x(t), v(t)) \end{cases} \quad (59)$$

where $x \in \mathbb{R}^n$ is the state vector $y \in \mathbb{R}^p$ is the output vector, $u \in \mathbb{R}^m$ the input vector, x_0 the initial condition at t_0 , $f : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^r \rightarrow \mathbb{R}^n$ and $h : \mathbb{R}^n \times \mathbb{R}^s \rightarrow \mathbb{R}^p$.

The unknown quantities $w \in \mathbb{R}^r$ and $v \in \mathbb{R}^s$ are characterised by their upper and lower bounds:

$$w^-(t) \leq w(t) \leq w^+(t) \quad \forall t \geq t_0 \tag{60}$$

$$v^-(t) \leq v(t) \leq v^+(t) \quad \forall t \geq t_0 \tag{61}$$

Remark: the operator \leq applies to vectors, it corresponds to inequalities between each component.

Based on the fixed model structure (\mathcal{S}_0) and on the set of known variables, a dynamical auxiliary system can be designed as follows:

$$(\mathcal{O}_0) \left\{ \begin{array}{l} \frac{dz^-}{dt} = f^-(z^-, z^+, u, y, w^-, w^+, v^-, v^+) \quad ; \quad z^-(t_0) = g^-(x_0^-, x_0^+) \\ \frac{dz^+}{dt} = f^+(z^-, z^+, u, y, w^-, w^+, v^-, v^+) \quad ; \quad z^+(t_0) = g^+(x_0^-, x_0^+) \\ x^- = h^-(z^-, z^+, u, y, w^-, w^+, v^-, v^+) \\ x^+ = h^+(z^-, z^+, u, y, w^-, w^+, v^-, v^+) \end{array} \right. \tag{62}$$

with $z^-, z^+ \in \mathbb{R}^q$, the other functions being defined in the appropriate domains.

Definition 8 (interval estimator) System (\mathcal{O}_0) is an interval estimator of system (\mathcal{S}_0) if for any pair of initial conditions $x_0^- \leq x_0^+$, there exists bounds $z^-(t_0), z^+(t_0)$ such that the coupled system ($\mathcal{S}_0, \mathcal{O}_0$) verifies:

$$x^-(t) \leq x(t) \leq x^+(t) \quad ; \quad \forall t \geq t_0 \tag{63}$$

The interval estimator comes from the coupling between two estimators providing each an under-estimate $x^-(t)$ and an over-estimate $x^+(t)$ of $x(t)$, The estimator provides a dynamical interval $[x^-(t), x^+(t)]$ containing the unknown value $x(t)$ (FIG. 4).

Of course, this interval can be very large and therefore useless. The next step consists in trying to reduce as far as possible this interval and increase the convergence rate toward this interval, for example with an exponential convergence rate. Then, we move back to classical observation problems, with the important difference that we don't require the observation error (the interval amplitude) to tend asymptotically *exactly* toward zero

6.2 The linear case up to an output injection

First, let us take a very simple case. We consider again the following system:

$$(\mathcal{S}) : \begin{cases} \frac{dx}{dt}(t) &= Ax(t) + \phi(t, y(t)) \\ y(t) &= Cx(t) \end{cases} \quad (64)$$

with $A \in \mathcal{M}^{n \times n}(\mathbb{R})$ ($n \geq 2$), $C \in \mathcal{M}^{1 \times n}(\mathbb{R})$. If the mapping $\phi : \mathbb{R}^+ \times \mathbb{R} \rightarrow \mathbb{R}^n$ is known, a Luenberger observer can be designed (Section 3.1).

What happens now if function ϕ is badly known ? We assume that it can be bounded and that the bounds are known. Thus, the functions $\phi^-, \phi^+ : \mathbb{R}^+ \times \mathbb{R} \rightarrow \mathbb{R}^n$, are known, sufficiently smooth, such that:

$$\phi^-(t, y) \leq \phi(t, y) \leq \phi^+(t, y), \quad \forall (t, y) \in \mathbb{R}^+ \times \mathbb{R} \quad (65)$$

Then we will use these bounds to design an upper and a lower estimator:

$$\frac{dx^+}{dt}(t) = Ax^+(t) + \phi^+(t, y(t)) + K(Cx^+(t) - y(t)) \quad (66)$$

$$\frac{dx^-}{dt}(t) = Ax^-(t) + \phi^-(t, y(t)) + K(Cx^-(t) - y(t)). \quad (67)$$

Let us consider now the “upper” error $e^+(t) = x^+(t) - x(t)$, we have:

$$\frac{de^+}{dt} = (A + KC)e^+ + b^+(t)$$

with

$$b^+(t) = \phi^+(t, y(t)) - \phi(t, y(t)).$$

It follows that b^+ is positive, and the following Lemma can be easily proven:

Lemma 2 *If the elements of matrix $(A + KC)$ are positive outside the diagonal (the matrix is said cooperative), then $e^+(0) \geq 0$ implies $e^+(t) \geq 0$ for any positive t .*

Of course, we have the same Lemma for the lower error: $e^-(t) = x(t) - x^-(t)$ and the total error $e(t) = e^-(t) + e^+(t)$. The following theorems can be deduced:

Theorem 5 *If the gains of vector K can be chosen such that matrix $(A + KC)$ is cooperative, and if we have an initial estimate such that*

$$x^-(0) \leq x(0) \leq x^+(0)$$

then equations (66),(67) provide an interval estimator for system (64).

Theorem 6 *If hypotheses of Theorem 5 are verified, if matrix $(A + KC)$ is stable, and if moreover the error on ϕ can be bounded, i.e. if we have:*

$$b(t) = \phi^+(t, y) - \phi^-(t, y) \leq B$$

where B is a positive constant, then the error $e(t)$ converges asymptotically toward an interval smaller (for each component) than the positive vector:

$$e_{max} = -(A + KC)^{-1}B$$

In particular, if the components of e_{max} are zero, then the corresponding components for $e(t)$ converge toward zero.

The proofs are straightforward; the proof of the first theorem follows directly from Lemma 2. The proof of the second theorem is due to the differential inequality

$$(A + KC)e + b(t) \leq (A + KC)e + B$$

which implies (with equal initial conditions)

$$e(t) \leq e_m(t), \quad \forall t \geq 0$$

where $e_m(t)$ is the solution of $\frac{de_m}{dt} = (A + KC)e_m + B$.

Remarks:

- We use in the observer design the fundamental hypothesis that it is possible to derive inequalities between the variables from inequalities on the left hand side of the differential equations. This hypothesis is connected with the comparison of the solutions of differential equations (see appendix). There exists other techniques to estimate the intervals, they are more precise but less explicit [23].
- We need also the assumption that the initial estimate is valid

$$x^-(0) \leq x(0) \leq x^+(0);$$

a large estimate can be chosen in practice.

- The problem of the tuning of the convergence rate has not been considered here; is it possible to choose a gain K that will ensure cooperativity, stability, and arbitrary convergence rate ? This is a complicated problem, we invite the reader to consult [22] for more details.

We illustrate this approach with an example of such an estimator for a biochemical process (see [24, 25]).

7 Interval estimator for an activated sludge process

We consider a very simplified model of an activated sludge process, used for the biological wastewater treatment. The objective is to process a wastewater, with an influent flow rate Q_{in} and a pollutant (substrate) concentration s_{in} . We want that the concentration of the effluent is lower than s_{out} . The process is composed by an aerator (bioreactor) followed by a settler separating the liquid and solid (biomass) phases. Then we recycle a part of the biomass toward the aerator. Let us denote x , s , and x_r the three state variables of this simple model, representing respectively the biomass and substrate concentrations in the aerator, and the recycled biomass in the settler. Q_{in} , Q_{out} , Q_r and Q_w are the flow rates, V_a and V_s the volumes (see Figure 5). We suppose that the biological reactions only take place in the aerator.

$$\frac{1}{Y}s \xrightarrow{\mu(\cdot)x} x$$

Y is a yield coefficient, and $\mu(\cdot)$ the bacterial growth rate. If we take into account the biomass recycling, we get:

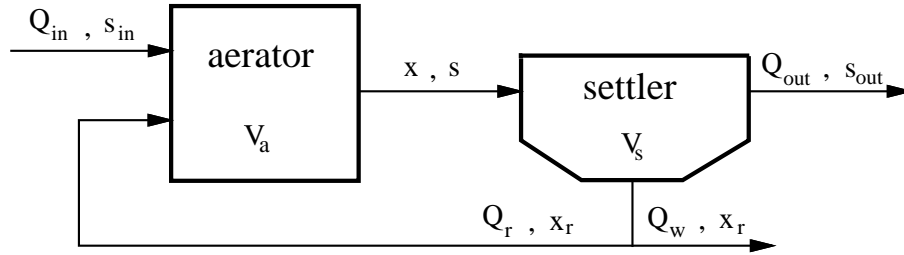


Figure 5: Diagram of an activated sludge process

$$\begin{cases} \frac{dx}{dt} = \mu(\cdot)x - (1+r)D(t)x + rD(t)x_r \\ \frac{ds}{dt} = -\frac{\mu(\cdot)x}{Y} - (1+r)D(t)s + D(t)s_{in}(t) \\ \frac{dx_r}{dt} = v(1+r)D(t)x - v(w+r)D(t)x_r \end{cases} \quad (68)$$

with

$$D(t) = \frac{Q_{in}}{V_a} \quad ; \quad r = \frac{Q_r}{Q_{in}} \quad ; \quad w = \frac{Q_w}{Q_{in}} \quad ; \quad v = \frac{V_a}{V_s}$$

We state the following hypotheses:

- We measure only s and we want to estimate x and x_r .
- We assume that $\mu(\cdot)$ is not known, and we want to design an asymptotic observer (see section 5.3)
- We know a bounding (even very loose) of the initial conditions for x and x_r .
- The substrate input for s_{in} fluctuates but is not known. However we know dynamical bounds for $s_{in}(t)$:

$$s_{in}^-(t) \leq s_{in}(t) \leq s_{in}^+(t) \quad \forall t \geq 0.$$

These hypotheses correspond to what happens in a urban wastewater treatment plant. The influent varies but is not measured. But it can be bounded by two functions corresponding to human activities. These bounds will probably evolve with respect to seasons.

We will design an asymptotic interval estimator, which will provide bounds for the variables to be estimated. First we perform a change of variable to eliminate $\mu(\cdot)$ (cf. section 5.3):

$$Z = X + \begin{bmatrix} Y \\ 0 \end{bmatrix} s; \quad Z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \quad ; \quad X = \begin{bmatrix} x \\ x_r \end{bmatrix} \quad (69)$$

and we get the 2-dimensional system:

$$\frac{dZ}{dt} = D(t) \left(A Z + B(s, t) \right) \quad ; \quad Z_0 = \begin{bmatrix} x_0 + Y s_0 \\ x_{r0} \end{bmatrix}$$

$$A = \begin{bmatrix} -(1+r) & r \\ v(1+r) & -v(w+r) \end{bmatrix} \quad ; \quad B(s, t) = \begin{bmatrix} Y s_{in}(t) \\ -Y v(1+r) s \end{bmatrix}$$

We can now build two estimators (upper and lower) which use unknown bounds on the influent concentration s_{in} :

$$\left\{ \begin{array}{l} \frac{d\hat{Z}^+}{dt} = D(t)(A \hat{Z}^+ + B^+(s, t)) \quad ; \quad \hat{Z}^+(0) = X_0^+ + \begin{bmatrix} Y \\ 0 \end{bmatrix} s_0 \\ \frac{d\hat{Z}^-}{dt} = D(t)(A \hat{Z}^- + B^-(s, t)) \quad ; \quad \hat{Z}^-(0) = X_0^- + \begin{bmatrix} Y \\ 0 \end{bmatrix} s_0 \\ \hat{X}^+ = \hat{Z}^+ - \begin{bmatrix} Y \\ 0 \end{bmatrix} s \\ \hat{X}^- = \hat{Z}^- - \begin{bmatrix} Y \\ 0 \end{bmatrix} s \end{array} \right. \quad (70)$$

with $B^+(s, t) = \begin{bmatrix} s_{in}^+(t) \\ -v(1+r)s \end{bmatrix} Y$; $B^-(s, t) = \begin{bmatrix} s_{in}^-(t) \\ -v(1+r)s \end{bmatrix} Y$

In this simple case, the convergence rate is fixed by the system. On Figure 6, we have represented the influent concentration and its bounds, the measurement s and the two estimates with the bounds. This very simple observer illustrates how to take into account the knowledge on the dynamical bounds.

Under additional hypotheses, it can be shown that this observer can be tuned [24].

8 Conclusion

We have seen a set of methods to design an observer for a bioreactor. Other techniques exist and we do not pretend to be exhaustive. Let us mention for example the methods based on neural networks, where the system and its observer are estimated at the same time. The convergence rate of the obtained neural network can not be tuned.

The presented observers assumed that the model parameters were known. In some cases these parameters can evolve. Algorithms to estimate the parameters must then be used, they lead to adaptive observers. Of course in that case, the convergence of the full system observer-parameter estimator must be demonstrated.

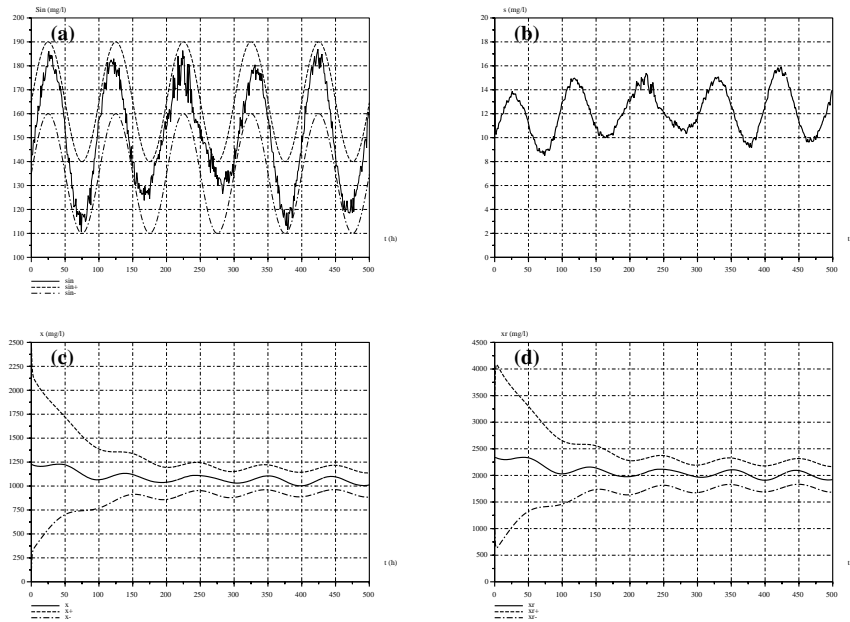


Figure 6: Interval observer. (a) Influent bounds, (b) Measurements of S , (c) interval estimations of X , (d) interval estimations of X_r

The choice of the type of observer to be found must be made above all by considering the reliability of the model and of the available measurements. A triple trade-off must then be managed between robustness with respect to modelling uncertainties, robustness with respect to disturbances and convergence rate.

Finally, to implement an observer in a computer, a discretising phase is required. This step will be based on Euler type algorithms. This step is not difficult, but it requires care. In particular, if the sampling rate is too high for the discretisation rate, continuous/discrete observers must be used [26].

To conclude, we insist that the observers must first be validated before they can be used. For this, their predictions must extensively be compared to direct measurements that were not used during the calibration process.

Appendix: a comparison theorem

We propose here a general theorem in the non linear case. It can be useful to apply the interval estimation techniques. The reader is invited to consult [35] for the details and for a general presentation.

Definition 9 *A non linear system in dimension n is said to be cooperative if its Jacobian matrix is positive outside its diagonal on a convex domain.*

We propose now the comparison theorem between $x(t)$ and $y(t)$ defined by the two systems

$$\begin{aligned}\frac{dx}{dt} &= f(x, t) ; & x(0) &= x_0 \\ \frac{dy}{dt} &= g(y, t) ; & y(0) &= y_0\end{aligned}$$

where $f, g : U \times \mathbb{R}^+ \rightarrow \mathbb{R}^n$ are sufficiently regular on a convex domain $U \subset \mathbb{R}^n$.

Property 3 *If*

- $\forall z \in U, \forall t \geq 0, f(z, t) \leq g(z, t)$
- g is cooperative
- $x_0 \leq y_0$

then $x(t) \leq y(t)$ for $t > 0$

The inequalities must be considered for each element. It means that, for a cooperative system the order between two solutions is conserved for any time. This property is fundamental for the set up of interval estimators.

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