European Journal of Control 21 (2015) 14–26

Contents lists available at ScienceDirect

European Journal of Control

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

High-order accurate continuous-discrete extended Kalman filter for chemical engineering

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ARTICLE INFO

Article history:
Received 8 February 2014
Received in revised form
21 November 2014
Accepted 30 November 2014
Recommended by M. Kano
Available online 8 December 2014

Keywords:
Extended Kalman filter
Continuous-discrete model
Moment differential equations
Adaptive ODE solver
Automatic local and global error control

ABSTRACT

This paper elaborates a new version of extended Kalman filtering (EKF) for state estimation in chemical nonlinear continuous-discrete stochastic systems. Such a state estimation always compounds real measurements of some system's variables (depending on the utilized technology) with computation of remaining (not measurable) parameters by means of appropriate filtering algorithms. Here, we consider the continuous-discrete EKF and show that its quality is raised by using the adaptive sixth-order nested implicit Runge–Kutta (NIRK) method of Gauss type with automatic local and global error controls. Through case studies the new filtering technology is compared to another EKF implementation based on an adaptive ODE solver but with the sole local error control. Our numerical results exhibit that the designed state estimation algorithm not only outperforms the earlier published adaptive EKF method, but also resolves the so-called "EKF failure" case reported recently.

1. Introduciton

Mathematical models in chemical research and industrial applications are often presented in the form of stochastic differential equation (SDE)

$$dx(t) = F(x(t), u(t))\,dt + G(x(t), u(t))\,dw(t) \tag{1}$$

where $x(t) \in \mathbb{R}^{n_1}$ is the n_1-dimensional vector of system's state at time t, $u(t) \in \mathbb{R}^{n_2}$ is the measurable input at time t, $F : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}^{n_1}$ is a nonlinear function representing the chemical reaction kinetics, $G(x(t), u(t))$ is a matrix of dimension $n_1 \times q$ and $\{w(t),\ t > 0\}$ is a Brownian process with square diffusion matrix $Q(t) \geq 0$ of the size q. We point out that chemical process models are based on conservation laws and described conventionally by ordinary differential equations (ODEs), whereas the stochastic term in SDE (1) simulates possible random disturbances and uncertainties in the reaction and also a plant-model mismatch always existing in reality.

Here, we deal with mathematical models of the form (1) where the measurable input $u(t)$ is assumed to be a known function of time. In other words, we consider that its value is known at any time instant. If the discussed chemical process model does not correspond to a particular situation, i.e. when the input of chemical system is unknown and should be measured in real experimentation, one can treat such a chemical system by augmenting the system's state with the unknown input entries. In this case, the input $u(t)$ is evaluated as a part of the augmented state vector $x(t)$. Then, removing the term $u(t)$ from all the below formulas allows the augmented chemical model to be estimated by the designed method as well.

The initial state x_0 of chemical process (1) is supposed to be a random variable. More precisely, $x_0 \sim \mathcal{N}(\bar{x}_0, \Pi_0)$ with $\Pi_0 \geq 0$, where the notation $\mathcal{N}(\bar{x}_0, \Pi_0)$ stands for the normal distribution with mean $\bar{x}_0$ and covariance Π_0.

The task of state estimation in chemical system (1) always compounds real measurements of measurable system's variables (depending on the utilized technology) with computation of remaining (not measurable) parameters by means of an appropriate nonlinear filtering algorithm. It is usually assumed that some observation information arrives discretely and in equidistant intervals of size $\delta = t_k - t_{k-1}$. This time interval δ is called the sampling period (or waiting time) in filtering theory. The relation of observations y_k to the state vector x_k in chemical system (1) is fixed by the formula

$$y_k = h(x_k) + v_k, \quad k \geq 1, \tag{2}$$

where k stands for a discrete time index (i.e. x_k means $x(t_k)$), $y_k \in \mathbb{R}^m$ is the information available at time t_k, $h : \mathbb{R}^{n_1} \to \mathbb{R}^m$ is a linear or nonlinear function and the measurement noise v_k is a zero-mean Gaussian white-noise process with covariance matrix $R_k > 0$. We emphasize that formula (2) covers both linear and nonlinear observation models. Also, all realizations of $w(t)$, v_k and x_0 are assumed to be taken from mutually independent Gaussian

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http://dx.doi.org/10.1016/j.ejcon.2014.11.003
0947-3580/

distributions. Thus, the continuous-discrete stochastic state-space model (1) and (2) is best suited for state estimation in chemical systems and widely used in chemistry research and industrial applications (see, for instance, [52,50,8,15,16,20,43–45]).

Concerning state estimation algorithms, we have to remark that, at present, there exist a great variety of different methods starting from a rigorous probabilistic approach solving Kolmogorov's (Fokker–Planck's) forward equation (as discussed, for instance, in [19,38]) till approximate approaches including various nonlinear modifications and implementations of the well-known Kalman filter (see [37,48,49,23,22,17,40,1–3,10,21,30,43–46]) as well as optimization based approaches usually referred to as the moving horizon estimation (studied in [18,42,15,16,43] and so on). Undoubtedly, the extended Kalman filter (EKF) still remains among the most popular and widely used numerical techniques for practical state estimation in nonlinear stochastic systems because of its implementation simplicity and good performance. It originates from the optimum state estimation theory developed by Kalman [25] in linear discrete-time stochastic state-space systems. The progress made in the Kalman filtering by now has resulted in a number of fast, numerically stable and many other algorithms (see, for instance, [37,24,12,11,38,47]).

Despite EKF's popularity, this method has been criticized on its performance for offline models and industrial applications in chemical research by Wilson et al. [52], Soroush [50], Dochain [8], Haseltine and Rawlings [15,16], Jørgensen [20], Rawlings and Bakshi [43], Romanenko and Castro [44], Romanenko et al. [45]. For example, Haseltine and Rawlings [15,16] report that their EKF fails for two types of chemical reactors meaning that wrong steady-states are calculated and negative concentrations are observed after convergence, which are of no physical sense. Jørgensen [20] claims that his EKF is not able to reconstruct offset free concentrations in the Van der Vusse reaction scenario on the basis of temperature measurements, only. One more difficulty mentioned in relation to the EKF is that it may fail for nonlinear systems with infrequent observations. So, Soroush [50] writes: "In the chemical/petrochemical and biochemical industries, there are many processes wherein the choice of sampling rate is limited by the availability of the output measurements. For example, composition analyzers such as gas chromatographs have a cycle time say 5–10 min compared to a desired control interval of say 0.1–1 min. If the control interval is increased to match the availability of measurements then control performance deteriorates significantly."

Recently, Kulikov and Kulikova [30] presented a way to resolve some cases of the "EKF failure" by means of adaptive ODE solvers with automatic error control. Therefore, the task of searching for the most appropriate ODE solver in the frame of EKF technology has arisen. We emphasize that the formulated task corresponds well to practitioners' expectations in control theory, as, for instance, stated in Arasaratnam et al. [3]. Below, we contribute to the research topic announced in the cited paper and conduct a detailed theoretical and numerical study of two efficient ODE solvers. The first one is grounded in the embedded pair of explicit-first-stage singly diagonal implicit Runge–Kutta (ESDIRK) methods of orders 3 and 4 and published in Kristensen et al. [26]. It is further denoted as `ESDIRK3(4)`. The second ODE solver is hybrid and designed here on the basis of two different schemes for computing the predicted state expectation and the predicted error covariance matrix. The predicted state mean is calculated by an embedded Runge–Kutta pair of orders 4 and 6. The higher-order method in this pair belongs to the family of nested implicit Runge–Kutta (NIRK) formulas of Gauss type. These NIRK schemes are introduced and studied by Kulikov and Shindin [33], Kulikov [27,29] at large. The predicted error covariance matrix is determined by the corresponding part of the numerical scheme designed and explored in Mazzoni [39], but it is modified for a square-root implementation of the EKF in this paper. So, the latter hybrid ODE solver is further referred to as `NIRK6(4)M2`. In the next section, we present the `ESDIRK3(4)` and `NIRK6(4)M2` based EKF variants with all necessary implementation particulars for a detailed theoretical and numerical comparison and study.

It is worthwhile to remark that our `NIRK6(4)M2` method distinguishes from what was used and published earlier in Kulikov and Kulikova [30]. First, the embedded NIRK pair of orders 2 and 4 with the global error control from Kulikov [29] was applied for the simultaneous solution of the state mean and error covariance equations in the earlier published research. This resulted in an accurate but time-consuming state estimator where the authors solved linear systems of size $n_1(n_1+3)/2$ with n_1 standing for the dimension of the state vector. The global error was controlled in all entries of the moment differential equations. Here, we design another method that treats the state mean and error covariance equations, separately. The global error control is also implemented in numerical integration of the first moment differential equation, only. All this reduces the cost of `NIRK6(4)M2` in comparison to the earlier published state estimator. Second, Kulikov and Kulikova [30] studied the standard continuous-discrete EKF technology whereas the present paper deals with a more stable square-root implementation of the EKF, as explained in Section 2.3.

At the end of this introduction, we point out that the purpose of the present paper is not to address the above-mentioned "EKF failure" phenomena, but to look for a more efficient version of the EKF, which may be successful in practice. In addition, we expose that the state estimator designed here works well for offline chemical models and, hence, may be potentially useful in industrial environment. Any comparison of our EKF technique to other effective nonlinear state estimation algorithms, as, for example, particle, unscented and ensemble filters, and its practical testing in real experimentation are beyond the scope of this paper and expected in future.

2. Theory and implementation

2.1. Continuous-discrete extended Kalman filter

Frogerais et al. [10] identify two main approaches for implementing the EKF method (namely, the continuous-discrete and discrete-discrete EKF implementations), and Kulikov and Kulikova [30] explain that the continuous-discrete EKF is more accurate and reliable in practice. Therefore, it is most suited for treating the continuous-discrete stochastic state-space model (1) and (2) arising often in chemical research and industrial applications. We restrict ourselves to the latter state estimation technology and present its implementation particulars, below.

It is well-known from the cited literature that the continuous-discrete EKF is based on replacement of the predicted values of state mean and error covariance matrix determined in the time-update step of the Kalman filtering with the values satisfying the moment differential equations (MDEs)

$$\frac{d\hat{x}(t)}{dt} = F(\hat{x}(t), u(t)), \tag{3a}$$

$$\frac{dP(t)}{dt} = J(\hat{x}(t), u(t))P(t) + P(t)J^T(\hat{x}(t), u(t)) + G(\hat{x}(t), u(t))Q(t)G^T(\hat{x}(t), u(t)) \tag{3b}$$

where $J(\hat{x}(t), u(t))$ denotes the Jacobian of the drift function $F(\hat{x}(t), u(t))$ from the SDE (1) (i.e. $J(\hat{x}(t), u(t)) = \partial F(\hat{x}(t), u(t))/\partial\hat{x}(t)$), $G(\hat{x}(t), u(t))$ is the matrix from the stochastic noise term of this equation, $Q(t)$ is the covariance matrix of the zero-mean Gaussian