Parameter Estimation of Nonlinear Systems

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Abstract

In this work, a continuous-time extended Kalman filter (EKF) is presented, which allows the parameters of nonlinear systems to be estimated. The idea of the extended Kalman filter is extending the linearized Kalman filter to directly estimate the states of a nonlinear system and linearizing the nonlinear system around the Kalman filter estimate. Two mathematical models, an interacting tank-in-series process and continuous stirred-tank reactor (CSTR), are introduced. EKF is used to estimate constants $k_{11}$ and $k_{22}$ for interacting tank-in-series process and temperature of reaction mixture $\vartheta$ and frequency factor $k_0$ for CSTR.

Keywords: Extended Kalman filter, nonlinear systems, parameters estimation

Introduction

State estimation is applicable to virtually all areas of engineering and science. Any discipline that is concerned with the mathematical modelling of its systems is a likely (perhaps inevitable) candidate for state estimation. State-space theory and state estimation was initially developed in the 1950s and 1960s, and since then there have been a huge number of applications.(Simon 2006)

State observation for linear differential-algebraic equations (DAEs) has been studied by, for example, (Nikoukhah et al. 1992) using the Kalman filter. Non-linear DAEs are considered in e.g. (Becerra et al. 2001), where an extension of the extended Kalman filter is used and also by (Zimmer and Meier 1997), where the original DAE model is rewritten as an ODE on a restricted manifold (Rheinboldt 1984). Other works include (Boutayeb and Darouach 1995) that uses linearization techniques and (Kidane et al. 2003) that, in addition to a linearization procedure, employs index reduction techniques to cope with high-index
models. In (Kaprielian and Turi 1992), a Lyapunov based approach is used in the design of the observer. In (Åslund et al. 2006) the state estimation for semi-explicit differential-algebraic models has been studied where the proposed observer is formulated as a differential-algebraic equation (DAE). Conditions on the design parameters in the observer are derived such that the index of the observer is 1. Linearization of the error dynamics is used to obtain local stability of the estimator error dynamics. This provides one possibility to design the observer by studying the linearized system and using available linear DAE techniques.

Model estimation using fast orthogonal search (FOS) is presented in (Eklund et al. 2007). FOS is an efficient and effective method of system identification that is able to find parsimonious models of systems from large numbers of candidate basis functions. The method is related to, but more efficient than, a technique proposed by Desrochers for approximating static nonlinear systems, where, amongst various differences, the computational cost is proportional to the square of the number of candidates, whereas in FOS it depends linearly on the number.

In this paper, extended Kalman filter is presented which allows the parameters of processes to be estimated. We will extend the linearized Kalman filter to directly estimate the states of a nonlinear system and linearize the nonlinear system around the Kalman filter estimate. EKF will be used to estimate unknown parameters of tank-in-series process and CSTR.

Theoretical

The continuous-time extended Kalman filter

Consider the following general nonlinear system model (Simon 2006):

\[ \dot{x} = f(x, u, w, t) \]
\[ y = h(x, v, t) \]
\[ w \sim (0, Q) \]
\[ v \sim (0, R) \]

(1)

The noise processes \( w \) and \( v \) are white, zero-mean, uncorrelated, and have known covariance matrices \( Q \) and \( R \). The system equation \( f(\cdot) \) and the measurement equation \( h(\cdot) \) are nonlinear functions. We will use Taylor series to expand these equations around a nominal control \( u_0 \), nominal state \( x_0 \), nominal output \( y_0 \), and nominal noise values \( w_0 \) and \( v_0 \). The Taylor series linearization of equation (1) gives
The definitions of the partial derivative matrices $A$, $B$, $C$, $L$, and $M$ are apparent from the above equations. Now we define the nominal system trajectory as

$$\begin{align*}
\dot{x}_0 &= f(x_0, u_0, w_0, t) \\
y_0 &= h(x_0, v_0, t)
\end{align*}$$

We define the deviation of the true state derivative from the nominal state derivative, and the deviation of the true measurement from the nominal measurement, as follows:

$$\begin{align*}
\Delta \dot{x} &= \dot{x} - \dot{x}_0 \\
\Delta y &= y - y_0
\end{align*}$$

With these definitions equation (2) becomes

$$\begin{align*}
\Delta \dot{x} &= A \Delta x + L w \\
\Delta y &= C \Delta x + M v
\end{align*}$$

The inputs to the filter consist of $\Delta y$, which is the difference between the actual measurement $y$ and the nominal measurement $y_0$. The $\Delta x$ that is output from the Kalman filter is an estimate of the difference between the actual state $x$ and the nominal state $x_0$. The Kalman filter equations for the linearized Kalman filter are

$$\begin{align*}
\Delta \dot{x} &= A \Delta x + K (\Delta y - C \Delta \dot{x}) \\
K &= PC^T \tilde{R}^{-1} \\
\dot{P} &= AP + PA^T + \tilde{Q} - PC^T \tilde{R}^{-1} CP \\
\dot{x} &= x_0 + \Delta \dot{x}
\end{align*}$$

For the Kalman filter, $P$ is equal to the covariance of the estimation error.

Combine the $\dot{x}_0$ in equation (3) with the $\Delta \dot{x}$ expression in equation (6) to obtain

$$\dot{x}_0 + \Delta \dot{x} = f(x_0, u_0, w_0, t) + A \Delta \dot{x} + K [y - y_0 - C (\dot{x} - x_0)]$$
Now choose \( x_0(t) = \hat{x}(t) \) so that \( \Delta \hat{x}(t) = 0 \) and \( \Delta \hat{\hat{x}}(t) = 0 \). In other words, our linearization trajectory \( x_0(t) \) is equal to our linearized Kalman filter estimate \( \hat{x}(t) \). Then the nominal measurement expression in equation (3) becomes

\[
y_0 = h(x_0, v_0, t) = h(\hat{x}, v_0, t)
\]

and equation (7) becomes

\[
\hat{x} = f(\hat{x}, u, w_0, t) + K[y - h(\hat{x}, v_0, t)]
\]

This is equivalent to the linearized Kalman filter except that we have chosen \( x_0 = \hat{x} \), and we have rearranged the equations to obtain \( \hat{x} \) directly. The Kalman gain \( K \) is the same as that presented in equation (6). But this formulation inputs the measurement \( y \) directly, and outputs the state estimate \( \hat{x} \) directly. The EKF can be summarized as follows:

1. The system equations are given as:
   \[
   \begin{align*}
   \dot{x} &= f(x, u, w, t) \\
y &= h(x, v, t) \\
w &\sim (0, Q) \\
v &\sim (0, R)
   \end{align*}
   \]

2. Compute the following partial derivative matrices evaluated at the current state estimate:
   \[
   \begin{align*}
   A &= \frac{\partial f}{\partial x} \\
L &= \frac{\partial f}{\partial w} \\
C &= \frac{\partial h}{\partial x} \\
M &= \frac{\partial h}{\partial v}
   \end{align*}
   \]

3. Compute the following matrices:
   \[
   \begin{align*}
   \tilde{Q} &= LQLT \\
\tilde{R} &= MRM^T
   \end{align*}
   \]

4. Execute the following Kalman filter equations:
   \[
   \begin{align*}
   \hat{x} &= f(\hat{x}, u, w_0, t) + K[y - h(\hat{x}, v_0, t)] \\
K &= PC^T \tilde{R}^{-1} \\
\dot{P} &= AP + PA^T + \tilde{Q} - PC^T \tilde{R}^{-1} CP
   \end{align*}
   \]

where the nominal noise values are given as \( w_0 = 0 \) and \( v_0 = 0 \).
Mathematical modelling

**Interacting tank-in-series process**

Consider the interacting tank-in-series process (Mikleš et al. 2007) shown in Fig. 1. The process input variable is the flow rate $q_0$.

![Fig.1. An interacting tank-in-series process.](image)

The process state variables are heights of liquid in tanks $h_1$, $h_2$. Assuming that liquid density, $F_1$ and $F_2$ are constant, mass balance for the process yields

$$F_1 \frac{dh_1}{dt} = q_0 - q_1$$  \hspace{1cm} (14)

$$F_2 \frac{dh_2}{dt} = q_1 - q_2$$  \hspace{1cm} (15)

where $F_1$ is cross-sectional area of the first tank, $F_2$ is cross-sectional area of the second tank, $h_1$ is height of liquid in the first tank, $h_2$ is height of liquid in the second tank, $q_0$ is inlet volumetric flow rate to the first tank, $q_1$ is inlet volumetric flow rate to the second tank, $q_2$ is outlet volumetric flow rate from the second tank.

Inlet flow rate $q_0$ is independent of tank states whereas $q_1$ depends on the difference between liquid heights

$$q_1 = k_{11} \sqrt{h_1 - h_2}$$  \hspace{1cm} (16)

where $k_{11}$ is valve constant.

Outlet flow rate $q_2$ depends on liquid height in the second tank

$$q_2 = k_{22} \sqrt{h_2}$$  \hspace{1cm} (17)

where $k_{22}$ is valve constant.

Substituting $q_1$ from equation (16) and $q_2$ from (17) into (14) and (15) we get
\[
\frac{dh_1}{dt} = \frac{q_0}{F_1} - \frac{k_{11}}{F_1} \sqrt{h_1 - h_2} \\
\frac{dh_2}{dt} = \frac{k_{11}}{F_2} \sqrt{h_1 - h_2} - \frac{k_{22}}{F_2} \sqrt{h_2}
\]

with arbitrary initial conditions
\[
h_1(0) = h_{10} \\
h_2(0) = h_{20}
\]

Assume that parameters \( k_{11} \) and \( k_{22} \) are unknown. To estimate constants \( k_{11} \) and \( k_{22} \), two more equations are needed
\[
\frac{dk_{11}}{dt} = 0 \quad k_{11}(0) = k_{11}^0 \\
\frac{dk_{22}}{dt} = 0 \quad k_{22}(0) = k_{22}^0
\]

Equations (18) and (20) are now nonlinear system model for parameters estimation. According to (11)

\[
A = \begin{pmatrix}
-\frac{\dot{k}_{11}}{2F_1\sqrt{\hat{h}_1 - \hat{h}_2}} & \frac{\dot{k}_{11}}{2F_1\sqrt{\hat{h}_1 - \hat{h}_2}} & -\frac{\sqrt{\hat{h}_1 - \hat{h}_2}}{F_1} \\
\frac{\dot{k}_{11}}{2F_2\sqrt{\hat{h}_1 - \hat{h}_2}} & -\frac{\dot{k}_{22}}{2F_2\sqrt{\hat{h}_1 - \hat{h}_2}} & -\frac{\sqrt{\hat{h}_1 - \hat{h}_2}}{F_2} \\
0 & \frac{\sqrt{\hat{h}_1 - \hat{h}_2}}{2F_2\sqrt{\hat{h}_2}} & 0 \\
0 & 0 & 0
\end{pmatrix}
\]

\[
C = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}
\]

Parameters of the interacting tank-in-series process are shown on Table 1.

<table>
<thead>
<tr>
<th>q0S / (m(^3)·h(^{-1}))</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>k11 / (m(^{5/2})·h)</td>
<td>0.8</td>
</tr>
<tr>
<td>k22 / (m(^{5/2})·h)</td>
<td>1.5</td>
</tr>
<tr>
<td>F1 / (m(^2))</td>
<td>0.8</td>
</tr>
<tr>
<td>F2 / (m(^2))</td>
<td>0.8</td>
</tr>
</tbody>
</table>
Continuous stirred-tank reactor

We consider CSTR (Mikleš et al. 2007) with a simple exothermal reaction \( A \rightarrow B \) (Fig. 2.).

![Diagram of a CSTR](image)

For the development of a mathematical model of the CSTR, the following assumptions are made: neglected heat capacity of inner walls of the reactor, constant density and specific heat capacity of liquid, constant reactor volume, constant overall heat transfer coefficient, and constant and equal input and output volumetric flow rates. As the reactor is well-mixed, the outlet stream concentration and temperature are identical with those in the tank.

A mass balance of component A can be expressed as

\[
V \frac{dc_A}{dt} = qc_{AV} - qc_A - Vr(c_A, \vartheta)
\]

where \( V \) is reactor volume, \( c_A \) is molar concentration of A in the outlet stream, \( q \) is volumetric flow rate of reaction mixture, \( c_{AV} \) is molar concentration of A in the inlet stream, \( r \) is rate of reaction, \( \vartheta \) is temperature of reaction mixture.

The rate of reaction is strong function of concentration and temperature (Arrhenius law)

\[
r(c_A, \vartheta) = kc_A = k_0 e^{-\frac{E}{R\vartheta} c_A}
\]

where \( k_0 \) is frequency factor, \( E \) is activation energy.

Heat balance gives

\[
V \rho c_p \frac{d\vartheta}{dt} = q \rho c_p \vartheta - q \rho c_p \vartheta - \alpha F(\vartheta - \vartheta_C) + V(-H)r(c_A, \vartheta)
\]
where \( \rho \) is liquid density, \( c_P \) is liquid specific heat capacity, \( \vartheta \) is temperature in the inlet stream, \( \alpha \) is overall heat transfer coefficient, \( F \) is heat transfer area, \( \vartheta_c \) is cooling temperature, \( \Delta H \) is heat of reaction.

Initial conditions are

\[
c_A(0) = c_{A0} \\
\vartheta(0) = \vartheta_0
\]

(26)

Assume that parameter \( \vartheta \) and \( k_0 \) is unknown. To estimate frequency factor \( k_0 \) one more equation is needed

\[
\frac{dk_0}{dt} = 0 \quad k_0(0) = k_0^0
\]

(27)

Equations (23), (25) and (27) are now nonlinear system model for parameters estimation.

According to (11)

\[
A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & 0 & 0 \end{pmatrix}
\]

(28)

\[
C = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}
\]

(29)

where

\[
a_{11} = -\frac{q}{V} - \frac{\hat{k}_0 e^{-\frac{\vartheta}{\vartheta_c}}}{\rho \vartheta} \quad a_{12} = -\frac{\hat{c}_A g k_0 e^{-\frac{\vartheta}{\vartheta_c}}}{R \vartheta^2} \quad a_{13} = -\hat{c}_A e^{-\frac{\vartheta}{\vartheta_c}}
\]

\[
a_{21} = \frac{\hat{k}_0 e^{-\frac{\vartheta}{\vartheta_c}} (-\Delta H) \hat{c}_A}{\rho c_P} \quad a_{22} = -\frac{q}{V} - \frac{\alpha F}{V \rho c_P} + \frac{\hat{k}_0 e^{-\frac{\vartheta}{\vartheta_c}} (-\Delta H) \hat{c}_A}{\hat{\vartheta}^2 \rho c_P}
\]

\[
a_{23} = -\frac{e^{-\frac{\vartheta}{\vartheta_c}} (-\Delta H) \hat{c}_A}{\rho c_P}
\]

Parameters of the reaction and reactor are shown on Table 2.

<table>
<thead>
<tr>
<th>Parameters of the reaction and reactor.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{A VS} ) (kmol m(^{-3}))</td>
<td>1.2</td>
</tr>
<tr>
<td>( c_P ) (kJ kg(^{-1}) K(^{-1}))</td>
<td>4.05</td>
</tr>
<tr>
<td>( E ) (kJ kmol(^{-1}))</td>
<td>107280</td>
</tr>
<tr>
<td>( F ) (m(^2))</td>
<td>6.08</td>
</tr>
<tr>
<td>( k_0 ) (min(^{-1}))</td>
<td>7.93e15</td>
</tr>
<tr>
<td>( \rho ) (kg m(^{-3}))</td>
<td>998</td>
</tr>
<tr>
<td>( \Delta H ) (kJ kmol(^{-1}))</td>
<td>-150000</td>
</tr>
</tbody>
</table>

\[\text{Acta Chimica Slovaca, Vol.1, No. 1, 2008, 309 – 320}\]
Results and Discussion

For the tank-in-series process parameters estimation simulation, the following values were tracked: \( q_0(t) = 1 \text{ m}^3\text{.h}^{-1} \) for \( t < 0 \text{ h} \) and \( q_0(t) = 1.1 \text{ m}^3\text{.h}^{-1} \) for \( t \geq 0 \text{ h} \), initial condition for the states is taken as [2.000 0.4444] and for estimated values of states \( \hat{k}_{11}, \hat{k}_{22} \) are [1 1]. Fig. 3,4,5,6 show the estimation results for tank-in-series process.

![Fig.3](image1.png)

Fig.3. Simulation (-) and estimation (--) of the height of liquid in the first tank.

![Fig.4](image2.png)

Fig.4. Simulation (-) and estimation (--) of the height of liquid in the second tank.
For the CSTR parameters estimation simulation, the following values were tracked: $c_{AV}(t) = 1.2 \text{ kmol.m}^{-3}$ for $t < 0 \text{ h}$ and $c_{AV}(t) = 1.1 \text{ kmol.m}^{-3}$ for $t \geq 0 \text{ h}$, initial condition for the states is taken as $[0.9923 \ 320.068]$ and for estimated value of state $\hat{k}_0$ is $[7e14]$. Fig. 7,8,9 show the estimation results for CSTR.
Fig. 7. Simulation (-) and estimation (--·) of the molar concentration of A in the outlet stream.

Fig. 8. Estimation of the temperature of reaction mixture.

Fig. 9. Estimation of the frequency factor.
The estimation of parameters and states is carried out in presence of noise. From the results on Fig. 3,4,5,6,7,8,9 it is observed that extended Kalman filter algorithm gives very high accuracy of parameters estimation and for flow processes parameters estimation can be successfully used. Parameters estimation converges in minimum time for most of the initial values. For the purpose of estimation is needed to provide a measurement such that process observability conditions are held.

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References