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Optimal Filtering For Bilinear System States And Its Application To Terpolymerization Process Identification*

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Abstract

This paper presents the optimal nonlinear filter for bilinear state and linear observation equations confused with white Gaussian disturbances. The general scheme for obtaining the optimal filter in case of polynomial state and linear observation equations is announced. The obtained bilinear filter is applied to solution of the identification problem for the bilinear terpolymerization process and compared to the optimal linear filter available for the linearized model and to the mixed filter designed as a combination of those filters.

1 Introduction

It is virtually the common opinion that the optimal nonlinear finite-dimensional filter exists and can be obtained in a closed form only in the case of linear state and observation equations. This famous construction is called the linear Kalman-Bucy filter [3]. However, the optimal nonlinear finite-dimensional filter can also be obtained in some other cases, if, for example, the state vector can take only a finite number of admissible states [8] or if the observation equation is linear and the drift term in the state equation satisfies the Riccati equation $f'(x) + f^2 = x^2$ (see [2]). The complete classification of the "general situation" cases (this means that there are no special assumptions on the structure of state and observation equations), where the optimal nonlinear finite-dimensional filter exists, is given in [9].

This paper studies a relatively simple (but important in practical applications, see [6]) case of polynomial system states, where the optimal nonlinear finite-dimensional filter can be obtained in a closed form. Indeed, if the observation equation is linear and the observation matrix is invertible, then, as shown below in the paper, it is possible to obtain the optimal finite-dimensional filter for a polynomial state equation, provided that the system coefficients depend on time only. In the case of a bilinear state equation, the corresponding filtering equations are derived in the paper directly. A similar filtering problem has been treated for cubic polynomial states and linear observations

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in [1], where the third degree of a vector is defined in a restrictive (componentwise) sense. The possibility to solve the optimal filtering problem for an arbitrary polynomial state and linear observations is underlined.

The obtained optimal filter for bilinear system states and linear observations is applied to solution of an identification problem for the terpolymerization process [6] in the presence of direct linear observations. The process equations are intrinsically nonlinear (bilinear), so their linearization leads to large deviations from the real system dynamics, as it can be seen from the simulation results. Numerical simulations are conducted for the optimal filter for bilinear system states, the optimal linear filter available for the linearized model, and the mixed filter designed as a combination of those filters. The simulation results show an advantage of the optimal bilinear filter in comparison to the other filters.

The paper is organized as follows. Section 2 establishes the procedure to obtain a closed system of the filtering equations for polynomial state and linear observation equations and gives the optimal filter for bilinear system states and linear observations in the explicit form. In Section 3, the obtained bilinear filter is applied to solution of an identification problem for the bilinear terpolymerization process and compared to the optimal linear filter available for the linearized model and to the mixed filter designed as a combination of those filters.

2 Optimal filtering for polynomial state and linear observations

Let a unobserved random process $x(t)$ satisfy a nonlinear polynomial equation

$$dx(t) = f(x(t))dt + b(t)dW_1(t), \quad x(t_0) = x_0, \tag{1}$$

and linear observations are given by

$$dy(t) = h(x(t))dt + B(t)dW_2(t). \tag{2}$$

Here, the drift function $f(x(t)) = a_0(t) + a_1(t)x + a_2(t)x^2 + ...$ is a polynomial, the observation function $h(x(t)) = A_0(t) + A(t)x$ is linear, and the observation matrix $A(t)$ is invertible, i.e., the inverse matrix $A^{-1}(t)$ exists; $W_1(t)$ and $dW_2(t)$ are Wiener processes, whose weak derivatives are Gaussian noises and which are assumed independent of each other and of the initial value x_0.

The estimation problem is to find the best estimate for the real process $x(t)$ at time t based on the observations $Y(t) = \{y(s), t_0 \le s \le t\}$, that is the conditional expectation $m(t) = E(x(t) \mid Y(t))$ of the real process $x(t)$ with respect to the observations $Y(t)$. Let $P(t) = E((x(t) - m(t))(x(t) - m(t))^T \mid Y(t))$ be the error variance (correlation function).

To find the solution to the stated problem, let us first note that, since the observation equation is linear, the innovations process

$$\vartheta(t) = y(t) - \int_{t_0}^{t} (A_0(s) + A(s)m(s))ds$$

$$= \int_{t_0}^{t} A(s)(x(s)-m(s))ds + \int_{t_0}^{t} B(s)dW_2(s)$$

is a Wiener process [5], and, since $\int_{t_0}^{t} B(s)dW_2(s)$ is also a Wiener process, the random variable $A(t)(x(t)-m(t))$ is Gaussian for every fixed t. If the inverse matrix $A^{-1}(t)$ exists, then the random vector $(x(t)-m(t))$ is also Gaussian [7].

Moreover, taking into account that the equality

$$[E(h(x(t))x^T(t)|Y(t)) - E(h(x(t))|Y(t))m^T(t)]^T(B(t)B^T(t))^{-1}[dy(t)-A(t)m(t)dt]$$
$$= P(t)A^T(t)(B(t)B^T(t))^{-1}[dy(t)-A(t)m(t)dt].$$

is valid for the linear observation function $h(x(t))$ in (2), the nonlinear filtering equation for the optimal estimate $m(t)$, first derived by Kushner [4], takes the form

$$dm(t) = E(f(x(t)) \mid Y(t))dt + P(t)A^T(t)(B(t)B^T(t))^{-1}[dy(t)-A(t)m(t)dt], \quad (3)$$

$$m(t_0) = E(x(t_0) \mid Y(t_0)).$$

Let us note now that if the function $f(x(t)) = a_0(t) + a_1(t)x + a_2(t)x^2 + ...$ is a polynomial, it should be possible to compute a finite-dimensional filter in a closed form for variables $m(t)$ and $P(t)$, using the fact that the random variable $(x(t)-m(t))$ is Gaussian. Since all the system coefficients in (1),(2) do not depend on state $x(t)$ and observations $y(t)$, the conditional moments of $(x(t)-m(t))$ with respect to observations $y(t)$ coincide with the unconditional ones. This implies that all odd central conditional moments of this Gaussian variable $\mu_1 = E((x(t)-m(t)) \mid Y(t))$, $\mu_3 = E((x(t)-m(t))^3 \mid Y(t))$, $\mu_5 = E((x(t)-m(t))^5 \mid Y(t)), ...$ are equal to 0, and all even central conditional moments $\mu_2 = E((x(t)-m(t))^2 \mid Y(t))$, $\mu_4 = E((x(t)-m(t))^4 \mid Y(t))$, $\mu_6 = E((x(t)-m(t))^6 \mid Y(t)), ...$ can be represented as functions of the variance $P(t)$. For example, $\mu_2 = P$, $\mu_4 = 3P^2$, $\mu_6 = 15P^3, ...$ (see [7]). Thus, all higher moments of $(x(t)-m(t))$ can be expressed using $P(t)$, and this yields additional relations for representing every higher initial moment of $x(t)$ and, finally, the possibility to obtain the optimal filter in a closed form, i.e., with respect to a finite number of filtering variables. In other words, the optimal finite-dimensional filter should exist in the polynomial-linear case.

2.1 Bilinear state equation

In a particular case, if the function

$$f(x) = a_0(t) + a_1(t)x + a_2(t)xx^T \quad (4)$$

is a bilinear polynomial, where x is now an n-dimensional vector, a_1 is an $n \times n$ - matrix, and a_2 is a 3D tensor of dimension $n \times n \times n$, the system of filtering equations is as follows

$$\begin{aligned} dm(t) &= (a_0(t) + a_1(t)m(t) + a_2(t)m(t)m^T(t) + a_2(t)P(t))dt \\ &\quad + P(t)A^T(t)(B(t)B^T(t))^{-1}[dy(t)-A(t)m(t)dt], \end{aligned} \quad (5)$$

$$m(t_0) = E(x(t_0) \mid Y(t_0)),$$

$$\begin{aligned} dP(t) &= (a_1(t)P(t) + P(t)a_1^T(t) + 2a_2(t)m(t)P(t) + 2(a_2(t)m(t)P(t))^T \\ &+ b(t)b^T(t))dt - P(t)A^T(t)(B(t)B^T(t))^{-1}A(t)P(t)dt, \end{aligned} \quad (6)$$

$$P(t_0) = E((x(t_0) - m(t_0))(x(t_0) - m(t_0))^T \mid Y(t_0)),$$

since the third central moment μ_3 is equal to 0, and the third initial moment of $x(t)$ can be expressed using its second and first moments, i.e., $P(t)$ and $m(t)$. In this bilinear-linear case, the variance equation is also independent of the observations $y(t)$, but has the bilinear terms $m(t)P(t)$ in its right-hand side and depends on $m(t)$, thus making both the equations interconnected. The estimate equation is bilinear with respect to m, as expected.

3 Terpolymerization process identification

The obtained optimal filter for bilinear system states and linear observations is applied to solution of an identification problem for the terpolymerization process [6] in the presence of direct linear observations. Let us rewrite the bilinear state equations (1),(4) and the linear observation equations (2) in the component form using index summations

$$\frac{dx_k(t)}{dt} = a_{0k}(t) + \sum_i a_{1ki}(t)x_i(t) + \sum_{ij} a_{2kij}(t)x_i(t)x_j(t) + \sum_i b_{ki}(t)\psi_{1i}(t), \; k = 1, \dots, n,$$

$$y_k(t) = \sum_i A_{ki}(t)x_i(t) + \sum_i B_{ki}(t)\psi_{2i}(t), \quad (7)$$

where $\psi_1(t)$ and $\psi_2(t)$ are white Gaussian noises. Then, the filtering equations (5),(6) can be rewritten in the component form as follows

$$\begin{aligned} \frac{dm_k(t)}{dt} &= a_{0k}(t) + \sum_i a_{1ki}(t)m_i(t) + \sum_{ij} a_{2kij}(t)m_i(t)m_j(t) + \sum_{ij} a_{2kij}(t)P_{ij}(t))dt \\ &+ \sum_{ijlps} P_{kj}(t)A_{jl}^T(t)(B_{lp}(t)B_{ps}(t))^{-1}[dy_s - \sum_r A_{sr}(t)m_r(t)dt], \end{aligned} \quad (8)$$

$$m_k(t_0) = E[x_k(t_0) \mid Y(t_0)];$$

$$\begin{aligned} dP_{ij}(t) &= \sum_k a_{1ik}(t)P_{kj}(t) + \sum_k P_{ki}(t)a_{1jk}(t) + 2\sum_{kl} a_{2ikl}(t)m_l(t)P_{kj} \\ &+ 2\sum_{kl} a_{2jkl}(t)m_l(t)P_{ki}(t) + \sum_k b_{ik}(t)b_{kj}(t) \\ &- \sum_{klpsr} P_{ik}(t)A_{kl}^T(t)(B_{lp}(t)B_{ps}(t))^{-1}A_{sr}(t)P_{rj}(t), \end{aligned} \quad (9)$$

$$P_{ij}(t_0) = E[(x_i(t_0) - m_i(t_0))(x_j(t_0) - m_j(t_0))^T \mid Y(t_0)].$$

The terpolymerization process model reduced to ten bilinear equations selected from [6] is given by

$$\frac{dC_{m1}}{dt} = \frac{1}{V} d\Delta_{m1}/dt - (1/\theta + K_{L1}C^* + K_{11}\mu_P^o + K_{21}\mu_Q^o + K_{31}\mu_R^o)C_{m1}; \quad (10)$$

$$\frac{dC_{m2}}{dt} = \frac{1}{V} d\Delta_{m2}/dt - (1/\theta + K_{L2}C^* + K_{12}\mu_P^o + K_{22}\mu_Q^o)C_{m2};$$

$$\frac{dC_{m3}}{dt} = \frac{1}{V} d\Delta_{m3}/dt - (1/\theta + K_{13}\mu_P^o)C_{m3};$$

$$\frac{dC^*}{dt} = \frac{1}{V} d\Delta_{m^*}/dt - (1/\theta + K_d + K_{L1}C_{m1} + K_{L2}C_{m2})C^*;$$

$$\begin{aligned}\frac{d\mu_P^o}{dt} &= (-1/\theta - K_{t1})\mu_P^o + K_{L1}C_{m1}C^* - (K_{12}C_{m2} + K_{13}C_{m3})\mu_P^o \\ &\quad + K_{21}C_{m1}\mu_Q^o + K_{31}C_{m1}\mu_R^o;\end{aligned}$$

$$\frac{d\mu_Q^o}{dt} = -\frac{1}{\theta}\mu_Q^o + K_{L2}C_{m2}C^* - (K_{21}C_{m1} + K_{t2})\mu_Q^o + K_{12}C_{m2}\mu_P^o;$$

$$\frac{d\mu_R^o}{dt} = -\frac{1}{\theta}\mu_R^o - (K_{31}C_{m1} + K_{t3})\mu_R^o + K_{13}C_{m3}\mu_P^o;$$

$$\begin{aligned}\frac{d\lambda_1^{100}}{dt} &= -\frac{1}{\theta}\lambda_1^{100} + K_{L1}C_{m1}C^* + K_{L2}C_{m2}C^* + K_{11}C_{m1}\mu_P^o \\ &\quad + K_{21}C_{m1}\mu_Q^o + K_{31}C_{m1}\mu_R^o;\end{aligned}$$

$$\frac{d\lambda_1^{010}}{dt} = -\frac{1}{\theta}\lambda_1^{010} + K_{L1}C_{m1}C^* + K_{L2}C_{m2}C^* + K_{12}C_{m2}\mu_P^o + K_{22}C_{m2}\mu_Q^o;$$

$$\frac{d\lambda_1^{001}}{dt} = -\frac{1}{\theta}\lambda_1^{001} + (K_{L1}C_{m1} + K_{L2}C_{m2})C^* + K_{13}C_{m3}\mu_P^o.$$

Here, the state variables are: C_{m1}, C_{m2}, and C_{m3} are the reagent (monomer) concentrations, C^* is the active catalyst concentration; μ_P^o, μ_Q^o, and μ_R^o are the zeroth live moments of the product MWD, and λ_1^{100}, λ_1^{010}, and λ_1^{001} are its first bulk moments. The reactor volume V and residence time θ, as well as all coefficients K's, are known parameters, and $\Delta_{m1}, \Delta_{m2}, \Delta_{m3}, \Delta_{m^*}$ stand for net molar flows of the reagents and active catalyst into the reactor.

The identification (filtering) problem is to find the optimal estimate for the unobserved states (10) assuming that the direct observations y_i contaminated with Gaussian noises ψ_2's are provided for each of the ten state components x_i

$$y_i = x_i + \psi_{2i}.$$

Here, x_1 denotes C_{m1}, x_2 denotes C_{m2}, and so on up to $x_{10} = \lambda_1^{001}$. In this situation, the bilinear filtering equations (8) for the vector of the optimal estimates $m(t)$ take the form

$$\begin{aligned}\frac{dm_1(t)}{dt} &= \frac{1}{V}d\Delta_{m1}/dt - ((1/\theta) + K_{L1}m_4(t) + K_{11}m_5(t) + K_{21}m_6(t)\\ &\quad +K_{31}m_7(t))m_1(t) - K_{L1}P_{14}(t) - K_{11}P_{15}(t) - K_{21}P_{16}(t)\\ &\quad -K_{31}P_{17}(t) + \sum_j P_{1j}[dy_j/dt - m_j];\end{aligned} \tag{11}$$

$$\begin{aligned}\frac{dm_2(t)}{dt} &= \frac{1}{V}d\Delta_{m2}/dt - ((1/\theta) + K_{L2}m_4(t) + K_{12}m_5(t) + K_{22}m_6(t))m_2(t)\\ &\quad -K_{L2}P_{24}(t) - K_{12}P_{25}(t) - K_{22}P_{26}(t) + \sum_j P_{2j}[dy_j/dt - m_j];\end{aligned}$$

$$\frac{dm_3(t)}{dt} = \frac{1}{V}d\Delta_{m3}/dt - ((1/\theta) + K_{13}m_5(t))m_3(t) - K_{13}P_{35}(t) + \sum_j P_{3j}[dy_j/dt - m_j];$$

$$\begin{aligned}\frac{dm_4(t)}{dt} &= \frac{1}{V}d\Delta_{m^*}/dt - ((1/\theta) + K_d + K_{L1}m_1(t)\\ &\quad +K_{12}m_2(t))m_4(t) - K_{L1}P_{14}(t) - K_{12}P_{24}(t) + \sum_j P_{4j}[dy_j/dt - m_j];\end{aligned}$$

$$\begin{aligned}\frac{dm_5(t)}{dt} &= (-1/\theta - K_{t1})m_5(t) + K_{L1}m_4(t)m_1(t) - K_{12}m_2(t)m_5(t)\\ &\quad +K_{21}m_6(t)m_1(t) + K_{31}m_7(t)m_1(t) - K_{13}m_5(t)m_3(t) + K_{L1}P_{14}(t)\\ &\quad +K_{21}P_{16}(t) + K_{31}P_{17}(t) - K_{12}P_{25}(t) - K_{13}P_{35}(t) + \sum_j P_{5j}[dy_j/dt - m_j];\end{aligned}$$

$$\begin{aligned}\frac{dm_6(t)}{dt} &= (-1/\theta - K_{t2} - K_{21}m_1(t))m_6(t) + K_{L2}m_4(t)m_2(t) + K_{12}m_5(t)m_2(t)\\ &\quad -K_{21}P_{16}(t) + K_{L2}P_{24}(t) + K_{12}P_{25}(t) + \sum_j P_{6j}[dy_j/dt - m_j];\end{aligned}$$

$$\begin{aligned}\frac{dm_7(t)}{dt} &= (-1/\theta - K_{t3} - K_{31}m_1(t))m_7(t) + K_{13}m_5(t)m_3(t)\\ &\quad -K_{31}P_{17}(t) + K_{13}P_{35}(t) + \sum_j P_{7j}[dy_j/dt - m_j];\end{aligned}$$

$$\begin{aligned}\frac{dm_8(t)}{dt} &= (-1/\theta)m_8(t) + (K_{L1}m_4(t) + K_{11}m_5(t) + K_{21}m_6(t) + K_{31}m_7(t))m_1(t)\\ &\quad +K_{L2}m_4(t)m_2(t) + K_{L1}P_{14}(t) + K_{11}P_{15}(t) + K_{21}P_{16}(t)\\ &\quad +K_{31}P_{17}(t) + K_{L2}P_{24}(t) + \sum_j P_{8j}[dy_j/dt - m_j];\end{aligned}$$

$$\frac{dm_9(t)}{dt} = -\frac{1}{\theta}m_9(t) + K_{L1}m_4(t)m_1(t) + K_{L2}m_4(t)m_2(t) + K_{12}m_5(t)m_2(t) + K_{22}m_6(t)m_2(t) + K_{L1}P_{14}(t) + K_{L2}P_{24}(t)K_{12}P_{25}(t) + K_{22}P_{26}(t) + \sum_j P_{9j}[dy_j/dt - m_j];$$

$$\frac{dm_{10}(t)}{dt} = -\frac{1}{\theta}m_{10}(t) + K_{L1}m_4(t)m_1(t) + K_{L2}m_4(t)m_2(t) + K_{13}m_5(t)m_3(t) + K_{L1}P_{14}(t) + K_{L2}P_{24}(t) + K_{13}P_{35}(t) + \sum_j P_{10j}[dy_j/dt - m_j].$$

Here, $m_1(t)$ is the optimal estimate for C_{m1}, $m_2(t)$ for C_{m2}, and so on up to $m_{10}(t)$. The fifty-five variance component equations are similarly generated by the equations (9).

In the simulation process, the initial conditions at $t = 0$ are equal to zero for the state variables $C_{m1}, \ldots, \lambda_1^{001}$, to 0.5 for the estimates $m_1(t), \ldots, m_{10}(t)$, to 1 for the diagonal entries of the variance matrix, and to zero for its other entries. For the purpose of testing the obtained filter, the system parameter values are all set to 1. The white Gaussian noises in the equations (7) are realized as sinusoidal signals: $\psi_i = \sin t$ for $i = 1, \ldots, 10$.

In Figure 1, the obtained values of the state variables $C_{m1}, \ldots, \lambda_1^{001}$ are given in the blue, and the values of the bilinear optimal filter estimates $m_1(t), \ldots, m_{10}(t)$ are depicted in the red.

The performance of the optimal bilinear filter (8),(9) is compared to the performance of the optimal linear Kalman-Bucy filter available for the linearized system. This linear filter consists of only the linear terms and innovations processes in the equations (8) (or (11)) for the optimal estimates and the Riccati equations for the variance matrix components corresponding to the equations (9):

$$\frac{dm_k(t)}{dt} = a_{0k}(t) + \sum_i a_{1ki}(t)m_i(t) + \sum_{jlps} P_{kj}(t)A_{jl}^T(t)(B_{lp}B_{ps}))^{-1}(t)[dy_s - \sum_r A_{sr}(t)m_r(t)dt], \quad (12)$$

$$m_k(t_0) = E[x_k(t_0) \mid Y(t_0)];$$

$$\frac{dP_{ij}(t)}{dt} = \sum_k a_{1ik}(t)P_{kj}(t) + \sum_k P_{ki}(t)a_{1jk}(t) + \sum_k b_{ik}(t)b_{kj}(t) - \sum_{klpsr} P_{ik}(t)A_{kl}^T(t)(B_{lp}B_{ps}))^{-1}A_{sr}P_{rj}(t), \quad (13)$$

$$P_{ij}(t_0) = E[(x_i(t_0) - m_i(t_0))(x_j(t_0) - m_j(t_0))^T \mid Y(t_0)].$$

The graphs of the estimates obtained using this linear Kalman-Bucy filter are shown in Figure 1 in the green.

Finally, the performance of the optimal bilinear filter (8),(9) is compared to the performance of the mixed filter designed as follows. The estimate equations in this filter coincide with the bilinear equations (8) (or (11)) from the optimal bilinear filter, and the variance equations coincide with the Riccati equations (13) from the linear Kalman-Bucy filter. The graphs of the estimates obtained using this mixed filter are shown in Figure 1 in the black. The initial conditions and white Gaussian noise realizations remain the same for all the filters involved in the simulation.

4 Discussion

Upon comparing all simulation results given in Figure 1, it can be concluded that the optimal bilinear filter gives the best estimates in comparison to two other filters. Although this conclusion follows from the developed theory, the numerical simulation serves as a convincing illustration. On the other hand, since the Kalman-Bucy estimates obtained for the linearized model do not converge to the real state values, it can be concluded that linearization fails and is not applicable even to simple bilinear systems.

It should finally be noted that the results obtained applying the mixed filter are actually very close to (and for the first two variables even better than) the results obtained using the optimal bilinear filter. The advantage of the mixed filter consists in its better realizability, since the matrix $P(t)$ for the mixed filter satisfies the conventional Riccati equation (13). Thus, the mixed filter could also be widely used to obtain reasonably good approximations of the optimal estimates for bilinear system states.

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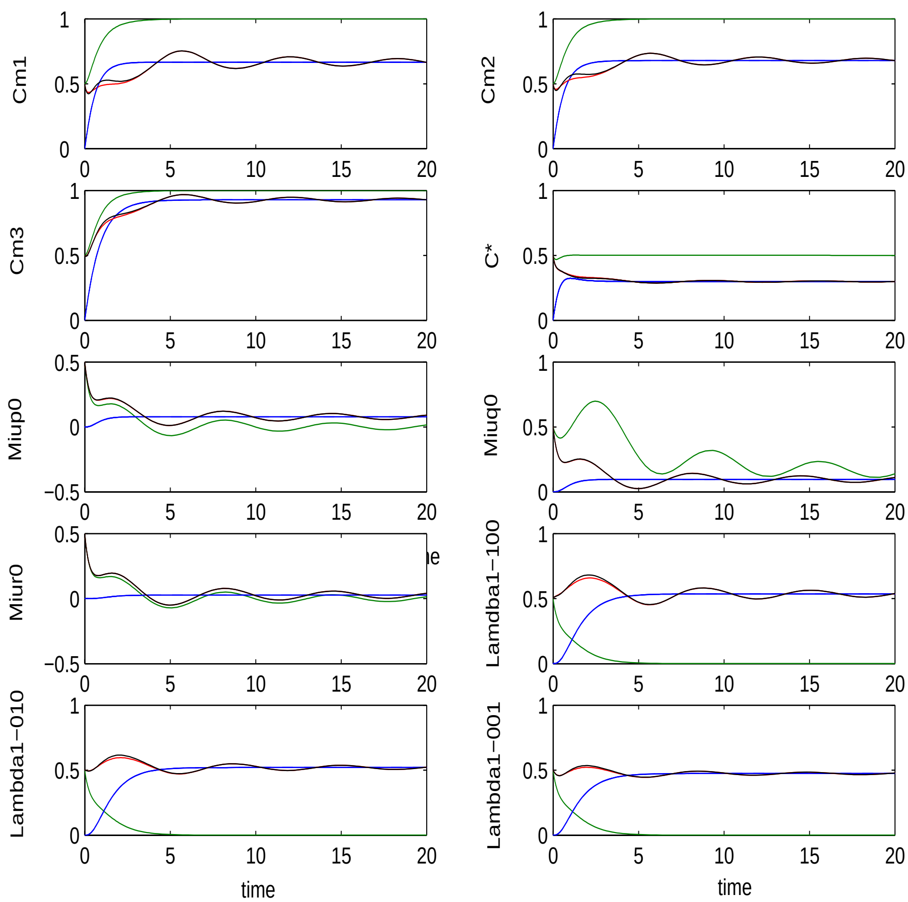

Figure 1: Graphs of the ten state variables (10) (blue),
the estimates given by the optimal bilinear filter (8),(9) (red),
the estimates given by the linear Kalman-Bucy filter (12),(13) (green),
the estimates given by the mixed filter (8),(13) (black).