A Critical Discussion of the Continuous-Discrete Extended Kalman Filter

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Abstract—In this paper, we derive and apply a novel numerically robust and computationally efficient extended Kalman filter for state estimation in nonlinear continuous-discrete stochastic systems. The continuous-discrete extended Kalman filter is applied to the Van der Vusse reaction example. This example is a well-known benchmark for nonlinear predictive control. Using the Van der Vusse example, we demonstrate inherent limitations of the extended Kalman filter and sensor structure for unbiased state estimation. In particular, we demonstrate that the convergence rate of the concentration estimate in the Van der Vusse system is limited by the frequency of concentration measurements. These limitations limit the achievable performance of any closed-loop system including nonlinear model predictive control.

I. INTRODUCTION

The objective of state estimation is to reconstruct the state of a system from process measurements given a model. State estimation has important applications in nonlinear continuous-discrete stochastic systems. The continuous-discrete extended Kalman filter is applied to the Van der Vusse reaction example. This example is a well-known benchmark for nonlinear predictive control. Using the Van der Vusse example, we demonstrate inherent limitations of the extended Kalman filter and sensor structure for unbiased state estimation. In particular, we demonstrate that the convergence rate of the concentration estimate in the Van der Vusse system is limited by the frequency of concentration measurements. These limitations limit the achievable performance of any closed-loop system including nonlinear model predictive control.

Consider the continuous-discrete stochastic nonlinear system

\[ dx(t) = f(t, x(t))dt + \sigma(t)d\omega(t) \]
\[ y_k = h(t_k, x(t_k)) + v_k \]

in which \( \{\omega(t), t \geq 0\} \) is a standard Wiener process, i.e. a Wiener process with incremental covariance \( Idt \), and the measurement noise is normally distributed, \( v_k = \nu(t_k) \sim N_{iid}(0, R_k) \). Assume that the mean and covariance of the initial state are known, i.e.

\[ x_{0|-1} \sim F(\hat{x}_{0|-1}, P_{0|-1}) \]

Then the extended Kalman filter for filtering and prediction in (1) may be stated as follows. The one-step ahead prediction of the measurement, \( \hat{y}_{k|k-1} = y_{k-1}(t_k) \), and its approximate covariance, \( R_{k|k-1} \), are computed as

\[ \hat{y}_{k|k-1} = h(t_k, \hat{x}_{k|k-1}) \]
\[ C_k = \frac{\partial h}{\partial x}(t_k, \hat{x}_{k|k-1}) \]
\[ R_{k|k-1} = C_k P_{k|k-1} C_k^T + R_k \]

The innovation, \( e_k \), is obtained by

\[ e_k = y_k - \hat{y}_{k|k-1} \]

and the state filter gain is computed using the expression

\[ K_{f,x,k} = P_{k|k-1} C_k^T R_{k|k-1}^{-1} \]

The filtered state, \( \hat{x}_{k|k} \), and its covariance, \( P_{k|k} \), are computed by

\[ \hat{x}_{k|k} = \hat{x}_{k|k-1} + K_{f,x,k} e_k \]
\[ P_{k|k} = P_{k|k-1} - K_{f,x,k} R_{e,k} K_{f,x,k}^T \]
The above formulas for the measurement update is structurally equivalent to the discrete-time case. The difference between the discrete-time case and the continuous-discrete time case arises in the one-step ahead propagation of the state estimate and its covariance. In the continuous-discrete case \( \dot{x}_{k+1|k} = \dot{x}_k(t_{k+1}) = \dot{x}(t_{k+1}; t_k, \hat{x}_{k|k}) \) and \( P_{k+1|k} = P_k(t_{k+1}) = P(t_{k+1}; t_k, \hat{x}_{k|k}, P_{k|k}) \) are computed as the solution to the system of differential equations

\[
\begin{align*}
\frac{d\hat{x}_k(t)}{dt} &= f(t, \hat{x}_k(t)) \\
\frac{dP_k(t)}{dt} &= A(t)P_k(t) + P_k(t)A(t)' + \sigma(t)\sigma(t)' \\
\end{align*}
\]

(6a) in which

\[
A(t) = \frac{\partial f}{\partial x}(t, \hat{x}_k(t))
\]

(6c) and with initial conditions \( \hat{x}_k(t_k) = \hat{x}_{k|k} \) and \( P_k(t_k) = P_{k|k} \). The main computational effort in the extended Kalman filter is the solution of (6). While this system can be solved using software for the standard initial value problem for systems of ordinary differential equations, it is highly inefficient to do so as (6) has additional structure that may be utilized for its efficient solution. We apply a specialized explicit singly diagonal implicit Runge-Kutta solver, ESDIRK, for solution of this system [16], [17].

\begin{algorithm}
\caption{Square root algorithm for \( P_{k+1|k} \) in (11)}
\begin{equation}
\begin{bmatrix}
X^{1/2} & 0
\end{bmatrix}
\leftarrow \Phi(t_{k+1}, t_k)P_{k+1/2}^{1/2}\Phi(t_{k+1}, T_i)\sqrt{\delta_i q_{1}^{1/2}} \Theta_i
\end{equation}
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Instead of computing the one-step ahead prediction of the states and the associated covariance by (6), ESDIRK computes these quantities by the following equivalent set of equations

\[
\begin{align*}
\frac{d\hat{x}_k(t)}{dt} &= f(t, \hat{x}_k(t)) \\
\frac{d\Phi_k(t)}{dt} &= A(t)\Phi_k(t) + \Phi_k(t)A(t)' + \sigma(t)\sigma(t)' \\
\end{align*}
\]

(10a) in which

\[
A(t) = \frac{\partial f}{\partial x}(t, \hat{x}_k(t))
\]

(10c) and

\[
P_k(t) = \Phi(t, t_k)P_{k|k} \Phi(t, t_k)'
\]

(10d) + \int_{t_k}^{t} \Phi(t, \sigma)\sigma(t)\sigma(t)'\Phi(t, \sigma)ds

The equivalence of (6) and (10) follows directly from the derivation of (6) [17], [18]. Equation (10b) has almost the same structure as the state sensitivity equation. However, in (10b) the initial time is also variable. If the integral of (10d) is computed by quadrature then it may be expressed as

\[
P_{k+1|k} = P_k(t_{k+1}) = \Phi(t_{k+1}, t_k)P_{k|k} \Phi(t_{k+1}, t_k)'
\]

\[
+ \int_{t_k}^{t_{k+1}} \Phi(t_{k+1}, s)\Phi(t_{k+1}, s)'Q(s)ds
\]

\[
\approx \Phi(t_{k+1}, t_k)P_{k|k} \Phi(t_{k+1}, t_k)'
\]

\[
+ \sum_{i=1}^{n_q} \delta_i \Phi(t_{k+1}, T_i)Q(T_i)\Phi(t_{k+1}, T_i)'
\]

in which \( Q(s) = \sigma(s)\sigma(s)' \) and \( n_q \) is the number of quadrature points. Let \( Q_i = Q(T_i) \). Then it is evident from (11) that the one-step ahead covariance square root, \( P_{k+1|k}^{1/2} \), can be computed by a sequence of orthogonal transformations as described in Algorithm 1. In this algorithm, \( \Theta_i \) are orthogonal transformation operators.

III. EXAMPLE: VAN DER VUSSE REACTION

In this section, we test the developed extended Kalman filter algorithm on the Van der Vusse reaction. The purpose is to provide a critical evaluation on the application of the ESDIRK based extended Kalman filter. We demonstrate the limitations that the sensor configuration imposes on the state estimation quality and its rate of convergence toward the true value. These limitations also limits the resulting closed-loop performance achievable by any controller including a
nonlinear predictive controller. The Van der Vusse reaction has been exploited in several controller benchmark studies [19]–[22]. The Van der Vusse reaction is

\[ A + \frac{k_1}{2} B \xrightleftharpoons{\kappa_2} C \]

in which B is the desired product, while C and D are unwanted by-products. The reaction is conducted in a CSTR with a cooling jacket. The reaction rates for this system are

\[ r_1(T, c_A) = k_1(T)c_A, \quad r_2(T, c_B) = k_2(T)c_B \]

and the model of the CSTR is

\[ \dot{c}_A = \frac{F}{V_R}(c_{A0} - c_A) - r_1(T, c_A) - r_3(T, c_A) \]
\[ \dot{c}_B = -\frac{F}{V_R} c_B + r_1(T, c_A) - r_2(T, c_B) \]
\[ \dot{c}_C = \frac{F}{V_R} (T_0 - T) + \frac{k_w A_R}{\rho C_p V_R} (T_J - T) - r_1(T, c_A) \Delta H_{r_1} - r_2(T, c_B) \Delta H_{r_2} - r_3(T, c_A) \Delta H_{r_3} \]
\[ \dot{T}_J = \frac{1}{m_C C_P J} \left( \dot{Q}_J + k_w A_R (T - T_J) \right) \]

The parameters and nominal operating point are provided in Tables I and II, respectively.

The model of the Van der Vusse system is a deterministic system of ordinary differential equations, i.e.

\[ \frac{dx(t)}{dt} = f(x(t), u(t), d(t)) \]

in which

\[ x = \begin{bmatrix} c_A \\ c_B \\ T \\ T_J \end{bmatrix}, \quad u = \begin{bmatrix} F \\ \dot{Q}_J \end{bmatrix}, \quad d = \begin{bmatrix} c_{A0} \\ T_0 \end{bmatrix} \]

and \( x \) is the state vector, \( u \) is the manipulable input vector, and \( d \) is the disturbance vector. The steady state yield of B as function of the feed flow rate for different values of the feed concentration of A is plotted in Figure 1. It should be noted that around the optimal point of operation (maximum yield), the gain from the feed flow rate to the concentration of B changes sign. Hence, the system is not integral controllable by a linear controller in that optimal operating point.

The deterministic system (14) is augmented by a stochastic term, \( \sigma d\omega(t) \), describing the random part of the state evolution. Consequently, the evolution of the Van der Vusse system is described by the following system of stochastic differential equations

\[ dx(t) = f(x(t), u(t), d(t))dt + \sigma d\omega(t) \]

A stochastic and deterministic simulation of the Van der Vusse system is plotted in Figure 2. At time \( t = 4.0 \), the feed concentration of A is increased by 20%. The diffusion term is selected as \( \sigma = 0.03 \text{diag}(x_0) \)

The stochastic differential equation (15) is observed by the stochastic measurement equation

\[ y(t_k) = h(x(t_k)) + \psi(t_k) \quad \psi(t_k) \sim N(0, R_k) \]

at the discrete times \( t_k = 0.01k : k = 0, 1, \ldots \). The measurement noise covariance, \( R_k \), is a diagonal matrix with the entries equal to 0.1 times the corresponding entries in \( \sigma \), i.e. for the full state measurement case \( R_k = 0.1\sigma \). The measurement scenario used for the simulations is illustrated in Figure 3. In the full state feedback all measurements

\[ \text{TABLE I} \]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_{10} )</td>
<td>1.287 \cdot 10^{12} \text{ hr}^{-1}</td>
</tr>
<tr>
<td>( k_{20} )</td>
<td>1.287 \cdot 10^{12} \text{ hr}^{-1}</td>
</tr>
<tr>
<td>( k_{30} )</td>
<td>9.043 \cdot 10^9 \text{ mol}^{-1} \text{ m}^{-3} \text{ hr}^{-1}</td>
</tr>
<tr>
<td>( E_{1/R} )</td>
<td>9758.3 K</td>
</tr>
<tr>
<td>( E_{2/R} )</td>
<td>9758.3 K</td>
</tr>
<tr>
<td>( E_{3/R} )</td>
<td>8560 K</td>
</tr>
<tr>
<td>( \Delta H_{r_1} )</td>
<td>4.2 kJ/mol</td>
</tr>
<tr>
<td>( \Delta H_{r_2} )</td>
<td>-11.0 kJ/mol</td>
</tr>
<tr>
<td>( \Delta H_{r_3} )</td>
<td>-41.85 kJ/mol</td>
</tr>
</tbody>
</table>

\[ \rho \quad 0.9342 \text{ kg/L} \]

\[ C_p \quad 3.01 \text{ J} \text{ K}^{-1} \text{ kg}^{-1} \]

\[ k_w \quad 4032 \text{ hr}^{-1} \text{ m}^{-3} \text{ mol}^{-1} \]

\[ A_R \quad 0.215 \text{ m}^2 \]

\[ m_c \quad 5 \text{ kg} \]

\[ \rho_c \quad 5.1 \text{ mol/L} \]

\[ T_0 \quad 378.05 \text{ K} \]

\[ m_J \quad 0.9342 \text{ kg/L} \]

\[ 0.215 \text{ m}^2 \]

\[ 387.34 \text{ K} \]

\[ 386.66 \text{ K} \]

\[ 386.06 \text{ K} \]

\[ 1.3 \text{ C}_{A0} \]

\[ 0.7 \text{ C}_{A0} \]

\[ 0.9342 \text{ kg/L} \]

\[ 5.1 \text{ mol/L} \]

The entries equal to 0.1 times the corresponding entries in \( \sigma \) are selected as \( \sigma_{x_0} \).

\[ \text{TABLE II} \]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_A )</td>
<td>2.1404 mol/L</td>
</tr>
<tr>
<td>( c_B )</td>
<td>1.0903 mol/L</td>
</tr>
<tr>
<td>( T )</td>
<td>387.34 K</td>
</tr>
<tr>
<td>( T_J )</td>
<td>386.66 K</td>
</tr>
</tbody>
</table>

\[ F \quad 141.9 \text{ L/hr} \]

\[ \dot{Q}_J \quad -1113.5 \text{ kJ/hr} \]

\[ c_{A0} \quad 5.1 \text{ mol/L} \]

\[ T_0 \quad 378.05 \text{ K} \]
mismatches in the case of unknown disturbances, i.e. plant-model
concentrations of model mismatch, a significant offset in the estimation of the
of Fig. 3. Noise corrupted measurements (dots) and actual states (full line)
Fig. 2. Stochastic and deterministic (dashed line) simulation of the Van
der Vusse system.
are used for the extended Kalman filter, while only the
temperature measurements are used for the extended Kalman
filter in the temperature feedback case.
Systematic procedures for identification of parameters in
continuous-discrete stochastic systems (15)-(16) exist but is
outside the topic of this paper [14], [15].
A. Temperature and Concentration Feedback
The first case considered is the case with full state feed-
back, i.e. all states are measured; though the measurements are corrupted by measurement noise. The filtered estimate
of the states, \( \hat{x}_{Kal} \), and true states are illustrated in Figure 4.
The filtered state estimate is close to the true state until time
t = 4.0 at which the disturbance in the feed concentration
of A occurs. After that time, at which there is a plant-
model mismatch, a significant offset in the estimation of the
concentrations of A and B persists.
To avoid the persistent offset of the concentration esti-
mates in the case of unknown disturbances, i.e. plant-model
mismatch, the model is augmented with integrators [24],
[25]. In this case, we augment the model with integrators in
the feed concentration of A, \( c_{A0} \), and the feed temperature,
\( T_0 \), i.e. integrators in the unmeasured disturbance vector, \( d \).
Hence, in the framework of stochastic differential equations,
the integrator states, \( x_d(t) \), used for estimating \( d \) is a random
such that the augmented model becomes
\[
d\begin{bmatrix} x(t) \\ x_d(t) \end{bmatrix} = \begin{bmatrix} f(x(t), u(t), x_d(t)) \\ 0 \end{bmatrix} dt + \begin{bmatrix} \sigma_x & 0 \\ 0 & \sigma_d \end{bmatrix} d\begin{bmatrix} \omega(t) \\ \omega_d(t) \end{bmatrix}
\]
(17)
This model augmented with integrators is used by the
extended Kalman filter for state estimation with \( \sigma_x = 0.01d, \)
\( (\hat{x}_d)_{0|0} = d \), and the corresponding covariance matrix equal
to the unity matrix. The filtered state estimates and the true
states are illustrated in Figure 5. The estimated disturbances
and their true values are plotted in Figure 6. In this case,
there is no persistent offset in the state estimates and the
estimates of the unknown disturbances converge to their true
values. In conclusion, the extended kalman filter performs
adequately as a state estimator for this system with full noise
corrupted state feedback and unknown disturbances in the
feed concentration of A.
B. Temperature Feedback
Consider the more realistic situation in which the concen-
trations of A and B are not measured. Only the temperatures
\( T \) and \( T_J \) are measured. The performance of the continuous-
discrete extended Kalman filter with input integrators dete-
riorate dramatically. This is illustrated in Figures 7 and 8.
The filtered state estimates for the concentrations as well
as the unknown input disturbances do not converge to their
true values. Provided that the system is locally detectable
with the available measurements and that the noise model is
locally stabilizable the estimated states converge in a mean
sense. However, even though it is in principle possible to
estimate the unmeasured states from the subset of measured states, it is often so in practice that in the face of model-plant mismatch the result is quite disappointing in the sense that one cannot substitute concentration measurements with a soft sensor such as the EKF [26]. There is simply no substitute for a good sensor (except for the Utopian wish for a perfect model).

C. Laboratory Measurement of the Concentrations

To overcome some of the limitations associated with an estimator based on only temperature measurements, we assume that the concentrations are measured every 15 minutes (25 times less frequent than the sample rate of the EKF). This setup is supposed to emulate the situation in which the concentrations, $c_A$ and $c_B$, are measured by a laboratory procedure\(^2\). The resulting performance of the extended Kalman filter with input disturbance integrators is illustrated in figures 9 and 10. While the filtered state and input disturbance estimates converge to their true values, the convergence is slower compared to the full state feedback case. This observation is not surprising, but points to the fact that the achievable performance of a closed-loop feedback system intended to control either the productivity or the concentration of $B$ is ultimately limited by the rate at which the estimates of $c_B$, $c_A$, and $c_{A0}$ converge. And the convergence rate is limited by the frequency at which the concentrations are measured.

IV. CONCLUSION

A numerically robust and efficient extended Kalman filter has been introduced as an approximative technique for state estimation in nonlinear stochastic continuous-discrete systems (1). The continuous-discrete extended Kalman filter is applied to the Van der Vusse benchmark example. In this example, temperature measurements are not sufficient
Fig. 9. The filter estimates and the true states (dotted line) for the case with frequent temperature measurements, infrequent concentration measurements, and two input disturbance integrators.

Fig. 10. The filter estimates of the two input integrators and their true value (dashed line) for the case with frequent temperature measurements and infrequent concentration measurements.

to provide steady-state offset free state estimation. The convergence rate of the concentration estimates is limited by the frequency of concentration measurements. This implies that the closed-loop performance of the Van der Vusse benchmark for any controller including nonlinear predictive control is limited by the concentration measurement frequency.

REFERENCES