

Set-membership Estimation using Ellipsoidal Ensembles

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Abstract: This paper is about a set-membership based state- and parameter estimation approach for nonlinear dynamic systems under the assumption that all measurement errors are bounded. In detail, we propose an outer approximation method, where the set of states and parameters that is consistent with the incoming measurement bounds is over-approximated by an intersection of ellipsoids. We introduce computationally tractable methods for propagating such ellipsoidal ensembles through dynamic systems and construct an associated recursive estimation algorithm. We also show how to select the past measurements such that the intersection problem remains tractable on long time horizons. The proposed approach is illustrated by applying it to a batch membrane process.

Keywords: Parameter and state estimation, Bounded error identification, Nonlinear system identification.

1. INTRODUCTION

The quality of model-based control, firstly, strongly depends on the accuracy of the models that are employed. This can normally be increased by the estimation of model parameters. Also, as not all the state variables are usually measured, they should be estimated to initialize the model predictions for model-based controllers. The successful estimation is inevitably impaired by the presence of measurement noise so that the estimates can only be known with uncertainty. Knowledge of guaranteed bounds of the estimation uncertainty can be exploited in robust control such that, e.g., violation of the constraints, can be avoided (Nagy and Braatz, 2003; Bertsimas et al., 2010).

Unlike the statistical estimation, *guaranteed* or *set-membership* estimation seeks to find the set of all possible state- and parameter values such that the predicted outputs match the corresponding measurements within prescribed error bounds (Schweppe, 1968; Jaulin and Walter, 1993). Thus, the set-membership estimation does not need to rely on usually unreliable approximations of the measurement error distributions and uses measurement error bounds, which are often known quite reliably or can be inferred likewise from the historical data.

Rigorous set-membership approaches use either set-based calculations (Chachuat et al., 2015) or global optimization techniques (Mukkula and Paulen, 2017; Walz et al., 2018). As the global dynamic optimization cannot tackle large-scale problems, set-based methods are more popular and generally more applicable. In general, the application of set-based methods has two ingredients: a) propagation

of the reachable set (possibly over-approximated) and b) its intersection with the (over-approximation of) measurement (error) set and over-approximation of the intersection. As these solution techniques rely heavily on over-approximation, one can conclude that the tighter the over-approximation, the lower the estimation conservatism.

The early contributions to set-membership estimation assumed linear models and used ellipsoids for set-based arithmetics (propagation, intersection, over-bounding of the intersections) to compute the enclosures of the solution of the set-membership estimation at each time step (Schweppe, 1968; Maksarov and Norton, 1996; Kurzhanski and Vályi, 1997). In Chabane et al. (2014), an approach was proposed for guaranteed parameter estimation for linear systems by minimizing the radius of the ellipsoidal estimation set. The problem of approximating the solution set by a box partition has been studied by Kieffer et al. (1998) using interval analysis. Other reachability methods include ellipsoidal calculus (Boyd et al., 1994; Kurzhanski and Varaiya, 2000), polytopic and zonotopic bounding techniques (Bitsoris, 1988) as well as general (non-)convex set propagation techniques (Chachuat et al., 2015; Villanueva et al., 2015).

This paper makes use of the propagation of an intersection of ellipsoid ensembles, where the ellipsoids represent state reachability tubes and measurement tubes. This way, a general nonlinear dynamic state- and parameter estimation problem can be treated with a moderate computational effort. We use the proposed method in the recursive settings. To improve estimation quality, we take into account several past measurements, where the considered

measurement set is propagated in time. We limit the number of past measurements to maintain computational tractability. We use a heuristic criterion to select the retained past measurements for estimation.

Notation

We use the notation L_1^n to denote the set of n -dimensional L_1 -integrable functions. The associated Sobolev space of weakly differentiable functions with L_1^n derivatives is denoted by $W_{1,1}^n$. Moreover, the set of $n \times n$ -dimensional positive semidefinite matrices is denoted by \mathbb{S}_+^n . For any given vector $q \in \mathbb{R}^n$ and any matrix $Q \in \mathbb{S}_+^n$ (with its Cholesky factor $Q^{\frac{1}{2}}$), the notation

$$\mathcal{E}(q, Q) = \left\{ q + Q^{\frac{1}{2}}v \mid v^\top v \leq 1 \right\},$$

is used to denote the associated ellipsoid. We additionally use the shorthand $\mathcal{E}(Q) = \mathcal{E}(0, Q)$ for centered ellipsoids.

2. SET-MEMBERSHIP ESTIMATION

This section briefly reviews the concept of set-membership based state and parameter estimation for uncertain nonlinear processes. Here, we focus in particular on methods that are based on ellipsoidal calculus.

2.1 Uncertain Dynamic Processes

This paper is concerned with nonlinear processes

$$\dot{x}(t) = f(x(t), p) \quad \text{with} \quad x(0) \in \mathbb{X}_0, \quad (1)$$

on a finite time horizon, $t \in [0, T]$. Here, $x : [0, T] \rightarrow \mathbb{R}^{n_x}$ denotes the state trajectory with initial value $\mathbb{X}_0 \subseteq \mathbb{R}^{n_x}$ denotes a compact set of potential initial states. Moreover, $p \in \mathbb{P}_0 \subseteq \mathbb{R}^{n_p}$ denotes unknown parameters or unmeasured disturbances. Throughout this paper we assume that $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \rightarrow \mathbb{R}^{n_x}$ is at least jointly continuous in all its variables and Lipschitz continuous in x . Moreover, we assume that \mathbb{P}_0 is a given compact set.

The developments in this paper can, almost trivially, be extended to uncertain processes whose dynamics depend on an exogenous disturbance signal. Here, the only assumption needed is that the disturbance is L_1 -integrable and takes its values on a known compact set.

2.2 Set Membership based State- and Parameter Estimation

The goal of this paper is to develop methods for computing bounds on the estimated states and parameters by taking measurements into account. Here, we assume that the measurements of n_y outputs

$$y_k = h(x(t_k), p) + v_k, \quad (2)$$

are taken at the time points $t_1, t_2, \dots, t_m \in [0, T]$. The measurement error, $v_k \in \mathbb{V}$ is assumed to be bounded by a given compact set $\mathbb{V} \subseteq \mathbb{R}^{n_y}$. Then, the set of states and parameters which are consistent with the measurements—in a set-membership sense—is given by

$$Z(t) = \left\{ (\xi, p) \in \mathbb{R}^{n_x} \times \mathbb{P}_0 \mid \begin{array}{l} \exists x \in W_{1,1}^{n_x} : \forall \tau \in [0, t], \\ \dot{x}(\tau) = f(x(\tau), p), \\ x(0) \in \mathbb{X}_0, \quad x(t) = \xi \\ \forall k \in \{1, \dots, m\}, t_i \in [0, t] : \\ h(x(t_k), p) - y_k \in \mathbb{V}, \end{array} \right\}. \quad (3)$$

Here, we additionally set $t_0 = 0$ and $t_{m+1} = T$. Therefore, the reachable set

$$X(t) = \{ \xi \in \mathbb{R}^{n_x} \mid \exists p \in \mathbb{R}^{n_p} : (\xi, p) \in Z(t) \}, \quad (4)$$

as well as the associated set of consistent parameters

$$P(t) = \{ p \in \mathbb{R}^{n_p} \mid \exists \xi \in \mathbb{R}^{n_x} : (\xi, p) \in Z(t) \}, \quad (5)$$

are projections of $Z(t)$ set onto the state and parameter space, respectively.

3. PROPAGATION AND UPDATES OF ELLIPSOIDAL ENSEMBLES

Since an exact characterization of $Z(t)$ is seldom possible, the focus of this section is on computing enclosures using ellipsoidal techniques, as introduced by Kurzhanski and Vályi (1997), further extended by Houska et al. (2012).

3.1 Propagation of Ellipsoidal Ensembles

One of the key ideas of this paper is to propagate an ensemble of ellipsoids that collectively enclose $Z(t) \subseteq \mathbb{R}^{n_z}$. That is, our goal is to construct sets $\bar{Z}(t)$ satisfying

$$\bar{Z}(t) = \bigcap_{i \in \{1, \dots, N\}} \mathcal{E}(q_i(t), Q_i(t)) \supseteq Z(t), \quad \forall t \in [0, T]. \quad (6)$$

Here, $q_i : [0, T] \rightarrow \mathbb{R}^{n_z}$ and $Q_i : [0, T] \rightarrow \mathbb{S}_+^{n_z}$, with $n_z = n_x + n_p$, denote the central path and the time-varying shape matrix of the ellipsoid $\mathcal{E}(q_i(t), Q_i(t))$. As we shall see in the following, these functions can be constructed by a systematic application of ellipsoidal calculus.

The first step towards the construction of these functions is to start with outer approximations,

$$\bar{Z}(0) = \bigcap_{i \in \{1, \dots, N\}} \mathcal{E}(q_i^0, Q_i^0) \supseteq \mathbb{X}_0 \times \mathbb{P}_0. \quad (7)$$

Notice that such enclosures can always be constructed, as both \mathbb{X}_0 and \mathbb{P}_0 are assumed to be compact.

The main idea of ellipsoidal methods is to construct a system of differential equations, such that, if these are satisfied by q_i and Q_i , we have $Z(t) \subseteq \mathcal{E}(q_i(t), Q_i(t))$ for all $t \in [0, T]$. Before these conditions are provided, we introduce the vector-valued auxiliary functions

$$\varphi_1(q) = \begin{pmatrix} f(q_1, q_2) \\ 0 \end{pmatrix} \quad \text{with} \quad q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad (8)$$

$$\varphi_3(\kappa, q, Q, r, R) = \kappa Q R^{-1} (r - q). \quad (9)$$

where $q_1 \in \mathbb{R}^{n_x}$ and $q_2 \in \mathbb{R}^{n_p}$. Likewise, we introduce the matrix-valued auxiliary functions

$$\Phi_1(A, B, Q) = \begin{pmatrix} A & B \\ 0 & \mathbb{1} \end{pmatrix} Q + Q \begin{pmatrix} A^\top & 0 \\ B^\top & \mathbb{1} \end{pmatrix}, \quad (10)$$

$$\Phi_2(\lambda, A, B, q, Q) = \frac{1}{\lambda} Q + \lambda \begin{pmatrix} \Omega(q, Q, A, B) & 0 \\ 0 & 0 \end{pmatrix}, \quad (11)$$

$$\Phi_3(\kappa, q, Q, r, R) = \kappa Q \left[I - R^{-1} Q - \|q - r\|_{R^{-1}, 2}^2 \right]. \quad (12)$$

Notice that φ_1, φ_3 as well as Φ_1, Φ_2 , and Φ_3 are defined for all $q, r \in \mathbb{R}^{n_z}$, all matrices $Q, R \in \mathbb{S}_+^{n_z}$, $A \in \mathbb{R}^{n_x \times n_x}$ and $B \in \mathbb{R}^{n_x \times n_p}$ as well as all scalars κ and $\lambda > 0$. In this context, we have additionally introduced a function

$$\Omega : \mathbb{R}^{n_z} \times \mathbb{S}_+^{n_z} \times \mathbb{R}^{n_x \times n_x} \times \mathbb{R}^{n_x \times n_p} \rightarrow \mathbb{S}_+^{n_z}, \quad (13)$$

which is assumed to be constructed such that it satisfies

$$f(x, p) - f(q_1, q_2) - (A \ B) (z - q) \in \mathcal{E}(\Omega(q, Q, A, B)), \quad (14)$$

for all $z = (x^\top, p^\top)^\top \in \mathcal{E}(q, Q)$ and $q = (q_1^\top, q_2^\top)^\top \in \mathbb{R}^{n_z}$, as well as matrices $Q \in \mathbb{S}_+^{n_z}$, $A \in \mathbb{R}^{n_x \times n_x}$, and $B \in \mathbb{R}^{n_x \times n_p}$.

The following theorem presents a generalization of a result for ellipsoidal propagation, originally developed for taking a-priori enclosures into account in reachability analysis Feng et al. (2020); Villanueva et al. (2019).

Theorem 1. Let the functions $q_1, \dots, q_N : \mathbb{R} \rightarrow \mathbb{R}^{n_z}$ and $Q_1, \dots, Q_N : \mathbb{R} \rightarrow \mathbb{S}_+^{n_z}$ be continuously differentiable and satisfy

$$\begin{aligned} \dot{q}_i(t) &= \varphi_1(q_i(t)) \\ &+ \sum_{k \neq i} \varphi_3(\kappa_{i,k}(t), q_k(t), Q_i(t), q_k(t), Q_k(t)), \end{aligned} \quad (15a)$$

$$\begin{aligned} \dot{Q}_i(t) &= \Phi_1(A_i(t), B_i(t), Q_i(t)) \\ &+ \Phi_2(\lambda_i(t), A_i(t), B_i(t), q_i(t), Q_i(t)) \\ &+ \sum_{k \neq i} \Phi_3(\kappa_{i,k}(t), q_i(t), Q_i(t), q_k(t), Q_k(t)), \end{aligned} \quad (15b)$$

$$q_i(0) = q_i^0 \quad \text{and} \quad Q_i(0) = Q_i^0, \quad (15c)$$

for all $t \in [0, T]$ and for any given integrable functions $\lambda_i : \mathbb{R} \rightarrow \mathbb{R}_+$, $\kappa_i : \mathbb{R} \rightarrow \mathbb{R}_+^{N-1}$, $A_i : \mathbb{R} \rightarrow \mathbb{R}^{n_x \times n_x}$, and $B_i : \mathbb{R} \rightarrow \mathbb{R}^{n_x \times n_p}$ for every index $i \in \{1, \dots, N\}$. Then,

$$\overline{Z}(t) = \bigcap_{i \in \{1, \dots, N\}} \mathcal{E}(q_i(t), Q_i(t)) \supseteq Z(t), \quad (16)$$

for all $t \in [0, T]$.

Proof. The statement of this theorem has been established for the case $N = 2$ in Feng et al. (2020, Thm. 3). The proof of the fact that the above statement also holds for any number intersected ellipsoids is, however, straightforward. Note that one can apply the Thm. 3 from Feng et al. (2020) to recursively intersect all ellipsoids pairwise until a bound on all N ellipsoids is obtained—leading directly to the statement of this theorem. \square

The construction of ellipsoids, or in this case ellipsoidal ensembles, enclosing the reachable set requires fixing the degrees of freedom introduced through the functions A_i , B_i , λ_i and κ_i , as well as constructing an appropriate nonlinearity bounder Ω . Here, we set A_i and B_i as

$$A_i(t) = \frac{\partial}{\partial x} f(q_{i,1}(t), q_{i,2}(t)), \quad (17)$$

$$B_i(t) = \frac{\partial}{\partial p} f(q_{i,1}(t), q_{i,2}(t)). \quad (18)$$

Here, the vectors $q_{i,1}(t) \in \mathbb{R}^{n_x}$ and $q_{i,2}(t) \in \mathbb{R}^{n_p}$ satisfy $q_i = (q_{i,1}(t)^\top, q_{i,2}(t)^\top)^\top$. Notice that, as long as f is at least Lipschitz continuous in x , we can always construct Ω (see, e.g. Houska et al., 2012; Villanueva et al., 2017). For example, one can consider Lipschitz constants or Hessian bounds (if f is twice continuously differentiable). The remaining degrees of freedom are chosen in such a manner that a suitable performance measure is optimized. Here, we minimize a Lagrangian functional involving the determinants of the shape matrices of the ellipsoids in the ensemble. That is, we solve

$$\inf_{\substack{q_1, \dots, q_N, \\ Q_1, \dots, Q_N, \\ \lambda_1, \dots, \lambda_N, \\ \kappa_1, \dots, \kappa_N}} \int_0^T \sum_i^N \det(Q_i(t)) dt \quad \text{s.t.} \quad \begin{cases} \forall t \in [0, T], \\ \forall i \in \{1, \dots, N\}, \\ \text{Eqs. (15) hold,} \\ \lambda_i(t) > 0, \kappa_i(t) \geq 0. \end{cases} \quad (19)$$

Notice that other constructions are also possible. For example, Villanueva et al. (2015) proposed an approach for constructing the right-hand side function on-the-fly, for the case $N = 1$. This approach relies on polynomial models together with heuristics designed to minimize the trace of the right-hand side function for choosing the remaining degrees of freedom.

3.2 Recursive Updates of Ellipsoidal Ensembles

Having the ability to propagate ellipsoids continuously in time, such that their intersection encloses the reachable sets $Z(t)$, we can proceed to summarize the set-membership estimation procedure. Each (uncertain) measurement can be transformed into an equivalent ellipsoid in the state space. The main idea of the proposed estimation procedure is then to recursively amend the ellipsoidal ensemble with the measurement ellipsoids. As this will mean an increase in computational burden of propagation, one can discard one of the N (past) ellipsoids before the amendment.

We will treat the case when $n_y = n_x$. If $n_y > n_x$, the outputs can be introduced as dummy states (see the case study in Section 4). If $n_y < n_x$, the output vector can be augmented by dummy outputs such that $\overline{Z}(t_k) \supseteq Z(t_k)$.

Let us assume the availability of a (measurement ellipsoid) set $\mathcal{E}(z_k, V_k) \supseteq h^{-1}(\mathbb{V} \oplus y_k)$. Once a new measurement at time t_k becomes available, the ellipsoidal ensemble can be updated. Note that a scheme that would mimic a traditional recursive-estimation settings would use $N = 2$ and replace the measurement ellipsoid propagated from time $k - 1$ by the (new) measurement ellipsoid at time k , i.e. $\mathcal{E}(z_k, V_k) \rightarrow \mathcal{E}(q_2(t_k), Q_2(t_k))$.

3.3 Moving Horizon Variant

As we possess the freedom of propagating (any number) N ellipsoids, we can retain arbitrary past information that improves the quality of estimation and keep it in the ensemble, similar to Artzová and Paulen (2019) in the set-membership parameter estimation context. We propose here a heuristic based on volume of intersection, provided by an ellipsoidal intersection formula from Ros et al. (2002). This scheme evaluates the intersection volume of all the possible $N + 1$ ensembles, i.e. combinations of N (past) ensemble ellipsoids with the current measurement ellipsoid. The retained N -ellipsoid ensemble takes the smallest volume of the intersection.

4. CASE STUDY

We study the performance of the proposed methodology on the case study of a batch membrane process. We will turn our attention towards the problem of state estimation, taking into account the uncertainty in the parameters that are treated as bounded time-varying disturbance.

4.1 Plant Description

The membrane process under the study is a batch diafiltration (see Fig. 1). We use the same plant as in Sharma et al. (2019). The batch is commenced with initial volume

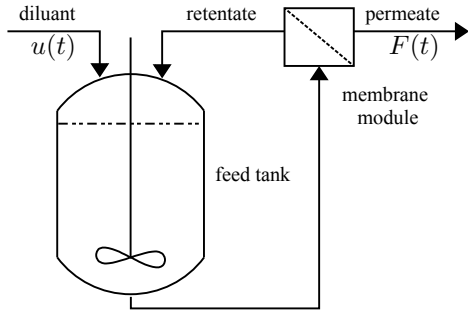


Fig. 1. Schematic representation of the membrane plant. V_0 of the filtered solution in the tank. The solution initially contains a diluant (solvent) and there-in dissolved species: micro-solute (low molecular weight component) and macro-solute (high molecular weight component). During the operation, the pump forces the feed from the tank into the membrane module, where the solution separates into two streams: a micro-solute-rich stream that passes through the membrane—a so-called permeate—and the retained stream—a so-called retentate. Permeate leaves the system with the flow rate F . The retentate stream is circulated back into the feed tank. The plant operates under constant transmembrane pressure and constant temperature (Sharma et al., 2019). The process control is achieved by adjusting the flow rate of solute-free diluant (water) to the feed tank. Control variable α is defined as a ratio between the inflow of diluant to the feed tank and the outflow of permeate F .

4.2 Process Model

The mass balances of the concentrations of the dissolved species are given by (Sharma et al., 2019)

$$\dot{c}_1 = c_1^2 \frac{F(c_1, c_2)}{c_{1,0} V_0} (1 - \alpha), \quad c_1(0) = c_{1,0}, \quad (20a)$$

$$\dot{c}_2 = -c_1 c_2 \frac{F(c_1, c_2)}{c_{1,0} V_0} \alpha, \quad c_2(0) = c_{2,0}, \quad (20b)$$

$$\text{with } F(c_1(t), c_2(t), k, c_{\text{lim}}, \gamma) = k \ln \left(\frac{c_{\text{lim}}}{c_1(t) c_2^\gamma(t)} \right), \quad (20c)$$

where c_1 and c_2 denote the concentrations of macro- and micro-solute with initial conditions $c_{1,0}$ and $c_{2,0}$, respectively, k is the mass-transfer coefficient, c_{lim} is the limiting concentration of the macro-solute, and γ is a dimensionless non-ideality factor.

As we can measure both the concentrations and the permeate flowrate, we reformulate the dynamic model as

$$\underbrace{\begin{pmatrix} \dot{c}_1(t) \\ \dot{c}_2(t) \\ \dot{F}(t) \end{pmatrix}}_x = \begin{pmatrix} \frac{c_1(t)^2}{c_{1,0} V_0} F(t) (1 - \alpha(t)) \\ -\frac{c_1(t) c_2(t)}{c_{1,0} V_0} F(t) \alpha(t) \\ \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}^\top \begin{pmatrix} 1 - \alpha(t) \\ -\alpha(t) \end{pmatrix} \frac{c_1(t) F(t)}{c_{1,0} V_0} \end{pmatrix}, \quad (21)$$

$$\begin{pmatrix} c_1(0) \\ c_2(0) \\ F(0) \end{pmatrix} = \begin{pmatrix} c_{1,0} \\ c_{2,0} \\ F(c_{1,0}, c_{2,0}, p) \end{pmatrix}, \quad (22)$$

where $x(t) = (c_1, c_2(t), F(t))^\top$ and the following reparametrization, using the logarithmic identities, is introduced

$$F(c_1(t), c_2(t), p) = p_0 + p_1 \log c_1(t) + p_2 \log c_2(t), \quad (23)$$

Table 1. Model parameters, their bounds, and problem attributes.

Parameter/Attribute	Value	Unit
$c_{1,0}$	50	g/L
$c_{2,0}$	5.3	g/L
V_0	100	L
k	8.33×10^{-4}	L/s
c_{lim}	3×10^3	g/L
γ	0.1	-
$[c_{1,0}^L, c_{1,0}^U]$	[49.5, 50.5]	g/L
$[c_{2,0}^L, c_{2,0}^U]$	[4.5, 5.5]	g/L
$[k^L, k^U]$	$[5.17 \times 10^{-4}, 1.10 \times 10^{-3}]$	L/s
$[c_{\text{lim}}^L, c_{\text{lim}}^U]$	$[0.6589 \times 10^3, 4.1163 \times 10^3]$	g/L
$[\gamma^L, \gamma^U]$	[-0.11, 0.17]	-
$\alpha(t)$	0	-

Table 2. Simulated scenarios.

	N	Tube selection	CPU [s]
Scenario 1	2	✗	0.2
Scenario 2	2	✓	0.2
Scenario 3	3	✓	1.0
Scenario 4	4	✓	4.1
Scenario 5	5	✓	10.5

The construction of an explicit nonlinearity estimate for the dynamic system (21) is established in Appendix A.

The studied setup is taken from our earlier experimental work (Sharma et al., 2018). The experimental data were used for a set-membership parameter estimation in Paulen et al. (2018). The resulting parameter bounds are used in this work. The summary of the problem parameters is given in Tab. 1.

4.3 Results

We consider new measurements to be available at each sampling period of the plant that is $T_s := 1$ s. We assume a realistic measurement noise for the measurements of concentrations (± 0.5 g/L) and of the permeate flowrate (± 0.5 L/h). To study the computational aspects and estimation performance of the proposed approach, we consider several scenarios summarized in Tab. 2. The scenarios differ in the number of intersected tubes, where one tube represents the model predictor and the rest of the tubes are taken from the past measurements. In Scenario 1, we use a standard recursive scheme, where the new measurement (tube) obtained at time k replaces the past measurement from time $k-1$. In Scenarios 2–5, the number of considered measurements varies and a selection procedure is included to heuristically decide about $N-1$ measurements (up to time k) that are retained for the estimation. The heuristics for selecting the retained measurements that is used in this paper is based on ellipsoidal intersection formula (Ros et al., 2002).

The proposed method was implemented in CasADi (Andersson et al., 2019) using its Matlab interface via MATLAB 2018b. We conducted 20 simulations for each scenario with different realizations of the measurement noises. Table 2 also shows the average computational effort in terms of CPU time obtained at a standard desktop worksta-

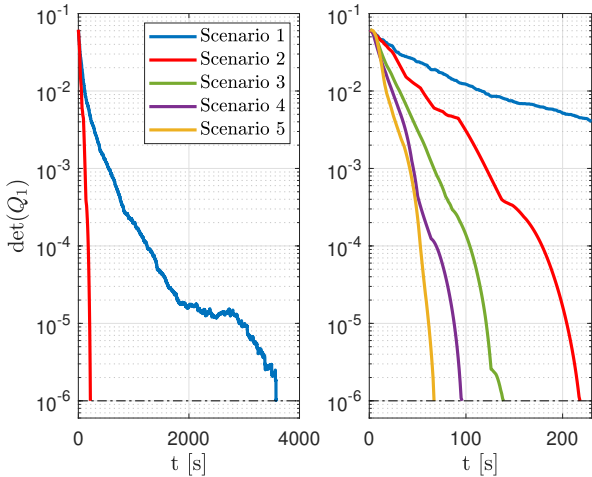


Fig. 2. Evolution of the estimation quality for each scenario with average values.

tion. The CPU times are not optimized and are relatively high as we exploit sequential approach to solve (19). We can clearly notice the increasing computational burden as the number of considered measurements increases. This effort increase is expected and similar to moving-horizon estimation (Rao et al., 2003). We can also conclude that Scenarios 1–3 are real-time feasible taking into account the sampling period. Though the sampling period can be prolonged for the problem at hand up to one minute if necessary as the batch operation would normally last several hours for the considered plant.

We report the results of the proposed approach in Figs. 2–4 via assessing the estimation performance by evaluating the $\det(\cdot)$ of the ellipsoidal shaping matrix Q_1 , which is related to the volume of the estimation set. We consider the estimation to be successful once $\det(Q_1) \leq 10^{-6}$. At such a point, we terminate the estimation procedure.

Figure 2 shows for each scenario the average evolutions over time of the determinant of the ellipsoidal shaping matrix Q_1 . The figure is split into two plots for clarity of the presentation. We can observe that the time necessary to reach the desired estimation performance is around 3,500 seconds for Scenario 1. For Scenario 2, in comparison with Scenario 1, the desired estimation performance is reached in much shorter time. This difference stems from the selection of appropriate measurements to retain for further estimation. In this the decision is between retaining a past measurement and using the newly obtained one. The right-hand plot in Fig. 2 shows that the number of tubes (retained measurements) influences the rate of convergence of the estimation procedure, where, as expected, the more tubes, faster the convergence.

Figure 3 shows the evolution of the determinant of the ellipsoidal shaping matrix Q_1 for all conducted simulations in Scenario 2. Minimum, average, and maximum are highlighted. We can clearly see that the variance in the convergence rate is quit high, i.e., the desired estimation quality is reached within [150, 300] seconds. This is attributed to the actual realization of the measurement noise and was shown previously in Artzová and Paulen (2019).

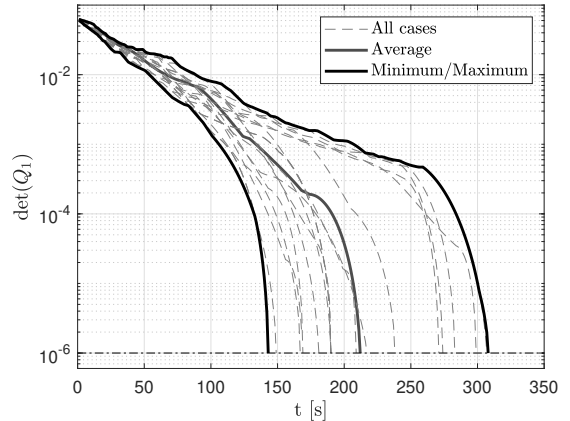


Fig. 3. Evolution of the estimation quality for Scenario 2.

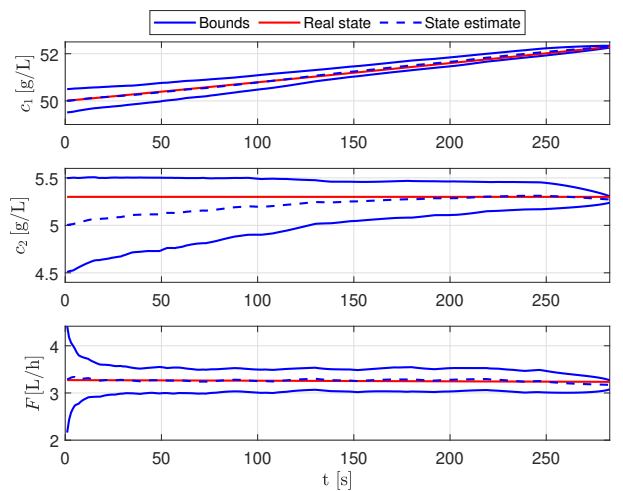


Fig. 4. Evolution of the bounds, real states and state estimates for Scenario 2.

Figure 4 shows the estimation performance for the state variables c_1 , c_2 and F for one of the simulation runs of Scenario 2. The blue solid lines represent the set-membership bounds (ellipsoids projected to 1D). The red solid line represents the real state value and the blue dashed line represents state estimate obtained via the proposed method. Real state and state estimate gradually converge to each other while the bounds shrink. At the end of the time window, the estimation almost yields a single point and can be thus claimed as successful.

5. CONCLUSION

In this paper, a new approach has been proposed to set-membership state- and parameter estimation for nonlinear dynamic systems. The proposed theory bounds the set of the states and parameters that are consistent with the output measurement by intersection of ellipsoids, which originate from uncertainty propagation and from the observed (uncertain) measurements. The potential of this approach, in terms of estimation performance and computational effort is illustrated on an example of a batch membrane process. The results suggest that a proper selection of the past measurements to enhance the standard recursive estimation is crucial for the good estimation quality.

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REFERENCES

- Andersson, J.A.E., Gillis, J., Horn, G., Rawlings, J.B., and Diehl, M. (2019). CasADi – A software framework for nonlinear optimization and optimal control. *Mathematical Programming Computation*, 11(1), 1–36.
- Artzová, P. and Paulen, R. (2019). Moving-horizon guaranteed parameter estimation. *IFAC-PapersOnLine*, 52(1), 112–117.
- Bertsimas, D., Brown, D.B., and Caramanis, C. (2010). Theory and applications of robust optimization. *SIAM Review*, 53, 464–501.
- Bitsoris, G. (1988). On the positive invariance of polyhedral sets for discrete-time systems. *Systems & Control Letters*, 11(3), 243 – 248.
- Boyd, S., El Ghaoui, L., Feron, E., and Balakrishnan, V. (1994). *Linear Matrix Inequalities in System and Control Theory*. SIAM.
- Chabane, S.B., Maniu, C.S., Alamo, T., Camacho, E., and Dumur, D. (2014). A new approach for guaranteed ellipsoidal state estimation. *IFAC Proceedings Volumes*, 47(3), 6533 – 6538. 19th IFAC World Congress.
- Chachuat, B., Houska, B., Paulen, R., Perić, N.D., Rajyaguru, J., and Villanueva, M.E. (2015). Set-theoretic approaches in analysis, estimation and control of nonlinear systems. *IFAC-PapersOnLine*, 48(8), 981–995.
- Feng, X., Villanueva, M.E., and Houska, B. (2020). Backward-forward reachable set splitting for state-constrained differential games. *Automatica*, 111, 108602.
- Houska, B., Logist, F., Van Impe, J., and Diehl, M. (2012). Robust optimization of nonlinear dynamic systems with application to a jacketed tubular reactor. *Journal of Process Control*, 22(6), 1152–1160.
- Jaulin, L. and Walter, E. (1993). Set inversion via interval analysis for nonlinear bounded-error estimation. *Automatica*, 29, 1053–1064.
- Kieffer, M., Jaulin, L., and Walter, E. (1998). Guaranteed recursive nonlinear state estimation using interval analysis. *Proceedings of the 37th IEEE Conference on Decision and Control*, 4, 3966–3971.
- Kurzhanski, A. and Vályi, I. (1997). *Ellipsoidal calculus for estimation and control*. Birkhäuser.
- Kurzhanski, A.B. and Varaiya, P. (2000). Ellipsoidal techniques for reachability analysis. In N. Lynch and B.H. Krogh (eds.), *Hybrid Systems: Computation and Control*, 202–214. Springer, Berlin, Heidelberg.
- Makarov, D. and Norton, J.P. (1996). State bounding with ellipsoidal set description of the uncertainty. *International Journal of Control*, 65, 847–866.
- Mukkula, A.R.G. and Paulen, R. (2017). Model-based design of optimal experiments for nonlinear systems in the context of guaranteed parameter estimation. *Computers & Chemical Engineering*, 99, 198–213.
- Nagy, Z.K. and Braatz, R.D. (2003). Robust nonlinear model predictive control of batch processes. *AIChE Journal*, 49(7), 1776–1786.
- Paulen, R., Sharma, A., and Fikar, M. (2018). Dynamic real-time optimization of batch membrane processes using pontryagin’s minimum principle. In *28th European Symposium on Computer Aided Process Engineering*, volume 28, 1045–1050. Elsevier.
- Rao, C.V., Rawlings, J.B., and Mayne, D.Q. (2003). Constrained state estimation for nonlinear discrete-time systems: stability and moving horizon approximations. *IEEE Trans Automat Contr*, 48(2), 246–258.
- Ros, L., Sabater, A., and Thomas, F. (2002). An ellipsoidal calculus based on propagation and fusion. *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, 32(4), 430–442.
- Schweppe, F.C. (1968). Recursive state estimation: Unknown but bounded errors and system inputs. *IEEE Transactions on Automatic Control*, 13, 22–28.
- Sharma, A., Valo, R., Kalúz, M., Paulen, R., and Fikar, M. (2018). Experimental validation and comparison of time-optimal and industrial strategy for membrane separation process. In *Preprints of the 9th Vienna International Conference on Mathematical Modelling, Vienna, Austria, February 21-23, 2018*, 869–874. IFAC.
- Sharma, A., Valo, R., Kalúz, M., Paulen, R., and Fikar, M. (2019). Implementation of optimal strategy to economically improve batch membrane separation. *Journal of Process Control*, 76, 155–164.
- Villanueva, M.E., Feng, X., Paulen, R., Chachuat, B., and Houska, B. (2019). Convex enclosures for constrained reachability tubes. *IFAC-PapersOnLine*, 52(1), 118–123.
- Villanueva, M.E., Houska, B., and Chachuat, B. (2015). Unified framework for the propagation of continuous-time enclosures for parametric nonlinear odes. *Journal of Global Optimization*, 62(3), 575–613.
- Villanueva, M.E., Quirynen, R., Diehl, M., Chachuat, B., and Houska, B. (2017). Robust mpc via min–max differential inequalities. *Automatica*, 77, 311–321.
- Walz, O., Djelassi, H., Caspari, A., and Mitsos, A. (2018). Bounded-error optimal experimental design via global solution of constrained min-max program. *Computers & Chemical Engineering*, 111, 92–101.

Appendix A. NONLINEARITY ESTIMATES

The explicit nonlinearity estimates for the system (21) can be constructed using the following expressions:

$$n_1(q, Q) := (1 - \alpha)Q_{1,1}\sqrt{Q_{3,3}} + |q_3|(1 - \alpha)Q_{1,1}, \quad (\text{A.1})$$

$$+ 2(1 - \alpha)|q_1|\sqrt{Q_{1,1}Q_{3,3}}, \quad (\text{A.2})$$

$$n_2(q, Q) := \alpha\sqrt{Q_{1,1}Q_{2,2}Q_{3,3}} + \alpha|q_3|\sqrt{Q_{1,1}Q_{2,2}}, \quad (\text{A.3})$$

$$+ \alpha|q_2|\sqrt{Q_{1,1}Q_{3,3}} + \alpha|q_1|\sqrt{Q_{2,2}Q_{3,3}}, \quad (\text{A.4})$$

$$n_3(q, Q) := ((1 - \alpha)|p_1| + \alpha|p_2|)\sqrt{Q_{1,1}Q_{3,3}}, \quad (\text{A.5})$$

$$\Omega(q, Q) = \frac{1}{c_{1,0}^2 V_0^2} \begin{pmatrix} n_1^2(q, Q) & 0 & 0 \\ 0 & n_2^2(q, Q) & 0 \\ 0 & 0 & n_3^2(q, Q) \end{pmatrix}. \quad (\text{A.6})$$