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Application of Advanced Estimation Techniques to a Chemical Plant Model

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The paper is aimed at comparing some of the most promising and novel advanced techniques for estimation by assessing their effectiveness on the chemical process benchmark. Global and distributed implementations of the extended Kalman filter are the key elements of the work. In addition, the paper is also aimed at describing and developing a recursive implementation of the autocovariance least square algorithm for the on-line updating of the tuning knobs of the filter, demonstrating its relevance in the performance monitoring of chemical processes.

1. Introduction

In process control, the state estimation problem is of paramount importance for monitoring and for the application of advanced control techniques, such as model predictive control, see e.g. Chen and Allgöwer (1998), Magni et al. (2001). One of the most effective widespread state estimation techniques for nonlinear systems is the Extended Kalman Filter (EKF), see e.g. Simon (2006) which, especially in case of application to large-scale systems, requires a considerable amount of on-line computations for the update of the filter gain and for the real-time simulation of the dynamic nonlinear model of the process. In this paper, a distributed implementation of the EKF is first proposed to deal with a complete process layout made by interconnected process units without overlapping states, as is often the case in chemical and petrochemical processes. More specifically, an independent EKF is designed for any subsystem based on the available local measurements and on the variables estimated by its neighboring units and referred to material and energy flows among the subsystems. In order to test the performance of this distributed EKF implementation, an ideal chemical plant consisting of a jacketed continuous stirred tank reactor (CSTR), a flash drum separator, and two distillation columns has been used as a benchmark (Figure 1). Its overall mathematical model includes 85 ODEs and 10 algebraic equations. For this system, a distributed architecture composed by three interconnected low-order EKFs has been designed and its performance has been compared to that guaranteed by a centralized EKF implementation. In both cases a mixed discrete/continuous-time filter implementation has been employed: specifically, predictions are computed by direct integration of the continuous-time system model, while corrections are provided, with period T, using discretized/linearized models, similarly to standard EKF implementations. In our benchmark example the distributed approach can reduce the computational time by a factor of 5 or more, without detriment of the quality of the estimation. Notably, the distributed EKF approach with recursive covariance update has been used also for the on-line estimation of a relevant process model parameter, i.e. the heat transfer coefficient of CSTR. Also in this case, simulation results emphasize the potentialities of the proposed approach. One of the main

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difficulties in the use of EKF is the definition of the characteristics of the noises acting on the system states and on the available measurements. For this reason, in the past many efforts have been devoted to the development of methods for the estimation of the noise covariance matrices, see e.g. Mehra (1970, 1972), Odelson et al. (2006a, 2006b). In particular, the Autocovariance Least Squares (ALS) algorithm described in Odelson et al. (2006a, 2006b) is one of the most promising approaches for off-line covariance estimation. The second contribution of this paper is the development and test of a simple recursive implementation of the ALS algorithm for the on-line update of the covariance matrices used in the distributed EKF. This method has been applied to the considered benchmark problem also for the on-line tuning of the covariances related to the dummy noise describing the uncertainty of unknown parameters that allows for fast and, at the same time, precise convergence of the parameter estimates.

2. Benchmark description

The selected system consists of a CSTR where the generic reaction 2A+B->2C+D takes place. Products and unreacted species are sent to a flash drum separator where the components are ideally split in vapor-phase compounds (A and C, light elements) and liquid-phase compounds (B and D, heavy elements). Both the vapor and liquid phase are sent to distillation towers, which we will refer to as A/C and B/D tower respectively, to separate reactants and products. Also, the compound A recovered at the bottom of A/C tower is recycled and mixed with the fresh stream of A entering the reactor. The CSTR subsystem is described by 9 state variables, 2 of which (the liquid level and the reactor temperature) are measured. On the other hand, the A/C tower is described by 30 state variables, 3 of which are measured (temperature of the liquid holdup on tray 7 and top and bottom compositions). Finally, the B/D tower is described by 46 state variables, 4 of which are measured (temperature on the trays 12 and 34; top and bottom compositions). As illustrated in Figure 1, the three subsystems are coupled through interconnection variables (flow rate, composition and temperature) The mathematical model consists of mass and energy balances for reactor, unit operations, and recycle stream, as discussed e.g., in (Luyben, Luyben, 1997; Buzzi-Ferraris, Manenti, 2009), leading to a sparse, partially-structured ordinary differential equation system, which can be represented in a centralized form (i.e., considering the overall model as a unique system) using a state space model of the type:

$$\begin{cases} \dot{x}(t) = & f\left(x(t), u(t)\right) + v_1(t) \\ y(t) = & h\left(x(t), u(t)\right) + v_2(t) \end{cases} \tag{1}$$

$x(t)$ and $u(t)$ are the state and the input vectors, respectively, while $y(t)$ is the vector of measured variables. The terms $v_1(t)$ and $v_2(t)$ have been introduced to account for the presence of unknown phenomena, such as system perturbations and unmodelled chemical-physical phenomena (i.e., $v_1(t)$) and measurement noise (i.e., $v_2(t)$), and are assumed to be independent Gaussian white noises with diagonal covariance matrices $Q \in R^{85\times85}$ and $R \in R^{9\times9}$, respectively.

In view of the clear physically-based system decomposability into three subsystems and in view of the presence of interconnection variables, the input, state, and output vectors, respectively, can be partitioned into non-overlapping low order input, state, and output sub-vectors $u_i(t)$, $x_i(t)$, and $y_i(t)$, respectively, with i=1,2,3, each corresponding to a subsystem (see, e.g., Farina *et al* 2010, 2011). By partitioning the model (1) into three sub-models, we obtain an equivalent set of three sub-systems:

$$\begin{cases} \dot{x}_i(t) = & f_i\left(x_i(t), u_i(t), \{x_j(t)\}_{j\neq i}\right) + v_{1i}(t) \\ y_i(t) = & h_i\left(x_i(t), u_i(t), \{x_j(t)\}_{j\neq i}\right) + v_{2i}(t) \end{cases} \tag{2}$$

where the possible effect of the subsystem $j \neq i$ upon subsystem i is accounted for, since $x_j(t)$ is an argument of both $f_i(\cdot)$ and $h_i(\cdot)$. The terms $v_{1i}(t)$ and $v_{2i}(t)$ are subvectors of $v_1(t)$ and $v_2(t)$, respectively, and are assumed to be independent Gaussian white noises with diagonal covariance matrices Q_i and R_i, respectively, which, in turn, are submatrices of Q and R of suitable dimensions. The

observability property is verified (for the linearized models around the nominal steady-state conditions of the process) for all three subsystems' states $x_i(t)$ from their respective output variables $y_i(t)$. Also, observability of the state of the overall linearized system model $x(t)$ is verified from the overall measurement set $y(t)$.

3. Centralized and distributed estimation

In this paper a mixed discrete/continuous-time filter implementation has been employed, similarly to that used in (Becerra et al., 2001): specifically, predictions (i.e., *a priori* estimates) are computed by direct integration of the continuous-time system model and by neglecting the uncertainty terms, and corrections (i.e., the *a posteriori* estimates) are provided, with period T, using discretized/linearized models, similarly to more standard EKF implementations (for details see Simon, 2006). The first scope of the work is to test two different estimation schemes based on EKF. Namely,

- first a standard *centralized EKF* (cEKF) is implemented, where the model (1) is accounted for and an estimate $\hat{x}(t)$ of the state variable $x(t)$ is recursively computed based on the collective measurement vector $y(t)$;
- secondly, a *distributed EKF* (dEKF) architecture is implemented where, at each time step,
  - each subsystem computes an *a priori* estimate of the local state variable $\hat{x}_i(t)$ based on the local model (2) where piecewise constant estimates of the state variables of the neighboring subsystems $\hat{x}_j(t), j \neq i$, computed in the previous time step by the neighboring subsystems, are used as input terms;
  - each subsystem performs the a posteriori estimate of the local state variable $\hat{x}_i(t)$ using the local measurement $y_i(t)$ and the local measurement equation (2).

As discussed, the second approach actually accounts for the process as a set of separated units. This, from the computational perspective, implies that three low-order EKFs are implemented, hence reducing the computational load; from the communication side, it implies broadcasting of information among subsystems, according to a communication topology which closely follows the "information/material/energy exchange" topology illustrated in Figure 1: in our example the state estimates computed by the CSTR are sent to the local estimators for the distillation towers and the state estimates of the A/C tower are sent back to the local estimator of the CSTR reactor as per recycle stream. Here we test the two estimators with sampling time T=0.02 h. A simulation plot is shown in Figure 2, where the time evolution of the level in the CTRS is depicted, and it is compared with its estimates computed with the cEKF and the dEKF.

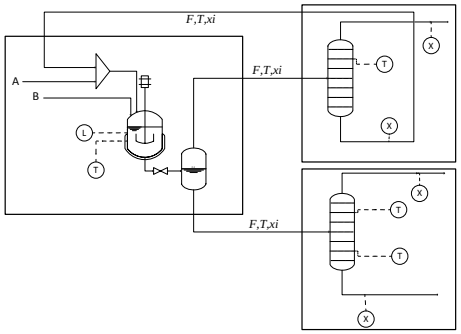

Figure 1: chemical process layout and dEKF structure.

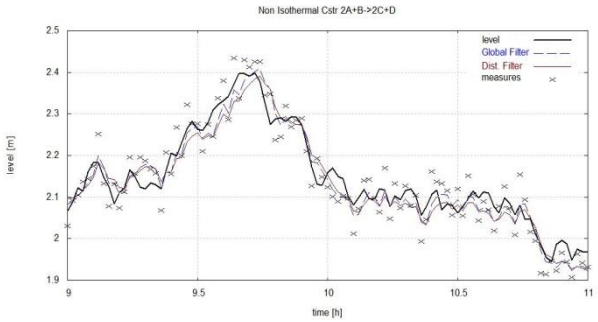

Figure 2: CSTR level (solid thick line), measurement, and estimates of the level obtained with a cEKF (dashed line) with a dEKF (solid thin line).

Table 1:normalized root mean square error (RMSE) of the estimates obtained with cEKF and dEKF.

	$x_1(t)$ (CSTR)	$x_2(t)$ (A/C tower)	$x_3(t)$ (B/D tower)	$x(t)$ (overall system)
cEKF	$1.50 \cdot 10^{-1}$	$1.78 \cdot 10^{-2}$	$5.33 \cdot 10^{-2}$	$6.35 \cdot 10^{-2}$
dEKF	$1.74 \cdot 10^{-1}$	$2.18 \cdot 10^{-1}$	$1.02 \cdot 10^{-1}$	$1.60 \cdot 10^{-1}$

Apparently, both the centralized and the distributed EKF provide accurate estimation results. Importantly, the computational time of the simulation decreases dramatically in dEKF as expected: the computational effort required is 800 to 840 s for cEKF and 130 to 160 s for dEKF, showing that the distributed EKF is significantly faster (5-6 times) than the classical approach; moreover, the gap is expected to increase with the size of the model and the complexity of the chemical process, making the dEKF the only effective technology for online estimation in many large-scale problems.

4. Application of cEKF and dEKF for parameter estimation

State estimators are a valid approach for parameter identification i.e., for providing reliable estimates of unknown model parameters. The rationale of parameter estimation methods based on this is to consider the model parameters as time-invariant state variables, and to estimate them through suitable state estimators. In this section we use EKF for the estimation of the overall heat transfer coefficient U for the CSTR, which is a key-parameter under several points of view. Actually, the possibility to estimate and monitor the trend of this parameter is essential to ensure the optimal conversion of chemical species, to prevent reactor runaways, to preserve the whole production efficiency (Fogler, 1992; Levenspiel, 1999). The CSTR sub-model has been modified by adding the equation $\dot{U}(t) = v_U(t)$ where v_U is a Gaussian white noise with variance Q_U. Figure 3 shows the results of application of EKF (results are equivalent for cEKF and dEKF). Notably, different values of Q_U correspond to different estimator convergence rates and, on the other hand, on different steady state uncertainty. Specifically, the smaller Q_U, the slower but more accurate the parameter estimation; conversely, the larger the variance, the faster but less reliable the estimation.

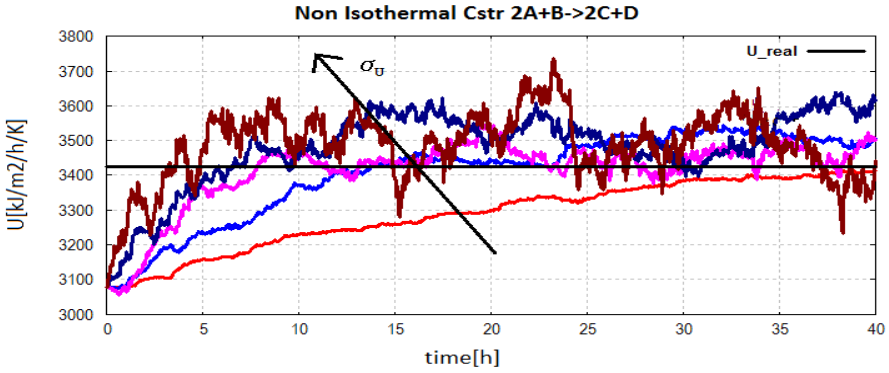

Figure 3: Dynamic behaviors of estimated parameters depend on standard deviation

In conclusion, an adaptive tuning of Q_U can be highly beneficial for providing fast convergence rates and reliable parameter estimates. An algorithm with this purpose is discussed next.

Recursive covariance estimation

In order to provide reliable state estimates, EKF generally requires the knowledge of the noise covariance matrices Q and R. Despite the estimates of these matrices can be, in some cases,

obtained by physical insight, in general they are unknown. Recently, the Autocovariance Least Squares (ALS) method has been proposed in (Odelson et al., 2006a, 2006b; Murali et al, 2007). In a few words, the ALS method consists in solving the following least square problems, with $\hat{Q}$ and $\hat{R}$ (estimates of covariance matrices Q and R, respectively) as arguments

$$Q^{opt}, R^{opt} = arg\min_{\hat{Q},\hat{R}} \left\| \gamma \begin{bmatrix} (\hat{Q})_s \\ (\hat{R})_s \end{bmatrix} - b \right\|^2 \quad \text{s.t.: } \hat{Q}, \hat{R} > 0; \;\; \hat{Q} = \hat{Q}^T; \;\; \hat{R} = \hat{R}^T \tag{3}$$

where $\left(\hat{Q}\right)_S$ and $\left(\hat{R}\right)_S$ denote vectors whose entries are the entries of $\hat{Q}$ and $\hat{R}$, respectively (i.e., $\hat{Q}$ and $\hat{R}$ "stacked"), γ is a (full column rank) matrix depending on system, and the entries of vector *b* are sampled covariances of the output estimation error, i.e., $b = \left[(\hat{C}_0)_s^T, ..., (\hat{C}_{N-1})_s^T \right]^T$ with:

$$\hat{C}_k = \frac{1}{N_d - k} \sum_{j=1}^{N_d - k} (y(t+k) - \hat{y}(t+k))(y(t) - \hat{y}(t))^T \tag{4}$$

where $\hat{y}(t)$ denotes the predicted output. In this paper we use a recursive version of this algorithm where the covariance matrices used for the EKF filter implementation at time *t*, and the covariance terms $\hat{C}_k$ are updated online at each sampling step according to the following equations

$$\begin{aligned} Q(t) = &\quad Q(t-1) + \rho_Q (Q^{opt}(t-1) - Q(t-1)) \\ R(t) = &\quad R(t-1) + \rho_R (R^{opt}(t-1) - R(t-1)) \end{aligned} \tag{5}$$

$$\hat{C}_k(t) = \hat{C}_k(t-1) + \rho_c \left(\left(y(t-k-1) - \hat{y}(t-k-1) \right) \left(y(t-1) - \hat{y}(t-1) \right)^T - \hat{C}_k(t-1) \right) \tag{6}$$

where $Q^{opt}(t-1), R^{opt}(t-1)$ are obtained by solving the ALS problem at time *t-1* and the parameters ρ_Q, ρ_R, ρ_C take values in the interval [0,1]. In this way we can obtain a smooth adaptive estimation of the covariance matrices and, at the same time, we can use an updated linearized model around the current operating point, for the computation of the weighting matrix γ.

Recursive covariance estimation of Q_U for adaptive parameter estimation

In this work, we have used the recursive ALS method detailed above for the online tuning of the variance Q_U, which basically represents the uncertainty of the estimate of parameter *U*. The idea developed in this section is to set the large initial values of Q_U to attain a rapid initial convergence to a neighborhood of the estimation. As expected (see Figure 4), the recursive ALS method reduces the values of Q_U iteratively, which at the same time guarantees a very good steady state accuracy of the parameter estimate.

5. Conclusions

The paper offered a qualitative and quantitative comparison of different advanced techniques for the state and parameter estimation in chemical processes. Specifically, global and distributed EKF implementations are described, tested, and compared according to the mandatory conciseness of the contribution. In addition, the combined EKF-ALS technique has been formulated and implemented. It is quite useful for the online reliable estimation of a wide set of parameters in chemical plants (e.g., fouling factors, cleanliness factors, unit operation efficiency). The next planned step is to apply the abovementioned novel and advanced techniques to an industrial case.

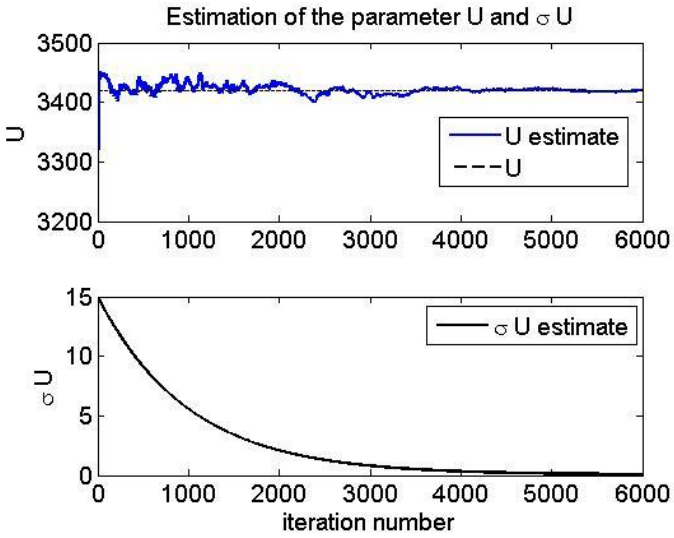

Figure 4: estimation of overall heat exchange coefficient U (up) using the proposed technique to combine EKF-ALS. The standard deviation is progressively reduced in the proposed technique (down).

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