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State estimation for nonlinear systems under model unobservable uncertainties: application to continuous reactor

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Abstract

The issue of this paper is the classical problem of state estimation, considering partially unknown, nonlinear systems with noise measurements. Estimation of system's state variables with observable and unobservable unstructured uncertain terms is performed simultaneously. An alternative system representation is proposed to transform the measured disturbance onto system disturbance, which lead a more adequate observer structure. The proposed methodology contains an uncertainty estimator based on the predictive contribution to infer the unobservable uncertainties and corrective contribution to estimate the observable uncertainties; which provides robustness against noisy measurements and model uncertainties. Convergence analysis of the proposed estimation methodology is realized, analyzing the dynamic equation of the estimation error, where asymptotic convergence is shown. This estimation scheme is applied to a continuous stirred chemical reactor. Numerical experiments illustrate the good performance of the proposed observer.

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1. Introduction

Observer schemes are widely used for the reconstruction of no measured state dynamics, some of them necessary for identification and feedback control. The only available information is the system's output, which represents a function of some current states. Usually, the dimension of the vector of output signals is smaller than the dimension of the corresponding vector of states; therefore it is necessary to develop estimation techniques, known as observer design dealing with on-line state estimation.

Early contributions for observer design in nonlinear systems were based on information of the complete nonlinear dynamics [1-3]. This approach assumes a hypothetical situation, where it is possible to obtain a set of rather restrictive conditions when the dynamics of the observation error

is linear and there are not observation disturbances (noises). Prevalent approach in observer design is related with dominate nonlinearities with high gain linear terms, or to eliminate them via geometric transformation. Gauthier and Bonard [4] stated a canonical form and necessary and sufficient observability conditions for a class of nonlinear systems that are linear with respect to inputs. Zeitz [5] designed the extended Luenberger observer for a class of SISO nonlinear systems, while Gauthier et al. [6] developed the exponential convergent observer. More complete results were showed in Ciccarella et al. [7], which employ a simple assumption on regularity, to prove global asymptotic convergence of the observer.

The most successful observation schemes need a nominal model for their implementation, but as is well known the exact knowledge of the nonlinearities of nonlinear plants is a hard task, this situation leads to new develops in estimation theory related with both state and uncertain terms observation. Other situation arises when the system's states and the uncertain terms are not observable, Alvarez and Hernández

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[8] presented an observer design which estimate only unobservable states of nonlinear plants under the assumption of nominal plant model availability, Aguilar et al. [9,10] develop high gain observers for uncertainty estimation in nonlinear systems and integral-type observer for state estimation for partially unknown nonlinear plants, however the problem of state estimation with unobservable uncertainties still remains. Following these ideas, research was oriented to the observation/estimation problem subjected to bounded nonlinearities or uncertainties [11]. If the plant model is uncertain or incomplete, which is the most common case, the implementation of high gain observers turns out to be adequate [12,13]. Besides, the design of new robust observers based on adaptive techniques, such as neural networks, has been proposed [13].

Hou et al. [14] provided a methodology to construct state observers by means of an injective map, which is a generalized coordinate change via a diffeomorphic relationship between a uniformly observable system and its triangular form transformation. This methodology generates a field of dimension higher than the original system. Nevertheless, this approach needs at least a nominal model of the system under study, which could be a potential drawback. The extended Kalman filters have been widely used in the process industry, because of their easy implementation and capabilities to deal with errors in the modeling and the measurements in its structure. Nonetheless, this design is based on linearized approaches of the nonlinear system, where robustness and convergence properties are difficult to prove [15].

Another approach related to the construction of observers (basically, asymptotic) for nonlinear processes, is geometric differential methods [16]. The main idea is to find some state transformation that represents the original system as a linear equation plus a nonlinear term, which is a function of the system output. However, finding a nonlinear transformation, that places a system of order n into observer form, requires simultaneous integration of n-coupled partial differential equations. Furthermore, this approach needs accurate knowledge of the nonlinear dynamics of the system; hence, turns to be inapplicable if the model for the process includes uncertainties.

Although algebraic differential methodologies [17,18] have been employed to construct asymptotic and even exponential observers, up to date these designs only include full order observers for state estimation and do not include uncertainty estimation. Other methodologies consider particular observer's design for control purposes, where the effect of uncertainties, state variables and/or disturbances are estimated and then coupled with a control laws [19–21].

The main objective of this paper is the design of an observer whose structure leads to estimate state variables despite of observable and unobservable uncertain terms. Estimation of states and unstructured uncertainty in partially known, lumped parameter, nonlinear systems is performed, considering corrupted (noisy) measurements of the system output. The convergence analysis is realized via the dynamics of the error estimation equation. The performance of the methodology proposed is illustrated taking as case study a continuous stirred tank reactor, where the heat generation by chemical reaction (observable uncertainty), the heat transfer of the cooled jacked (observable uncertainty), the kinetic rate (unobservable uncertainty) and three state variables (reactive concentration, reactor and cooled jacket temperatures) are estimated using continuous temperature measurements at the reactor outlet and the cooled jacket, as usual in this processes, leading to more realistic situation.

2. Problem description

Consider the following nonlinear plant with linear output which can be described by Eqs. (1a) and (1b):

$$\dot{Z} = f(Z, U) = \aleph(Z) + \ell(Z, \mathbf{U}) \tag{1a}$$

$$\mathbf{Y} = h(Z, \varpi) = CZ + \varpi \tag{1b}$$

Here $Z \in \Re^n$ is the vector of states, $\mathbf{U} \in \Re^q$ the control input vector, $\aleph(\circ) : \Re^n \to \Re^n$ a nonlinear, partially known vector field, $\ell(\circ) : \Re^{n+q} \to \Re^n$ a linear vector of arguments, $\varpi \in \Re^m$ an additive bounded measurement noise, and $\mathbf{Y} \in \Re^m$ is the system output. Now, consider that the unknown part of the nonlinear vector field $\aleph(\circ) : \Re^n \to \Re^n$ contains observable (\aleph_0) and unobservable (\aleph_U) uncertain terms, such that

$$\aleph(\circ) = \begin{cases} \aleph_{\mathrm{O}}(\circ) \\ \aleph_{\mathrm{U}}(\circ) \end{cases}$$

where \aleph_0 is a sub-set of observable uncertainties and \aleph_U is a sub-set of unobservable uncertainties.

Now, let us consider the following hypothesis:

(H1). The system given by ((1a) and (1b)) satisfies the observability rank condition:

$$\operatorname{rank}\left\{\frac{\partial}{\partial x}\vartheta\right\} = n$$

Here ϑ is the observability vector function defined as $\vartheta = (dL_{\rm f}^0 h_1, \ldots, dL_{\rm f}^0 h_m, \ldots, dL_{\rm f}^1 h_1, \ldots, dL_{\rm f}^1 h_m, \ldots, dL_{\rm f}^{n-1} h_1, \ldots, dL_{\rm f}^{n-1} h_m)^{\rm T}$, being $L_{\rm f}^r h_s$ (s = 1, 2...m) the *r*-order Lie derivatives, therefore it is locally uniformly state observable for all $z \in \Re^n$ and $u \in \Re^q$.

(H2). For the realized control input vector $\mathbf{U}(Z(t))$, $(\|\mathbf{U}(Z(t))\| \leq \overline{\mathbf{U}})$, the nominal closed-loop nonlinear system (1a) and (1b) is quadratically stable; therefore there exists a Lyapunov function $V \geq 0$ that satisfies that:

$$\frac{\partial V}{\partial Z} [\aleph(Z) + \ell(Z, \mathbf{U})] \le -\alpha_1 \|Z\|^2,$$
$$\left\|\frac{\partial V}{\partial Z}\right\| \le \alpha_2 \|Z\|, \quad \alpha_1, \alpha_2 > 0$$

(H3). ϖ is a vector function representing an external (maybe unknown), bounded perturbation:

$$\|\varpi\|_{\Delta}^2 = \Sigma < \infty, 0 < \Delta = \Delta^{\mathrm{T}}$$

The normalized matrix Δ is introduced to ensure the possibility to deal with components of different physical structure and is assumed as given a priori; Σ represents the power of the corresponding perturbation.

(H4). All the trajectories $Z(t, Z_0), Z_0 \in \Re^n_+$ of the system ((1a) and (1b)) are bounded.

(H5). The linear vector field $\ell(Z, \mathbf{U})$ is bounded, i.e. for any $Z \in \mathfrak{N}^n$, $\|\ell(Z, \mathbf{U})\| \le \ell^+ < \infty$.

(H6). A nominal model for the unobservable uncertainties is available, i.e. $\aleph_U = \varphi_0(Z)$, consequently, $\dot{\aleph}_U = \frac{\partial \varphi_0}{\partial Z} \frac{\partial Z}{\partial t} = \frac{\partial \varphi_0}{\partial Z} \dot{Z}$

The task is to design an observer to estimate the vector of state variables Z, despite of the unknown part of the nonlinear vector \aleph (which will be estimated, also); considering that Y and U are measured on-line at each time interval *t*.

3. Observer synthesis

In order to avoid the standard proportional observer drawbacks, the following modifications to its structure are proposed:

- (a) An uncertainty estimator based on corrective output term is introduced in the observation methodology, in order to estimate the unknown observable uncertainties of the nonlinear vector ℵ (1a).
- (b) An uncertainty estimator based on predictive term is considered on the observation methodology, in order to estimate the unknown unobservable uncertainties of the nonlinear vector ℵ (1a).

Furthermore, it is well known that classical proportional observers tend to amplify the noise of on-line measurements, which can lead to degradation of the observer performance. In order to save these drawbacks [10], the following representation of the system ((1a) and (1b)) is done:

$$\dot{Z} = \aleph(Z) + \ell(Z, \mathbf{U}) \tag{2a}$$

$$\dot{Z}_* = CZ + \varpi \tag{2b}$$

 $\dot{\aleph}_{\rm O} = \Theta(Z) \tag{2c}$

$$\dot{\aleph}_{\rm U} = \frac{\partial \varphi_0}{\partial Z} \frac{\partial Z}{\partial t} \tag{2d}$$

$$\mathbf{Y}_* = Z_* \tag{2e}$$

The main issue of this new representation of the system is to eliminate the additive noise from the new system output \mathbf{Y}_* , transforming the original output disturbance into a system disturbance. So the observable and unobservable uncertain terms of the vector \aleph , are considered as a new states, which obey the following assumption:

(H7). The dynamics of the uncertain terms, \aleph_0 and \aleph_U are bounded, therefore:

$$|\Theta(Z)| \le v \text{ for } v > 0 \text{ and } \left| \frac{\partial \varphi_0}{\partial Z} \frac{\partial Z}{\partial t} \right| \le \mu \text{ for } \mu > 0$$

Proposition 1. The following dynamic system is an asymptotic-type observer of the system given by Eqs. (2a)–(2d):

$$\hat{Z} = \hat{\aleph} + \ell(\hat{Z}, \mathbf{U}) + k_1 (\mathbf{Y}_* - \mathbf{C}\hat{Z}_*)$$
(3a)

$$\hat{\mathbf{Z}}_* = \mathbf{C}\hat{\mathbf{Z}} + k_2(\mathbf{Y}_* - \mathbf{C}\hat{\mathbf{Z}}_*) \tag{3b}$$

$$\dot{\hat{\aleph}}_{\rm O} = k_3 (\mathbf{Y}_* - \mathbf{C}\hat{Z}_*) \tag{3c}$$

$$\dot{\aleph}_{\rm U} = \frac{\partial \varphi_0}{\partial Z} \mathop{}_{Z=\hat{Z}} \dot{\hat{Z}}$$
(3d)

The vector of proportional observer gains, $\mathbf{K} = (k_1, k_2, k_3, 0)^{\mathrm{T}}$, is proposed as

$$\mathbf{K} = -N_{\pi}^{-1}C^{\mathrm{T}}, \quad N_{\pi} = \left(\frac{1}{\pi^{i+j-1}}N_{ij}\right)_{i,j=1,n+2}$$
(4)

The parameter $\pi > 0$ determines the desired convergence velocity. More over, in order to assure stabilizing properties, N_{π} should be a positive solution of the algebraic Riccati equation:

$$N_{\pi} \left(R + \frac{\pi}{2} \mathbf{I} \right) + \left(R^{\mathrm{T}} + \frac{\pi}{2} \mathbf{I} \right) N_{\pi} = C^{\mathrm{T}} C,$$
$$R = \begin{pmatrix} 0 & \mathbf{I}_{n-1,n-1} \\ 0 & 0 \end{pmatrix}$$
(5)

3.1. Stability remarks

3.1.1. Sketch of proof of Proposition 1

In accordance to Eqs. (2) and (3), the corresponding dynamic error equation, can be written as

$$\dot{\xi} = \mathbf{A}\xi + \Omega(Z, \mathbf{U}, \varpi) \tag{6}$$

Here

$$\xi = \begin{bmatrix} \frac{(Z_* - \hat{Z}_*)}{(\pi_{i,j=1,n+2}^{i+j-1})} \\ \frac{(Z - \hat{Z})}{(\pi_{i,j=1,n+2}^{i+j-1})} \\ \frac{(\aleph_0 - \hat{\aleph}_0)}{(\pi_{i,j=1,n+2}^{i+j-1})} \\ (\aleph_U - \hat{\aleph}_U) \end{bmatrix}; \quad A = \begin{bmatrix} 0 & -k_1 & 1 & 0 \\ 1 & -k_2 & 0 & 0 \\ 0 & -k_3 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix};$$

$$\Omega = \begin{bmatrix} \bar{\omega} \\ \Delta \ell \\ \Theta \\ \Delta \left(\frac{\partial \varphi_0}{\partial Z_{Z} = \hat{Z}} \hat{Z} \right) \end{bmatrix}; \quad |\Omega| \le \begin{bmatrix} \Sigma \\ \Gamma \\ \nu \\ \rho \end{bmatrix} = \Psi$$

Consider the following assumptions:

(H8). The function $\Delta \ell = \ell(\mathbf{X}, \mathbf{U}) - \ell(\hat{\mathbf{X}} - \mathbf{U})$ is bounded, i.e. $\|\ell(\mathbf{X}, \mathbf{U}) - \ell(\hat{\mathbf{X}} - \mathbf{U})\| \leq \Gamma$ for $\Gamma > 0$.

(H9). There exist two positive constants j > 0 and $\lambda > 0$, which satisfy:

$$\|\exp(\pi_{i,j=1,n+2}^{i+j-1} \operatorname{A} t)\xi\| \le j \exp(-\pi_{i,j=1,n+2}^{i+j-1} \lambda t) \|\xi\|$$

Now, solving Eq. (6), the following expression is obtained:

$$\xi = \exp(\pi_{i,j=1,n+2}^{i+j-1} \operatorname{At})\xi_0 + \int_0^t \exp\{\pi_{i,j=1,n+2}^{i+j-1} A(t-s)\}\Omega \,\mathrm{d}s$$
(7)

Considering the assumptions (H7)–(H9) and taking norms for both sides of Eq. (7), the following equation is generated:

$$\|\xi\| \le j \exp(-\pi_{i,j=1,n+2}^{i+j-1} \lambda t) \left[\|\xi_0\| - \frac{j\Psi}{\pi_{i,j=1,n+2}^{i+j-1} \lambda} \right] + \frac{j\Psi}{\pi_{i,j=1,n+2}^{i+j-1} \lambda}$$
(8)

Taking the limit, when $t \to \infty$:

$$\|\xi\| \le \frac{j\Psi}{\pi_{i,j=1,n+2}^{i+j-1}\lambda} \tag{9}$$

The above inequality implies that the estimation error can be as small as is desired, if the parameter gain of the observer, π , is chosen large enough.

4. Application example

On-line estimation of state variables, concentrations, mainly, in chemical reactors is very important. Concentrations are related to process productivity; however their direct measurement is often expensive or even impossible considering the current sensor technology. In order to show the improved features of the observer proposed, a continuous stirred chemical reactor is chosen as study case. The mathematical model of the reactor [21] (see Appendix A) consists of the dimensionless mass balance of the reactive chemical and the energy balances of the reactor and the cooled jacket, note that more complex process can be employed, such that it obey the corresponding assumption mentioned above. The proposed observer is applied to the CSTR model, considering the following situation: the observable uncertain terms are the reaction heat and the heat transfer to the cooled jacket, note that these both uncertainties are present in reactor energy balance and the cooled jacket energy balance, the corresponding unobservable uncertainty is the reaction rate, related with the mass balance. The uncertainties considered are terms very complex to evaluate due the complexity of the physic and chemical phenomena related in this kind of process, such that the uncertainty selection is a real situation in process operation. The state estimated are the reactive concentration, the reactor temperature and the jacket temperature, this is done by means of reactor temperature and cooled jacket temperature measurements, as usual. Previous work has shown that heat generation by chemical reaction is observable from reactor temperature measurements [17,18]. In industrial applications the monitoring of these uncertainties and variables is very important for process security and politic operation.

The temperature measurements are corrupted by a bounded noisy of $\varpi = \pm 0.1$ around the current temperature value, the initial conditions of the reactor are $X_1(0) = 0.58$, $X_2(0) = 2.67$, $X_3 = 0.12$; the corresponding initial conditions for the states observed are $\hat{X}_1 = 0.1$; $\hat{X}_2 = 2.0$; $\hat{X}_3 = 0.05$, zero as initial conditions for the observer equations for the observable uncertainties was considered. The observer gains for the observed states are [10,1.0, 1000] for reactive concentration, reactor temperature and cooled jacket temperature, respectively. The gains for the observable uncertainties



Fig. 1. Concentration estimation.



Fig. 2. Temperature estimation.







Fig. 4. Uncertainties estimation.

are [1.0, 0.3] for the reaction heat and the cooled jacket heat transfer, respectively.

Fig. 1 shows the performance of the concentration estimation; note the satisfactory performance of the proposed observer at 20 time units, the estimation of this state variable is one of the main tasks of the observation methodology. Figs. 2 and 3 are related with the filtering performance of the other state variables, reactor and cooled jacked temperatures, where an adequate estimation is done; finally, the estimation time evolution of the observable and unobservable uncertainties given by the proposed methodology can be seen in Fig. 4.

5. Concluding remarks

An observer is presented in this paper in order to perform state estimation despite of observable and unobservable model uncertain terms. It follows an alternative representation of the original system, where the output disturbances (noise measurements) are transformed into state disturbances, in order to decouple the observer's gains from the output disturbances to avoid the noise amplification, which is characteristic of the standard proportional observers. The unobservable uncertainty is estimated via predictive term, which is based on nominal model of the plant.

Despite of considers a simple model as application example; the methodology proposed can be applied to more complex systems, i.e. more complex reaction networks or even other kind of systems under the assumptions mentioned.

Appendix A

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The mathematical model of a jacketed CSTR, where a mass balance with a first-order kinetic, reactor energy balance and cooled jacket energy balance, presented in dimensionless form was taken from [21] and is the follows:

Reactor mass balance:

$$_{1} = q(X_{1in} - X_{1}) - \wp_{1} \tag{A.1}$$

Reactor energy balance:

 $\dot{X}_2 = q(X_{2in} - X_2) + \wp_2 + \wp_3 \tag{A.2}$

Cooled jacket energy balance:

$$\dot{X}_3 = \delta_1 \left[q_c (X_{3in} - X_3) \right] - \wp_3$$
 (A.3)

Measured system outputs:

$$Y_1 = X_2 + \overline{\omega}, \qquad Y_2 = X_3 + \overline{\omega} \tag{A.4}$$

where k is the kinetic constant (Arrhenius model) exp { $X_2/(1 + (X_2/20))$ }, X_1 the concentration of the chemical reactive (dimensionless), X_{1in} the reactive input concentration = 1.0 (dimensionless), X_2 the reactor temperature (dimensionless), X_{2in} the input reactor temperature = 0.0 (dimensionless), X_3 the cooled jacket temperature (dimensionless), X_{3in} the input cooled jacket temperature = -1.0 (dimensionless), \wp_1 the reaction rate = $0.072kX_1$ (unobservable uncertainty), \wp_2 the reaction heat = $0.072\Delta HkX_1 = 8.0(0.072)kX_1$ (observable uncertainty), \wp_3 the heat transfer to the cooled jacket = $10(X_2 - X_3)$ (observable uncertainty), q the inverse of the residence time = 1.0, q_c the inverse of the residence time of the cooled jacket = 0.28, δ_1 the parameter = 10.

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