Efficient Polynomial-Time Outer Bounds on State Trajectories for Uncertain Polynomial Systems Using Skewed Structured Singular Values

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***Abstract*—Outer bounds for the evolution of state trajectories of uncertain systems are useful for many purposes such as robust control, state and parameter estimation, model invalidation, safety evaluation, fault diagnosis, and experimental design. Obtaining tight outer bounds is, however, a challenging task. This technical note proposes a new approach to obtaining such bounds for discrete-time polynomial systems with uncertain initial state, uncertain parameters, and bounded disturbances. To obtain outer bounds, the nonlinear map describing the uncertain dynamical system is represented via linear fractional transformation. The bounds on the trajectories are obtained by computing polynomial-time upper and lower bounds for the skewed structured singular value of the linear fractional transformation. Algorithms with different tradeoffs between computational complexity and conservatism are outlined. The tradeoffs as well as efficiency of the approach are illustrated in a numerical example, which shows small conservatism of the obtained bounds.**

***Index Terms*— Discrete-time polynomial systems.**

I. INTRODUCTION

Outer bounds on the evolution of the states of nonlinear dynamical systems subject to disturbances and uncertain initial conditions play an important role in many control and analysis problems. Examples are model invalidation and parameter estimation [2], [3], model analysis [4], fault diagnosis [5], [6], robust model predictive control [7]–[10], the analysis of batch and semibatch processes [11], [12], and the safety analysis of plant operations [13]. The computation of tight outer bounds on the state is challenging in general. Various approaches to calculate outer bounds for the time evolution of the states in dynamical systems have been developed, e.g., based on set-based methods [14]–[16]; interval methods [17]–[19]; relaxation and feasibility reformulation [20], [21]; and barrier certificates [2].

This technical note proposes a new approach for computing tight outer bounds for discrete-time polynomial systems with uncertain parameters, initial conditions, and bounded disturbances. To bound the evolution of the states, the map defining the system dynamics is reformulated as a linear fractional transformation (LFT) [22]. Outer bounds on the states for each time instant are then computed employing *skewed structured singular values*, for which upper and lower bounds can be computed in polynomial time [23], [24] (note that the exact computation is NP-hard cf. [25]). An algorithm and two variants are proposed that differ in the tradeoff between computational complexity versus conservatism. Furthermore, it is described how to modify the overall approach to include the effect of time-varying uncertain parameters and bounded disturbances. Besides providing a new viewpoint on how to calculate tight bounds, the key advantages of the approach are an efficient and unified treatment of fixed and time-varying uncertain parameters, uncertain initial conditions, and bounded disturbances.

The technical note is organized as follows. Section II provides the notations and mathematical background including a theorem on the skewed structured singular value that is critical to understanding the main idea behind the proposed approach. Section III mathematically defines the considered problem. Section IV presents the approach to tightly outer bound the state trajectories. The algorithms are applied and compared in a numerical example in Section V. Section VI concludes the technical note.

II. MATHEMATICAL PRELIMINARIES

The maximum singular value of a matrix N is denoted by $\bar{\sigma}(N) = \sqrt{\lambda_{\max}(N^*N)}$, where "$N^*$" denotes the conjugate transpose of the matrix N, $\lambda_{\max}(N)$ denotes its maximum eigenvalue, and $|N|$ denotes its determinant. The uncertain nonlinear system will be reformulated using a (lower) Linear Fractional Transformation (LFT), which is defined for a block matrix $N = \left[\begin{array}{c|c} N_{11} & N_{12} \\ \hline N_{21} & N_{22} \end{array}\right]$ and a structured perturbation matrix Δ by $F_u(N, \Delta)$ and given by $F_u(N, \Delta) = N_{22} + N_{21}\Delta_u(I - N_{11}\Delta_u)^{-1}N_{12}$, cf. [22]. The unit ball in the space of the structured perturbation is defined as $B\Delta = \{\Delta : \bar{\sigma}(\Delta) \leq 1\}$. The structured singular value μ of N with respect to a structured perturbation matrix Δ is denoted by $\mu_\Delta(N)$, cf. [22]. "$\preceq$" denotes element-wise vector inequality. $x_{i,k}$ denotes the ith element of the state vector x_k at time instant k.

Definition 1 (Skewed Structured Singular Value [23], [26]): The skewed structured singular value ν of N with respect to structured perturbation matrices Δ_1 and Δ_2 is defined by[1]

$$\nu_{\Delta_1,\Delta_2}(N) = \begin{cases} 0, \\ \text{if } \forall\kappa < \infty, \nexists\Delta = \operatorname{diag}\{\Delta_1, \kappa\Delta_2\}, \\ \Delta_i \in B\Delta_i \text{ s.t. } |I - N\Delta| = 0, \\ 1/\min\{\kappa \geq 0 : \exists\Delta = \operatorname{diag}\{\Delta_1, \kappa\Delta_2\}, \\ \Delta_i \in B\Delta_i \text{ s.t. } |I - N\Delta| = 0\}, \text{otherwise.} \end{cases}$$

This structured singular value is said to be "skewed" because only a part of the structured perturbation matrix is stretched, while keeping

[1] As can be seen in the definition, $\nu_{\Delta_1,\Delta_2}(N)$ can be infinity. The value does not occur in this technical note because it is assumed that the LFT in Lemma 3 is well-posed, which ensures that $\kappa \neq 0$.

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the rest fixed. Upper and lower bounds on ν can be computed in polynomial time, with no more effort than non-skewed structured singular value calculations [24], [26], by a variety of methods including power iterations and linear matrix inequalities (LMIs). This gap between the upper/lower bounds has been observed to be small for most matrices [27]. The following results relate the LFT to ν.

Theorem 2 (Main Loop Theorem [22]): The following equivalence holds:

$$\mu_{\mathrm{diag}[\Delta_1,\Delta_2]}(N) < 1 \Leftrightarrow \begin{cases} \mu_{\Delta_1}(N_{11}) < 1 \\ \max\limits_{\bar{\sigma}(\Delta_1)\le 1} \mu_{\Delta_2}\left(F_u(N,\Delta_1)\right) < 1. \end{cases} \quad (1)$$

Proof: See [22]. ■

Lemma 3: For any well-posed LFT in which $F_u(N,\Delta_1)$ is a scalar

$$\max_{\bar{\sigma}(\Delta_1)\le 1} |F_u(N,\Delta_1)| = \nu_{\Delta_1,\Delta_2}(N). \quad (2)$$

Proof: The skewed version of Theorem 2

$$\nu_{\Delta_1,\Delta_2}(N) < \alpha \Leftrightarrow \begin{cases} \mu_{\Delta_1}(N_{11}) < 1 \\ \max\limits_{\bar{\sigma}(\Delta_1)\le 1} \mu_{\Delta_2}\left(F_u(N,\Delta_1)\right) < \alpha \end{cases} \quad (3)$$

can be obtained in a similar manner as in [26], for any $\alpha > 0$. This implies that $\max_{\bar{\sigma}(\Delta_1)\le 1} \overline{\sigma}(F_u(N,\Delta_1)) = \nu_{\Delta_1,\Delta_2}(N)$ and the maximum singular value of a scalar is equal to its absolute value. ■

In this technical note, Δ_1 represents the uncertainty in the system and $\Delta_2 = \delta$ is a complex scalar.

III. Problem Setup

Consider a discrete-time dynamical system of the form

$$x_k = f(x_{k-1},p) = \sum_n a_n \prod_{i,j} x_{i,k-1}^{\alpha_{ni}} p_{j,k-1}^{\beta_{nj}} \quad (4)$$

where $x_k \in \mathbb{R}^{n_x}$ denotes the state vector at time $k \in \{1,2,3,\cdots\}$, $p \in \mathbb{R}^{n_p}$ is a vector of uncertain parameters, and $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$ is polynomial in its arguments.

Problem 4: Given a system (4) with interval bounds on the initial state x_0 and parameter vector p, i.e., $x_{0,\min} \preceq x_0 \preceq x_{0,\max}$, $p_{\min} \preceq p \preceq p_{\max}$, find the tightest possible outer bounds (i.e., elementwise maximum and minimum bounds) on the trajectory bundle x_k.

This work proposes a method to solve Problem 4 based on the theory of skewed structured singular values. Before presenting the method, consider the following result.

Lemma 5: Solving Problem 4 is NP-hard.

Proof: Consider a problem in which the polynomial in the right-hand side of (4) is a quadratic function of $[x_{k-1}, p_{k-1}]^T$ for each element of the vector x_k, with an indefinite Hessian. The computation of a maximum or a minimum bound for any of the elements of x_1 is an indefinite quadratic program with box constraints, which is an NP-hard problem [28]. ■

Problem 4 is also NP-hard when there is uncertainty only in the initial condition x_0 (no uncertain parameters p).[2] The NP-hardness of Problem 4 motivates the derivation of polynomial-time algorithms for computing lower and upper bounds that have some conservatism but are rigorous and tight.

IV. Main Algorithm and Its Variants

This section proposes an algorithm to compute upper and lower bounds on each state at each time instant in Problem 4. The idea of the algorithm is to reformulate the polynomial map f such that maximum and minimum bounds of its range can be derived using the *skewed structured singular value*. This approach is repeatedly performed to bound the future evolution of the system states starting from an uncertain initial condition.

Step 0 is a normalization step, whereas Step 4 initializes the steps for future time instants. Steps 1–3 are the core of the Algorithm to bound the trajectories based on LFT reformulations of the system (4) using skewed structured singular values.

Step 1: A polynomial system can always be represented by an LFT [22].[3] Each element of the state vector x_k is expressed in the form of an LFT [29]–[31] so that (2) can be used in Step 2. Here the LFT relates the state x_k with the uncertain state vector x_{k-1} and uncertain parameter p, which is in contrast to the standard application of LFTs that expresses the input-output relation of transfer functions (e.g., $y = F_u(N,\Delta)w$). Subscript i indicates ith element of the state vector and subscript $k-1$ indicates the time instant at $k-1$. The subblock $N_{i,k-1,22}$ corresponds to the nominal state of $x_{i,k}$, and $\Delta_{i,k-1}$ is the structured perturbation that expresses uncertainties in the state $x_{i,k}$ and parameter p.

Algorithm: Compute bounds on the uncertain state trajectory from $k = 1$ to n

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Input: $x_{0,\max}, x_{0,\min}, p_{\max}, p_{\min}$
Output: $x_{1,\max}, x_{1,\min}, \cdots, x_{n,\max}, x_{n,\min}$
1: Step 0 (initialize): $p_c = (1/2)(p_{\max}+p_{\min})$, $w_p = (1/2)(p_{\max} - p_{\min})$, $x_{0,c} = (1/2)(x_{0,\max}+x_{0,\min})$, $w_{x_0} = (1/2)(x_{0,\max} - x_{0,\min})$.
2: **for** $k = 1$ to n **do**
3: **for** $i = 1$ to n_x **do**
4: Step 1 (write as an LFT):
Find $N_{i,k-1}$ and $\Delta_{i,k-1}$ by using p_c, w_p, $x_{k-1,c}$, and $w_{x_{k-1}}$ such that

$$x_{i,k} = F_u(N_{i,k-1}, \Delta_{i,k-1})$$

5: Step 2 (write in shifted forms):
Choose large enough $c_{i,k-1,\max} > 0$ and small enough $c_{i,k-1,\min} < 0$ and write

$$\begin{aligned} x_{i,k} &= \underbrace{F_u(N_{i,k-1}, \Delta_{i,k-1}) + c_{i,k-1,\max}}_{:=F_u(N_{i,k-1,\max},\Delta_{i,k-1})} - c_{i,k-1,\max} \\ &= \underbrace{F_u(N_{i,k-1}, \Delta_{i,k-1}) - c_{i,k-1,\min}}_{:=F_u(N_{i,k-1,\min},\Delta_{i,k-1})} + c_{i,k-1,\min} \end{aligned}$$

6: Step 3 (apply skewed structured singular value to define bounds)

$$x_{i,k,\max} = \nu_{\Delta_{i,k-1},\delta}(N_{i,k-1,\max}) - c_{i,k-1,\max}$$
$$x_{i,k,\min} = -\nu_{\Delta_{i,k-1},\delta}(N_{i,k-1,\min}) - c_{i,k-1,\min}$$

7: **end for**
8: Step 4 (update the maximum and minimum of the uncertain state):

$$x_{k,c} = \frac{1}{2}(x_{k,\max} + x_{k,\min}), \quad w_{x_k} = \frac{1}{2}(x_{k,\max} - x_{k,\min}).$$

9: **end for**

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[2]This is proved by replacing $[x_{k-1}, p_{k-1}]^T$ with $[x_{k-1}]^T$ in the proof.

[3]Note that LFT representations are not unique [22]. Namely, there are degrees of freedom in the formulations, but we do not further investigate here.

As an example, consider the logistic map $x_k = px_{k-1}(1-x_{k-1})$ where $p>0$ is an uncertain parameter, $x_{k-1}\in(0,1)$ is the population at year $k-1$, and x_0 is the initial population. An LFT of form $x_k = F_u(N_{k-1},\Delta_{k-1})$ can be found by combining the three LFTs

$$p = \underbrace{p_c}_{N_{p,22}} + \underbrace{w_p}_{N_{p,21}}\delta\bar{p},$$

$$N_{p,11}=0,\quad N_{p,12}=1,\quad |\delta\bar{p}|\le 1,$$

$$x_{k-1} = \underbrace{x_{k-1,c}}_{N_{x_{k-1},22}} + \underbrace{w_{x_{k-1}}}_{N_{x_{k-1},21}}\delta\bar{x}_{k-1},$$

$$N_{x_{k-1},11}=0,\quad N_{x_{k-1},12}=1,\quad |\delta\bar{x}_{k-1}|\le 1,$$

$$1-x_{k-1} = \underbrace{1-x_{k-1,c}}_{N_{x_{k-1},22}}\underbrace{-w_{x_{k-1}}}_{N_{x_{k-1},21}}\delta\bar{x}_{k-1},$$

$$N_{x_{k-1},11}=0,\quad N_{x_{k-1},12}=1$$

by using LFT algebra [22], which gives

$$N_{k-1} = \begin{bmatrix} N_{11} & N_{k-1,12} \\ N_{21} & N_{k-1,22}\end{bmatrix},\quad \Delta_k = \begin{bmatrix} \delta\bar{x}_{k-1} & 0 & 0 \\ 0 & \delta\bar{x}_{k-1} & 0 \\ 0 & 0 & \delta\bar{p}\end{bmatrix},$$

where

$$N_{11} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0\end{bmatrix},\quad N_{k,12} = \begin{bmatrix} -w^2_{x_{k-1}} \\ (1-2x_{k-1,c})w_{x_{k-1}} \\ x_{k-1,c}(1-x_{k-1,c})\end{bmatrix},$$

$$N_{21} = [0\quad p_c\quad w_p],\quad N_{k-1,22} = p_c x_{k-1,c}(1-x_{k-1,c}).$$

Any polynomial can be decomposed into factors and sets of terms, an LFT can be realized for each of those simpler components, and the overall LFT can be composed from the simpler LFT using block-diagram algebra [22]. For a scalar polynomial that consists of N terms, with the highest degree of each term being M, an LFT of maximum size $M+1$ can be derived for each of the N terms, and the overall LFT has maximum size $N(M+1)$. Polynomial-time multidimensional realization algorithms (e.g., [32]) can construct LFTs for complicated polynomials and use factorizations to obtain much smaller LFT realizations. Multidimensional model reduction algorithms (e.g., see [33] and references therein) can be applied to the obtained LFT so as to minimize the dimensions of Δ_k, which will reduce the computational cost of Step 3.

Step 2: The biases $c_{i,k,\max}>0$ and $c_{i,k,\min}<0$ are introduced so that the maximum and minimum can be expressed in terms of the absolute value while ensuring the sign to be positive and negative, respectively, as follows:[4]

$$\begin{aligned}&\max_{\Delta_{k-1}} F_u(N_{i,k-1,\max},\Delta_{k-1})\\ &\quad= \max_{\Delta_{k-1}} |F_u(N_{i,k-1,\max},\Delta_{k-1})|, \qquad (5)\\ &\min_{\Delta_{k-1}} F_u(N_{i,k-1,\min},\Delta_{k-1})\\ &\quad= -\max_{\Delta_{k-1}} |F_u(N_{i,k-1,\min},\Delta_{k-1})|. \qquad (6)\end{aligned}$$

Each $N_{i,k-1,\max}$ is equal to $N_{i,k-1}$ with $N_{i,k-1,22}$ replaced by $N_{i,k-1,22}+c_{i,k-1,\max}$ and each $N_{i,k-1,\min}$ is equal to $N_{i,k-1}$ with $N_{i,k-1,22}$ replaced by $N_{i,k-1,22}+c_{i,k-1,\min}$. From those expressions, it can be seen that

$$\max_{\Delta_{k-1}} x_k = \max_{\Delta_{k-1}} |F_u(N_{i,k-1,\max},\Delta_{k-1})| - c_{i,k,\max}, \qquad (7)$$
$$\min_{\Delta_{k-1}} x_k = -\max_{\Delta_{k-1}} |F_u(N_{i,k-1,\min},\Delta_{k-1})| - c_{i,k,\min}. \qquad (8)$$

Step 3:[5] Lemma 3 implies that bounds on the worst-case deviation of the 2-norm of the state vector of the uncertain polynomial system (4) at each time instant k can be computed by computing bounds on ν applied to the matrices N and Δ_1 associated with the LFT. With

$$\max_{\Delta_{k-1}} |F_u(N_{i,k-1,\max},\Delta_{k-1})| = \nu_{\Delta_{k-1},\delta}(N_{i,k-1,\max}), \qquad (9)$$
$$\max_{\Delta_{k-1}} |F_u(N_{i,k-1,\min},\Delta_{k-1})| = \nu_{\Delta_{k-1},\delta}(N_{i,k-1,\min}), \qquad (10)$$

for a scalar δ, bounds on ν directly translate into bounds on each state

$$\max_{\Delta_{k-1}} x_k = \nu_{\Delta_{k-1},\delta}(N_{i,k-1,\max}) - c_{i,k,\max}, \qquad (11)$$
$$\min_{\Delta_{k-1}} x_k = -\nu_{\Delta_{k-1},\delta}(N_{i,k-1,\min}) - c_{i,k,\min}. \qquad (12)$$

Each skewed structured singular value is not computed exactly, but is represented by its upper and lower bounds. The closeness of the upper and lower bounds can be used to verify their tightness.

Remark 6: The Algorithm allows the uncertain parameter to change at each time instant. Some conservatism may be introduced as the bounds on the state, rather than the state itself, are propagated to the computations of ν at the subsequent time instants. One can reduce this effect considering a variant of the Algorithm:

Variant A:

Instead of updating $x_{k,c}$ and w_{x_k} in the for loop, construct an LFT that uses only $x_{0,\max}$, $x_{0,\min}$, $p_{\max}$, $p_{\min}$ at each time step. This algorithm applies to fixed uncertain parameters and removes the conservatism of the Algorithm by propagating the state instead of the state bounds between time instants.

Variant A utilizes the fact that the recursion of a polynomial function is also polynomial. The computational cost of Variant A is much higher than the original Algorithm. Indeed, the reformulation of the uncertain system as ν problems is exact for Variant A, so the only potential conservatism is introduced by the gap between the upper and lower bound of ν.

Remark 7: By introducing a moving horizon, another variant combines the update strategies of the Algorithm and Variant A, so as to be more computationally efficient than Variant A, but with the introduction of potential conservatism.

Variant B:

Choose a moving horizon s. Do the same as Variant A until $k=s$; initialize with $x_{k-s,\max}$ and $x_{k-s,\min}$ for $k>s$.

Variant B produces the same bounds as Variant A up to horizon s, retaining the information on the past states for all time instants. The bounds computed by Variant B with $s=1$ are the same as the

[4]One way of finding satisfactory biases is to compute $c=\nu_{\Delta_{i,k-1},\delta}(N_{i,k-1})$, and set $c_{i,k,\max}=1.2c$ and $c_{i,k,\min}=-1.2c$, for example (the value 1.2 was chosen arbitrary, any value greater than 1 would work). Easy-to-implement polynomial-time methods are available for determining such $c_{i,k-1,\max}$ and $c_{i,k-1,\min}$ [34].

[5]Upper and lower bounds on $x_{i,k,\max}$ and $x_{i,k,\min}$ are immediately computed from upper and lower bounds on ν.

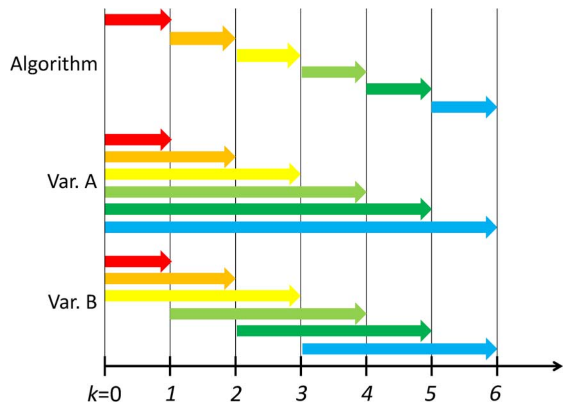

Fig. 1. The propagation of information in Algorithm and Variants A and B.

TABLE I
COMPARISON OF ALGORITHMS*

At kth step	Algorithm	Variant A	Variant B
$\dim\{N_{i,k}\}$	$\dim\{\Delta_0\}+1$	$k\dim\{\Delta_0\}+1$	$\le s\dim\{\Delta_0\}+1$
Bounds	possibly loose	tight	moderate
Dependency	x_{k-1}	x_0	x_{k-1-s} to x_{k-1}

*$N_{i,k}$ is square so only the row dimension is shown.

bounds computed by the original Algorithm. The bounds computed by Variant B converge to the bounds obtained by Variant A as the horizon increases; becoming the same for $s = S$, where S is the final time step of the simulation.

Fig. 1 and Table I summarize the properties and dependencies of the proposed Algorithm and its variants for computing the bounds on one state. The maximum computational cost at each time step of the Algorithm and Variant B is independent of k and the computation of the bounds on ν are polynomial-time in $\dim\{N\}$, which implies that the Algorithm and Variant B are polynomial-time. Numerical studies for dense matrices have observed a computational cost for the upper and lower bounds on ν that is approximately cubic as a function of the row dimension of N [27]; the computational cost should be much lower when sparse-matrix algebra is used.

Remark 8: The proposed approach also directly applies to fixed or time-varying disturbances that enter polynomially in the state equation, and it is straightforward to include any mix of parameters and disturbances that are time-varying or fixed. The latter approach also applies for more exotic uncertainty descriptions, such as restricting the parameters or disturbances to be fixed for short time intervals and allowed to vary in others.

Remark 9: A system that is linear in its states that can be written as an LFT, i.e., $x_k = F_u(N,\Delta)x_{k-1}$, is closely related to a *diagonal nonlinear differential inclusion* (DNLDI) [35]. Whereas theories on reachable or attainable sets have been developed for DNLDIs, they treat Δ as a function of time, which corresponds to the Algorithm. In contrast, Variants A and B treat fixed uncertain parameters Δ. This technical note can handle more flexible uncertainty descriptions than existing DNLDI theory (see also the discussion in Section VI), and this technical note computes bounds on the state for each time instant, instead of computing signal norms that sum up over all future time instants such as the L_2- and RMS-norms [35].

Remark 10: The proposed algorithms can be applied to compute bounds on the minimum diameter of an outer bounding ellipsoid by modifying N in Step 3 [36]. Another alternative is approximation by a zonotope [37], which is a superset of the axis-aligned orthotope presented here. A zonotope has a higher flexibility for tightly bounding the set of states but also has a higher complexity that increases at each time step unless pruned [37]. The bounding shape that best trades off computational cost with conservatism will depend on the specific application.

V. NUMERICAL EXAMPLE

Consider the polynomial model of a non-minimum phase quadruple-tank process presented in [38]. A discrete-time approximation of the dynamics is obtained by Euler discretization with a step size of 50 s. Furthermore, based on the linearization in [38] a output-feedback is introduced such that the zero is (locally) asymptotically stable. For additional parametric uncertainty, the uncertain parameters p_1, p_2 are included. The resulting model is

$$\begin{bmatrix} x_{1,k+1} \\ x_{2,k+1} \\ x_{3,k+1} \\ x_{4,k+1} \end{bmatrix} = \begin{bmatrix} x_{1,k} + 50\left(0.00073x_{1,k}^2 - 0.016x_{1,k} \right. \\ \left. \quad - 0.0047x_{2,k}^2 + 0.02x_{2,k} - p_1x_{1,k}\right) \\ x_{2,k} + 50\left(0.0047x_{2,k}^2 - 0.02x_{2,k} \right. \\ \left. \quad - 0.00375x_{3,k}\right) \\ x_{3,k} + 50\left(0.00052x_{3,k}^2 - 0.011x_{3,k} \right. \\ \left. \quad - 0.0033x_{4,k}^2 + 0.014x_{4,k} - p_2x_{3,k}\right) \\ x_{4,k} + 50\left(0.0033x_{4,k}^2 - 0.014x_{4,k} \right. \\ \left. \quad - 0.02795x_{1,k}\right) \end{bmatrix}$$

with the interval bounds on the initial conditions and parameters given by

$$x_{0,\min} = \begin{bmatrix} 0.27 \\ 0.18 \\ -0.12 \\ 0.08 \end{bmatrix}, \quad x_{0,\max} = \begin{bmatrix} 0.33 \\ 0.22 \\ -0.08 \\ 0.12 \end{bmatrix},$$
$$p_{\min} = [0,0]^T, \quad p_{\max} = [0.01, 0.01]^T.$$

Numerical experiments were performed for three different methods, namely the proposed algorithm, polynomial optimization, and interval analysis. A short description of the setting for each method is presented next.

Proposed Algorithm: Following the Algorithm, first the uncertainties in parameters and initial conditions are normalized (Step 0). Then the model is written as an LFT (Step 1). As an example, consider the LFT formulation of state x_1

$$N_{1,0,11} = \begin{bmatrix} 0 & 0.0365w_{x_{1,0}} & -50w_{p_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & w_{x_{2,0}} \end{bmatrix},$$

$$N_{1,0,12} = \begin{bmatrix} 0.0365x_{1,0,c} - 50p_{1,c} + 0.02 \\ 1 \\ 1 \\ 1 \\ 0 \end{bmatrix},$$

$$N_{1,0,21} = \begin{bmatrix} w_{x_{1,0}} \\ 0.0365w_{x_{1,0}}x_{1,0,c} \\ -50w_{p_1}x_{1,0,c} \\ -w_{x_{2,0}}(0.47x_{2,0,c} - 1) \\ -0.2350w_{x_{2,0}} \end{bmatrix}^T,$$

$$N_{1,0,22} = x_{2,0,c} - 0.235x_{2,0,c}^2 + x_{1,0,c}(0.0365x_{1,0,c} - 50p_{1,c} + 0.2),$$

$$\Delta_{1,0} = \operatorname{diag}[\delta x_{1,0}I_2, \delta p_1, \delta x_{2,0}I_2].$$

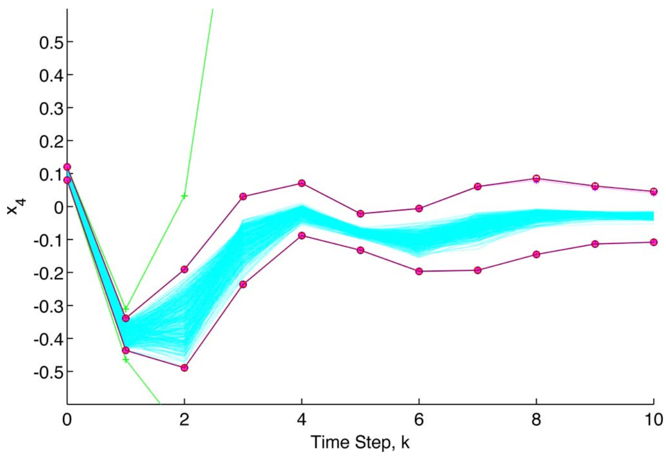

Fig. 2. Bounds on x_4. The results of the proposed Algorithm are blue lines with "$\circ$". The results of interval analysis and GloptiPoly3 are indicated by green dashed lines with "$+$" and magenta with "$*$," respectively. The cyan dotted lines are trajectories with randomly generated uncertain time-varying parameters.

As described in Step 1 in Section IV, this LFT was obtained by first writing each of the uncertain parameter/state in the form $u = u_c + w_u\delta\bar{u} = F_u\left(\left[\begin{array}{c|c} 0 & w_u \\ \hline 1 & u_c \end{array}\right], \delta\bar{u}\right)$, then using LFT multiplication and addition formulas [22], applying the reduction algorithms [33], and finally ordering the perturbation matrix by using permutation matrices so that the same uncertain parameter appears as a block. After deriving the shifted formulation (Step 2) with appropriately chosen constants (see footnote 4), lower and upper bounds on ν (Step 3) were computed using the Skew Mu Toolbox (SMT) [39].

Polynomial Optimization: For computing the bounds on each state, a minimization (respectively, maximization) of the right-hand side of the model was stated over the constraints defined by the bounds on parameters and initial conditions. GloptiPoly3 [40] was employed to solve the optimization problems to global optimality. GloptiPoly3 is a Matlab toolbox to solve polynomial optimization problems that is based on a convergent hierarchy of semidefinite relaxations.

Interval Analysis: Similarly to the previous method, interval analysis [41] was employed to compute bounds on each state and then propagating the bounds to the next time step. Here, only the basic rules of interval arithmetic and no advanced techniques for reducing the propagated error were employed.

Results: The bounds on x_4 obtained by the Algorithm, GloptiPoly3 [40], and interval analysis [41] are provided in Fig. 2. Overall, the proposed Algorithm and GloptiPoly3 provide almost the same bounds. The average absolute deviation (over all states and time steps) between the numerically global optimal bounds obtained by GloptiPoly3 and the proposed algorithm is 0.0018. The maximal absolute deviation is 0.0188. Comparing lower and upper bounds on ν as obtained by SMT showed that the upper bounds obtained by LMIs are generally closer to the bounds of GloptiPoly3 than the lower bounds obtained by power iteration. The interval analysis gives diverging bounds for all states. For this example and 10 time steps, the computation time for the ν upper bounds was 2.576 s, the ν lower bounds was 1.70 s (for given LFTs), while GloptiPoly3 was 60.46 s and interval analysis was 0.032 s. The upper bound of the proposed Algorithm was about a factor of 20–25 times faster than GloptiPoly3 with nearly identical accuracy.[6]

[6]The comparative speedup of the proposed Algorithm will vary somewhat depending on the chosen tolerances for each method, the Matlab version, the operating system, and the microprocessor.

The upper and lower bounds on the states were tight in additional numerical examples, including a chaotic system and a coordinate transformation [1].

VI. Conclusion

Skewed structured singular value-based approaches are proposed for bounding state trajectories for polynomial systems with uncertainty in the initial state and either time-varying (Algorithm) or fixed (Variants A and B) uncertainties in the parameters. The first proposed algorithm has the lowest computational cost, but can be conservative if the parameters are fixed instead of time-varying. Variant A provides tight bounds for polynomial systems with fixed parameter uncertainties but is computationally expensive. Variant B employs a moving horizon to reduce the computational cost for computing the state bounds for fixed parameter uncertainties, while increasing conservatism. The value of the moving horizon can be varied in Variant B to trade off computational cost with tightness of the bounds, and this algorithm is the most practical and attractive for polynomial systems with fixed parameter uncertainties. In the numerical examples in Section V and [1], the upper and lower bounds of the skewed structured singular value were tight.

The proposed approach and numerical algorithms have multiple possibilities for expansion to new systems. For example, the generalization to uncertain rational systems [36], to computing ellipsoidal bounds on the states [36], and to systems where the polynomial system can change at each time instant are straightforward.

References

[1] M. Kishida, P. Rumschinski, R. Findeisen, and R. D. Braatz, "Efficient polynomial-time outer bounds on state trajectories for uncertain polynomial systems using skewed structured singular values," in *Proc. IEEE Int. Symp. Computer Aided Control Syst. Design*, Denver, CO, 2011, pp. 216–221.

[2] S. Prajna, "Barrier certificates for nonlinear model validation," *Automatica*, vol. 42, pp. 117–126, 2006.

[3] P. Rumschinski, S. Streif, and R. Findeisen, "Combining qualitative information and semi-quantitative data for guaranteed invalidation of biochemical network models," *Int. J. Robust Nonlin. Control*, vol. 22, pp. 1157–1173, 2012.

[4] J. Hasenauer *et al.*, "Guaranteed steady state bounds for uncertain (bio-)chemical processes using infeasibility certificates," *J. Proc. Control*, vol. 20, pp. 1076–1083, 2010.

[5] P. Rumschinski *et al.*, "Complete fault diagnosis of uncertain polynomial systems," in *Proc. 9th IFAC DYCOPS*, Leuven, Belgium, 2010, pp. 127–132.

[6] M. Blanke, M. Kinnaert, J. Lunze, and M. Staroswiecki, *Diagnosis and Fault-Tolerant Control*, 2nd ed. New York, NY, USA: Springer, 2006.

[7] D. Q. Mayne, M. M. Seron, and S. V. Raković, "Robust model predictive control of constrained linear systems with bounded disturbances," *Automatica*, vol. 41, no. 2, pp. 219–224, 2005.

[8] Z. K. Nagy and R. D. Braatz, "Robust nonlinear model predictive control of batch processes," *AIChE J.*, vol. 49, pp. 1776–1786, 2003.

[9] S. V. Raković, B. Kouvaritakis, R. Findeisen, and M. Cannon, "Homothetic tube model predictive control," *Automatica*, vol. 48, pp. 1631–1638, 2012.

[10] J. M. Bravo, T. Alamo, and E. F. Camacho, "Robust MPC of constrained discrete-time nonlinear systems based on approximated reachable sets," *Automatica*, vol. 42, pp. 1745–1751, 2006.

[11] Z. K. Nagy and R. D. Braatz, "Worst-case and distributional robustness analysis of finite-time control trajectories for nonlinear distributed parameter systems," *IEEE T. Control Syst. T.*, vol. 11, pp. 494–504, 2003.

[12] D. L. Ma and R. D. Braatz, "Worst-case analysis of finite-time control policies," *IEEE T. Control Syst. T.*, vol. 9, pp. 766–774, 2001.

[13] H. Huang, C. S. Adjiman, and N. Shah, "Quantitative framework for reliable safety analysis," *AIChE J.*, vol. 48, pp. 78–96, 2002.

[14] H. Witsenhausen, "Sets of possible states of linear systems given perturbed observations," *IEEE Trans. Autom. Control*, vol. 13, no. 5, pp. 556–558, 1968.

[15] F. Blanchini and S. Miani, *Set-Theoretic Methods in Control*. Boston, MA, USA: Birkhäuser, 2007.

[16] T. Alamo, J. M. Bravo, M. J. Redondo, and E. F. Camacho, "A set-membership state estimation algorithm based on DC programming," *Automatica*, vol. 44, pp. 216–224, 2008.

[17] L. Jaulin, M. Kieffer, O. Didrit, and E. Walter, *Applied Interval Analysis*. London, U.K.: Springer, 2001.

[18] J. K. Scott and P. I. Barton, "Tight, efficient bounds on the solutions of chemical models," *Comput. Chem. Eng.*, vol. 34, pp. 717–731, 2010.

[19] D. Limon, J. Bravo, T. Alamo, and E. F. Camacho, "Robust MPC of constrained nonlinear systems based on interval arithmetic," *Proc. Inst. Elect. Eng.*, vol. 152, pp. 325–332, 2005.

[20] P. Rumschinski, S. Borchers, S. Bosio, R. Weismantel, and R. Findeisen, "Set-base dynamical parameter estimation and model invalidation for biochemical reaction networks," *BMC Syst. Biol.*, vol. 4, p. 69, 2010.

[21] S. Streif, A. Savchenko, P. Rumschinski, S. Borchers, and R. Findeisen, "ADMIT: A toolbox for guaranteed model invalidation, estimation, and qualitative-quantitative modeling," *Bioinformatics*, vol. 28, no. 9, pp. 1290–1291, 2012.

[22] K. Zhou, J. C. Doyle, and K. Glover, *Robust and Optimal Control*. Upper Saddle River, NJ, USA: Prentice-Hall, 1995.

[23] R. S. R. Smith, "Model Validation for Uncertain Systems," Ph.D. dissertation, California Institute of Technology, Pasadena, CA, USA, 1990. [Online]. Available: http://thesis.library.caltech.edu/4244/

[24] M. K. H. Fan and A. L. Tits, "A measure of worst-case H_∞ performance and of largest acceptable uncertainty," *Syst. Control Lett.*, vol. 18, pp. 409–421, 1992.

[25] R. D. Braatz, P. M. Young, J. C. Doyle, and M. Morari, "Computational complexity of μ calculation," *IEEE Trans. Autom. Control*, vol. 39, pp. 1000–1002, 1994.

[26] G. Ferreres, *A Practical Approach to Robustness Analysis With Aeronautical Applications*. New York, NY, USA: Springer, 1999.

[27] P. M. Young, M. P. Newlin, and J. C. Doyle, "Computing bounds for the mixed μ problem," *Int. J. Robust Nonlin. Control*, vol. 5, pp. 573–590, 1995.

[28] K. G. Murty and S. N. Kabadi, "Some NP-complete problems in quadratic and nonlinear programming," *Mathematical Programming*, vol. 39, pp. 117–129, 1987.

[29] J.-F. Magni, "Presentation of the linear fractional representation toolbox (LFRT)," in *Proc. IEEE Int. Symp. Computer Aided Control Syst. Design*, 2002, pp. 248–253.

[30] S. Hecker, A. Varga, and J.-F. Magni, "Enhanced LFR-toolbox for MATLAB," *Aerosp. Sci. Technol.*, vol. 9, pp. 173–180, 2005.

[31] J.-F. Magni, J.-M. Biannic, and C. Doll, LFRT With Simulink Interface Toolbox. [Online]. Available: http://jm.biannic.free.fr/software.html

[32] E. L. Russell, C. P. H. Power, and R. D. Braatz, "Multidimensional realizations of large scale uncertain systems for multivariable stability margin computation," *Int. J. Robust Nonlin. Control*, vol. 7, pp. 113–125, 1997.

[33] E. L. Russell and R. D. Braatz, "Model reduction for the robustness margin computation of large scale uncertain systems," *Comput. Chem. Eng.*, vol. 22, pp. 913–926, 1998.

[34] M. Kishida and R. D. Braatz, "Worst-case analysis of distributed parameter systems with application to the 2D reaction-diffusion equation," *Optim. Control Appl. Met.*, vol. 31, pp. 433–449, 2010.

[35] S. Boyd, L. E. Ghaoui, E. Feron, and V. Balakrishnan, *Linear Matrix Inequalities in System and Control Theory*. Philadelphia, PA, USA: SIAM, 1994.

[36] M. Kishida and R. D. Braatz, "Ellipsoid bounds on state trajectories for discrete-time systems with time-invariant and time-varying linear fractional uncertainties," in *Proc. IEEE Conf. Decision Control*, Orlando, FL, 2011, pp. 5671–5676.

[37] T. Alamo, J. M. Bravo, and E. F. Camacho, "Guaranteed state estimation by zonotopes," *Automatica*, vol. 41, pp. 1035–1043, 2005.

[38] B. Labibi, H. J. Marquez, and G. Chesi, "Decentralized robust output feedback control for control affine nonlinear interconnected systems," *J. Process Control*, vol. 19, no. 5, pp. 865–878, 2009.

[39] G. Ferreres and J.-M. Biannic, Skew Mu Toolbox (SMT), 2009. [Online]. Available: http://www.onera.fr/staff-en/jean-marc-biannic/

[40] D. Henrion and J. B. Lasserre, "GloptiPoly 3: Moments, optimization and semidefinite programming," *Optim. Methods Softw.*, vol. 24, pp. 761–779, 2009. [Online]. Available: http://homepages.laas.fr/henrion/software/gloptipoly/

[41] R. E. Moore, *Interval Analysis*. Englewood Cliffs, NJ, USA: Prentice-Hall, 1996.