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SUMMARY

This paper concerns the simulation of a class of nonlinear continuous-time systems under a set of initial conditions described by an ellipsoid. By getting inspiration from Lyapunov theory, we show that it is possible to derive a procedure allowing the computation of a bounding ellipsoidal envelope which will enclose all the states that can be reached from the set of initial conditions. This numerical procedure is based on convex optimisation, and it makes it possible to set a guaranteed hard bound on the evolution of the state of the system for all the possible initial conditions. At the end of the paper, we show an application of the method through an academic example.

KEY WORDS: Systematic or robust simulation; rational systems; linear matrix inequalities; sum of squares

1. INTRODUCTION

Simulation is a tool that is quite often used in the industry in order to validate the functionality and safety of a system. As the systems are often supposed to work in several different situations, it is important to run simulations which can validate them for all the possible cases, to make sure that no special condition may cause malfunctioning or danger. A practical approach to this problem is the use of systematic simulation, which consists ideally in checking the behaviour of the system with respect to all the possible initial conditions and for all the values of the non-constant parameters; however, this is strictly impossible if initial conditions and parameter values are assumed to belong to a dense set, as it would require running an infinite number of simulations. This leads to approaches based on selected tests or Monte Carlo methods [1], or approaches based on random exploration [2], or sensitivity analysis [3]. All of these methods unfortunately have the shortcoming on being a sort of "statistical" validation, in the sense that they do not offer a hard bound on the evolution of the system, if not for a computational complexity going to infinity. Another possibility consists in evaluating the effect of the initial condition with respect to an output index that is an indicator of such effects, but this approach does not establish precise bounds on each state variable [4, 5, 6].

In this article we present a radically different approach to the problem, based on the so called "robust simulation" or simulation of sets [7, 8, 9, 10, 11], which offers instead mathematically guaranteed bounds for the evolution of dynamical systems. Whereas almost all such existing works approach the problem of systematic simulation for discrete-time systems only, we focus here on *continuous-time systems*. In fact, the necessity of working in discrete-time can be a disadvantage, as it requires a discretisation of the original physical equations (usually, differential equations), which can introduce approximation errors in itself.

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The specific method developed in this paper focuses on a class of nonlinear systems, and it is based on the search of a Lyapunov-like function which allows bounding the state vector within an ellipsoid that evolves with time. The method can work on differential equations with polynomial or rational expressions thanks to the use of the sum of squares (SOS) relaxation [12], which leads to efficiently solvable convex optimisation problems in the form of linear matrix inequalities (LMIs) [13]. This approach can subsequently be considered "safe", as the evolution of all the possible trajectories of the state are hardly bounded, but on the other hand it is conservative, i.e. the bounds are not necessarily tight.

Robust simulation is a problem that shares several similarities with many works on stability, reachability and search for regions of attractions of nonlinear dynamical systems, like those based on moments [14, 15, 16] or Koopman operators [17]. We would like to stress here that the goal of this paper is to find the envelope containing the state *at each time instant*, and not to understand whether it is stable or whether it will eventually converge to a set.

The paper is organised as follows. Section 2 contains the preliminaries and the problem formulation. Sections 3 and 4 provide background on the two main tools used throughout the paper, whereas the two main theoretical results can then be found in Section 5 and Section 6, in the form of theorems. These results are then applied to an example in Section 7 and then conclusions are drawn in Section 8.

2. PRELIMINARIES

2.1. Notation

We denote by $\mathbb{R}$ the set of real numbers, and by $\mathbb{R}^{n\times m}$ the set of real $n \times m$ matrices. $A^\top$ indicates the transpose of a matrix A, I_n is the identity matrix of size n. The notation $A \succeq 0$ ($A \preceq 0$) indicates that all the eigenvalues of the symmetric matrix A are positive (negative) or equal to zero, whereas $A \succ 0$ ($A \prec 0$) indicates that all such eigenvalues are strictly positive (negative). The symbol $\binom{n}{k}$ indicates the binomial coefficient, for which we have

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

We also define $\mathcal{E}(P, c)$ as the ellipsoid of dimension n with matrix $P \in \mathbb{R}^{n\times n}$, $P = P^\top \succ 0$ and centered in $c \in \mathbb{R}^n$, i.e. $\mathcal{E}(P, c) = \{x \in \mathbb{R}^n \mid (x - c)^\top P(x - c) \leqslant 1\}$. At last, $\otimes$ indicates the Kronecker product, and we employ the symbol $*$ to complete symmetric matrix expressions avoiding repetitions.

2.2. Problem formulation

As stated in the introduction, we are interested in the problem of finding ellipsoidal hard bounds for the evolution of the state of dynamical continuous-time system. Namely, assume we have a differential equation

$$\dot{x}(t) = f(x(t)) \tag{1}$$

where $x \in \mathbb{R}^n$ is the state vector, $t \in \mathbb{R}$ it the time and f is a generic (nonlinear) function. Let us assume that the initial state vector is bound to belong to a given ellipsoid, i.e. $x(0) \in \mathcal{E}(P(0), c(0))$, with $P(0)$, $c(0)$ given. The general problem we are interested in is to find the smallest possible ellipsoid $\mathcal{E}(P(t), c(t))$ such that $x(t) \in \mathcal{E}(P(t), c(t))$ for $t \in [0, t_f]$, i.e. to find functions $P(t)$ and $c(t))$ defining such an ellipsoid, with $t_f > 0$ given. In this article, we propose a possible approach to such problem for f belonging to two different classes.

Problem 1
Consider the linear time-invariant system

$$\dot{x}(t) = Ax(t) \tag{2}$$

with $A \in \mathbb{R}^{n\times n}$, $x(0) \in \mathcal{E}(P(0), c(0))$), i.e. $(x(0) - c(0))^\top P(0)(x(0) - c(0)) \leqslant 1$, for given $c(0)$ and $P(0) \succ 0$. Find the smallest ellipsoid $\mathcal{E}(P(t), c(t))$ with $P(t)$, $c(t)$ such that

$$(x(t) - c(t))^\top P(t)(x(t) - c(t)) \leqslant 1, \quad \text{for } t \in [0, t_f]. \tag{3}$$

This problem can also be extended to rational systems, whose dynamics can be described as

$$\dot{x}(t) = \frac{N(x)}{d(x)}, \tag{4}$$

with $x = [x_1, x_2, \ldots, x_n]^\top$, $N(x) \in \mathbb{R}^n$ a vector of polynomials of degree up to m_x, and $d(x) \in \mathbb{R}$ a polynomial of degree up to $2m_x - 2$. If we define the vector $\chi \in \mathbb{R}^\rho$ which contains all the possible monomials obtainable from x from degree 0 up to m_x (for example, if $n = 2$, $m_x = 2$, then $\chi = [x_1, x_2, x_1^2, x_1x_2, x_2^2, 1]^\top$), with

$$\rho = \binom{n + m_x}{n}. \tag{5}$$

then we have that any polynomial in the variables of x up to degree m_x can be formulated as a linear function of χ; so namely we have

$$N(x) = F^\top \chi(t), \tag{6}$$

with $F \in \mathbb{R}^{\rho\times n}$. So, the second class of problems that we consider is formulated as follows.

Problem 2
Consider the rational system (4) where $F \in \mathbb{R}^{\rho\times n}$ is defined in (6) and $\chi(t) \in \mathbb{R}^\rho$ expresses all the possible monomials of $x(t)$ up to degree m_x, with $x(0) \in \mathcal{E}(P(0), c(0))$, i.e. $(x(0) - c(0))^T P(0)(x(0) - c(0)) \leqslant 1$, for given $c(0)$ and $P(0) \succ 0$. Find the smallest ellipsoid $\mathcal{E}(P(t), c(t))$ with $P(t)$, $c(t)$ such that

$$(x(t) - c(t))^\top P(t)(x(t) - c(t)) \leqslant 1, \quad \text{for } t \in [0, t_f]. \tag{7}$$

Notice that obviously Problem 1 is a special case of Problem 2; we have chosen to separate the two cases in order to be able to tackle the simpler Problem 1 first, and then extend the results to Problem 2. This greatly simplifies the reading and understanding of this paper.

Notice also that we do not assume any special stability properties for (2) or (4), i.e. the systems we are interested in simulating can be stable or unstable. Nevertheless, the approach that we follow for finding a possible solution for this problem is inspired by Lyapunov's work on the stability of systems. We recall the relevant results, and show how to exploit them, in the next section.

3. LYAPUNOV STABILITY AND PSEUDO-LYAPUNOV FUNCTIONS

We first restrict to a linear time-invariant system as in (2), and we define the quadratic form $V(x(t))$ as

$$V(x(t)) = x(t)^T P x(t), \tag{8}$$

where $P = P^\top \in \mathbb{R}^{n\times n}$. According to Lyapunov's theory [18], system (2) is asymptotically stable iff there exists $V(x(t))$ such that

$$\begin{cases} V(x(t)) > 0 \\ \dot{V}(x(t)) < 0 \end{cases} \quad \forall x \neq 0 \tag{9}$$

which is equivalent to the existence of a $P = P^T$ such that

$$\begin{cases} P \succ 0 \\ A^T P + PA \prec 0. \end{cases} \tag{10}$$

In this case $V(x(t))$ is called a Lyapunov function. There is an interesting interpretation for this approach: besides asymptotic stability, the existence of a P satisfying (10) allows defining the class of ellipsoidal sets $\vartheta_\beta = \{x|V(x) \leqslant \beta\}$ whose boundaries (also known as level curves) can only be crossed by a state trajectory in an inward motion, since $\dot{V}(x(t)) < 0$ for an x following (1). This means that, if at a given t_i, we have that $x(t_i) \in \mathcal{E}(P, 0)$, i.e. $x(t_i)^\top P x(t_i) \leqslant 1$, then $x(t)^\top P x(t_i) \leqslant 1$ for all $t \geqslant t_i$, i.e. $x(t)$ will never get out of the initial ellipsoid. Moreover, intuitively, if the value of the Lyapunov function decreases strictly with time, the state is necessarily brought to its only value for which $V(x(t)) = 0$, i.e. the origin.

We can adapt this approach to our problem by neglecting the necessity of proving the asymptotic stability (not our goal) and focusing on the aspect of the level curves. As we do not require anymore the system state to converge to the origin, we do not need the decreasing value of V to drag the state there, so we can account for just a non-positive derivative of $V(x(t))$, which is enough to ensure that the initial level curves are never crossed outwards; we can also account for a time-varying $\tilde{V}$ (i.e. with direct dependence with respect to time) in order to let these level curves accommodate the evolution of the state. These ideas let us formulate the following preliminary lemma, which is valid both for stable and unstable systems.

Lemma 3
Consider the system in (2), with $x(0)^\top P_0 x(0) \leqslant 1$. If there exists a matrix function $P(t) = P(t)^\top \in \mathbb{R}^{n\times n}$, with $P(0) = P_0$, such that

$$\begin{cases} P(t) \succ 0 \\ A^\top P(t) + P(t)A + \dot{P}(t) \preceq 0 \end{cases} \quad \text{for } t \in [0, t_f] \tag{11}$$

then $x(t)^\top P(t) x(t) \leqslant 1$ for $t \in [0, t_f]$.

Proof
The first equation in (11), left- and right-multiplied by $x(t)$, implies that the pseudo-Lyapunov function $\tilde{V}(x(t), t) = x(t)^\top P(t) x(t) > 0$, which guarantees the existence of the ellipsoids. The second equation in (11), again left- and right-multiplied by $x(t)$, yields $\frac{d}{dt}(x(t)^\top P(t) x(t)) \leqslant 0$. By integrating with respect to time, we have that $x(t)^\top P(t) x(t) - x(0)^\top P(0) x(0) = \int_0^t \frac{d}{dt}(x(t)^\top P(t) x(t)) dt \leqslant 0$ if $0 \leqslant t \leqslant t_f$, which implies that $x(t)^\top P(t) x(t) \leqslant x(0)^\top P(0) x(0) \leqslant 1$. □

Notice that there is no loss of generality in setting the initial time value as $t = 0$, as a shift or change of coordinates in the time axis is always possible.

Lemma 3 contains the key idea which will lead to the main results of this paper; in fact, finding a $P(t)$ satisfying (11) is quite close to finding a solution to Problem 1. Finding such a matrix function satisfying (11) is quite close to a classical LMI problem, with the relevant issue that the unknown $P(t)$ is not a constant but a function of a parameter, namely t. By searching through the literature, we can see that there are a number of similar problems with parameter-dependent LMIs, with a known computationally feasible solution [19, 20, 21, 22]. For the sake of this work, we will use a generalised version of the famous Kalman-Yakubovich-Popov (KYP) lemma [23], which is the topic of the next section.

4. THE KALMAN-YAKUBOVICH-POPOV LEMMA

The Kalman-Yakubovic-Popov lemma or KYP [23] is a widely celebrated result for dynamical systems that allows turning frequency-dependent inequalities into frequency-independent ones, by exploiting a state-space formulation. It turns out that such a result can be adapted and generalised to inequalities depending on any scalar parameter. Namely, we will use the following generalised version of the KYP.

Lemma 4 (Generalized KYP [19])
Consider

$$M(\xi) = M_0 + \sum_{i=1}^{l} \xi_i M_i, \tag{12}$$

with $\xi \in \mathbb{R}^l$ a vector of decision variables and $M_i = M_i^\top \in \mathbb{R}^{n_M \times n_M}, i = 1, ..., l$. The quadratic constraint

$$\phi(\theta)^\top M(\xi)\ \phi(\theta) \prec 0 \text{ for } \theta \in [\underline{\theta}, \overline{\theta}] \tag{13}$$

is verified if and only if there exist $\mathcal{D} = \mathcal{D}^\top \succ 0$ and $\mathcal{G} = -\mathcal{G}^\top$ such that

$$\begin{aligned} &\begin{bmatrix} \tilde{C}^\top \\ \tilde{D}^\top \end{bmatrix} M(\xi) \begin{bmatrix} \tilde{C} & \tilde{D} \end{bmatrix} \\ &+ \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix}^\top \begin{bmatrix} -2\mathcal{D} & (\underline{\theta}+\overline{\theta})\mathcal{D} + \mathcal{G} \\ (\underline{\theta}+\overline{\theta})\mathcal{D} - \mathcal{G} & -2\underline{\theta}\overline{\theta}\mathcal{D} \end{bmatrix} \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix} \prec 0 \end{aligned} \tag{14}$$

with $\tilde{A}$,$\tilde{B}$, $\tilde{C}$ and $\tilde{D}$ such that

$$\phi(\theta) = \tilde{D} + \tilde{C}\theta I(I - \tilde{A}\theta I)^{-1}\tilde{B} = \theta I \star \begin{bmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{bmatrix}, \tag{15}$$

where the operator $\star$ implicitly defined above is known as the Redheffer product [24].

The lemma applies as well if the sign $\prec$ in (13) is replaced by $\preceq$: in this case replace $\prec$ with $\preceq$ in (14) as well.

Notice that the lemma above can only be applied if the unknowns ξ are not depending on the parameter θ (t, in our case). So this means that this lemma cannot be applied to find a solution for Lemma 3 as the $P(t)$ there depends on time. This problem can be overcome by assuming a pre-established form for the time-dependence of $P(t)$. For example, we can assume $P(t)$ to be a polynomial of degree $2m$, with $m \geqslant 1$, i.e. $P(t) = \sum_{i=0}^{2m} P_i t^i, (P_i = P_i^\top, i = 0, \cdots, 2m)$ (this of course adds some conservatism, which can be progressively reduced by increasing the degree of the polynomial). In this way, the constant terms P_i (for $i = 1, \cdots, 2m$) are the unknowns, and $\dot{P}(t)$ can be explicitly expressed (notice that P_0 instead is a known constant, corresponding to the initial ellipsoid). Subsequently, any affine expression in $P(t)$ (degree $2m$) or $\dot{P}(t)$ (degree $2m-1$) can be expressed in the form of (13), i.e. as $\phi(t)^\top M(\xi)\,\phi(t)$ with $M(\xi)$ affine in the unknowns ξ, with

$$\phi(t) = \begin{bmatrix} t^m I \\ \vdots \\ I \end{bmatrix} = \tilde{D} + \tilde{C}tI(I - \tilde{A}tI)^{-1}\tilde{B} = tI \star \begin{bmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{bmatrix} \tag{16}$$

and

$$\begin{aligned} \tilde{A} = U_m \otimes I_n, \qquad \tilde{B} = \begin{bmatrix} z_{m-1} \\ 1 \end{bmatrix} \otimes I_n, \\ \tilde{C} = \begin{bmatrix} I_m \\ z_m^\top \end{bmatrix} \otimes I_n, \qquad \tilde{D} = \begin{bmatrix} z_m \\ 1 \end{bmatrix} \otimes I_n. \end{aligned} \tag{17}$$

where $U_i \in \mathbb{R}^{i \times i}$ is a matrix containing 1's in the first upper diagonal and 0's elsewhere, and $z_i \in \mathbb{R}^i$ is a column vector containing 0's in all its entries.

For example, for $m = 1$, we have

$$P(t) = P_0 + P_1 t + P_2 t^2 = \begin{bmatrix} tI \\ I \end{bmatrix}^\top \begin{bmatrix} P_2 & \frac{1}{2}P_1 \\ * & P_0 \end{bmatrix} \begin{bmatrix} tI \\ I \end{bmatrix} \tag{18}$$

$$A^\top P(t) + P(t)A + \dot{P}(t) = \begin{bmatrix} tI \\ I \end{bmatrix}^\top \begin{bmatrix} A^\top P_2 + P_2 A & P_1 A + P_2 \\ * & A^\top P_0 + P_0 A + P_1 \end{bmatrix} \begin{bmatrix} tI \\ I \end{bmatrix} \tag{19}$$

where $\dot{P}(t) = P_1 + 2P_2 t$ and

$$\phi(t) = \left[\begin{array}{c} tI \\ I \end{array}\right] = tI \star \left[\begin{array}{c|c} 0 & I \\ \hline I & 0 \\ 0 & I \end{array}\right]. \tag{20}$$

5. ROBUST SIMULATION: LINEAR CASE

Employing the tools of the two previous section, we can arrive at our first main result, in the form of a theorem.

Theorem 5
Consider the continuous linear time-invariant system in (2). If there exists $\mathcal{D}_1 = \mathcal{D}_1^\top \succ 0$, $\mathcal{G}_1 = -\mathcal{G}_1^\top$, $\mathcal{D}_2 = \mathcal{D}_2^\top \succ 0$ and $\mathcal{G}_2 = -\mathcal{G}_2^\top$ such that

$$\begin{bmatrix} \tilde{C}^\top \\ \tilde{D}^\top \end{bmatrix} M_1 \begin{bmatrix} \tilde{C} & \tilde{D} \end{bmatrix} + \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix}^\top \begin{bmatrix} -2\mathcal{D}_1 & t_f\mathcal{D}_1 + \mathcal{G}_1 \\ * & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix} \prec 0 \tag{21}$$

$$\begin{bmatrix} \tilde{C}^\top \\ \tilde{D}^\top \end{bmatrix} M_2 \begin{bmatrix} \tilde{C} & \tilde{D} \end{bmatrix} + \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix}^\top \begin{bmatrix} -2\mathcal{D}_2 & t_f\mathcal{D}_2 + \mathcal{G}_2 \\ * & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix} \preceq 0 \tag{22}$$

with $\phi(t) = \left[\begin{array}{c} t^m I \\ \vdots \\ I \end{array}\right] = \tilde{D} + \tilde{C}tI(I - \tilde{A}tI)^{-1}\tilde{B} = tI \star \left[\begin{array}{cc} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{array}\right]$, $P(t) = \sum_{i=0}^{2m} P_i t^i, (P_i = P_i^\top, i = 0, \cdots, 2m)$, M_1 and M_2 (affine in the coefficients of $P(t)$) such that

$$\phi(t)^\top M_1 \phi(t) = -P(t), \tag{23}$$

$$\phi(t)^\top M_2 \phi(t) = \dot{P}(t) + A^\top P(t) + P(t)A \tag{24}$$

then

$$x(0)^\top P(0) x(0) \leq 1 \Rightarrow \tilde{V}(x(t), t) = x(t)^\top P(t) x(t) \leqslant 1, \quad \forall t \in [0, t_f]. \tag{25}$$

Proof
The direct application of Lemma 4 (generalized KYP) means that the inequalities (21) and (22) imply the ones in Lemma 3, for $P(t)$ in the chosen polynomial form. This subsequently proves the theorem statement. □

Algorithm 6
As conditions (21) and (22) are LMIs with respect to the unknowns ($P_1, \ldots, P_{2m}$, $\mathcal{D}_1, \mathcal{D}_2, \mathcal{G}_1$and $\mathcal{G}_2$), we can find the solution of Problem 1 for ellipsoids centered in the origin, i.e. ellipsoids $\mathcal{E}(P(t), 0)$ containing all the points for $t \in [0, t_f]$ for given $P(0) = P_0$ and m, making sure that the end points for $t = t_f$ are enclosed by the smallest possible ellipsoid, by maximizing the trace of $P(t_f)$ (i.e. minimizing the sum of the semiaxes of the ellipsoid) under (21) and (22). Such a maximization is an optimization problem under LMI constraints, a convex problem solvable with standard tools [25, 26]. Notice that the ellipsoids found in this way are not necessarily tight. The value of m should be high enough to ensure that the polynomial matrix can accurately describe the evolution of the system, but not too high in order to keep the computational complexity of the LMI low.

Remark 7
Notice also that, even if not explicitly stated in the theorem, we can also search for ellipsoids not centered in the origin. It is sufficient to extend the state vector $x(t)$ to a state $\overline{x}(t) = [x(t)^\top \; 1]^\top$, with

A replaced by

$$\overline{A} = \begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix}. \tag{26}$$

An ellipsoid of matrix $\overline{P}$ defined for such a state is equivalent to an off-centered ellipsoid, as

$$(x-c)^\top P(x-c) \leqslant 1 \Leftrightarrow \begin{bmatrix} x \\ 1 \end{bmatrix}^\top \underbrace{\begin{bmatrix} P & -Pc \\ -c^\top P & c^\top Pc \end{bmatrix}}_{\overline{P}} \begin{bmatrix} x \\ 1 \end{bmatrix} \leqslant 1. \tag{27}$$

This lets Theorem 5 to be used also for computing any ellipsoids with respect to any initial condition, not only for those centered in the origin.

6. ROBUST SIMULATION: RATIONAL CASE

Theorem 5 can be extended to systems with rational dynamics, leading to a practical solution for Problem 2. In order to do so, as said previously, we make use of the techniques which can be found in the sum of squares (SOS) literature [12], which basically allow relaxing polynomial problems into linear algebra ones. As seen before, we define the vector $\chi \in \mathbb{R}^\rho$ as the vector containing all the possible monomials obtainable from x from degree 0 up to m_x, allowing us to write polynomial expressions up to degree m_x as a linear combination of χ. Moreover, it is also possible to express polynomials up to degree $2m_x$ as quadratic forms with respect to χ, i.e. $p(x) = \chi^\top \mathcal{S} \chi$, with $\mathcal{S} = \mathcal{S}^\top \in \mathbb{R}^{\rho \times \rho}$. This quadratic expression of a polynomial is not unique, due to the fact that different products of monomials can yield the same result, for example x_1^2 is either x_1^2 times 1 or x_1 times x_1. This implies that there exist linearly independent slack matrices $Q_k = Q_k^\top \in \mathbb{R}^{\rho \times \rho}$, with $k = 1, \ldots, \iota$ such that $\chi^\top Q_k \chi = 0$. The number of such matrices is

$$\iota = \frac{1}{2}\left(\binom{m_x+n}{m_x}^2 + \binom{m_x+n}{m_x}\right) - \binom{n+2m_x}{2m_x}. \tag{28}$$

This implies that, for a given $\mathcal{S}$, a polynomial of degree $2m$ or less can be expressed as

$$p(x) = \chi^\top \left(\mathcal{S} + \sum_{k=1}^{\iota} \psi_k Q_k\right) \chi \tag{29}$$

for any $\psi \in \mathbb{R}^\iota$, $\psi = [\psi_1, \psi_2, \ldots \psi_\iota]^\top$.

We can then formulate the theorem below, which can be used to tackle Problem 2. This theorem has the same structure of Theorem 5 with some important modifications.

Theorem 8

Consider the continuous time-invariant system described by the differential equation (4), where $\chi(t)$ expresses all the possible monomials of $x(t)$, Γ is such that $x(t) = \Gamma\chi(t)$ and $F \in \mathbb{R}^{\rho \times n}$. If 1) there exist $\mathcal{D}_1 = \mathcal{D}_1^\top \succ 0$, $\mathcal{G}_1 = -\mathcal{G}_1^\top$, $\mathcal{D}_2 = \mathcal{D}_2^\top \succ 0$, $\mathcal{G}_2 = -\mathcal{G}_2^\top$, $\alpha_i \in \mathbb{R}^\iota$, $\Omega \in \mathbb{R}^{\rho \times \rho}$ such that

$$\begin{bmatrix} \tilde{C}'^\top \\ \tilde{D}'^\top \end{bmatrix} M_1 \begin{bmatrix} \tilde{C}' & \tilde{D}' \end{bmatrix} + \begin{bmatrix} I & 0 \\ \tilde{A}' & \tilde{B}' \end{bmatrix}^\top \begin{bmatrix} -2\mathcal{D}_1 & t_f\mathcal{D}_1 + \mathcal{G}_1 \\ * & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ \tilde{A}' & \tilde{B}' \end{bmatrix} \prec 0, \tag{30}$$

$$\begin{bmatrix} \tilde{C}''^\top \\ \tilde{D}''^\top \end{bmatrix} M_2 \begin{bmatrix} \tilde{C}'' & \tilde{D}'' \end{bmatrix} + \begin{bmatrix} I & 0 \\ \tilde{A}'' & \tilde{B}'' \end{bmatrix}^\top \begin{bmatrix} -2\mathcal{D}_2 & t_f\mathcal{D}_2 + \mathcal{G}_2 \\ * & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ \tilde{A}'' & \tilde{B}'' \end{bmatrix} \preceq 0, \tag{31}$$

$$\Omega + \sum_{i=1}^{\iota} \alpha_i Q_i \succeq 0 \tag{32}$$

where

$$\phi'(t) = tI \star \begin{bmatrix} \tilde{A}' & \tilde{B}' \\ \tilde{C}' & \tilde{D}' \end{bmatrix} = \begin{bmatrix} t^m I_n \\ \vdots \\ I_n \end{bmatrix},$$

$$\phi''(t) = tI \star \begin{bmatrix} \tilde{A}'' & \tilde{B}'' \\ \tilde{C}'' & \tilde{D}'' \end{bmatrix} = \begin{bmatrix} t^m I_\rho \\ \vdots \\ I_\rho \end{bmatrix},$$

M_1 and M_2 are such that

$$\phi'(t)^\top M_1 \phi'(t) = -P(t), \tag{33}$$

$$\phi''(t)^\top M_2 \phi''(t) = F^\top P(t)\Gamma + \Gamma^\top P(t) F + \Theta(t) + \Sigma(t) + \sum_{i=1}^{\iota} v_i(t) Q_i \tag{34}$$

(the matrix M_1 is affine in the coefficients of $P(t)$, whereas the matrix M_2 is affine in the coefficients of $P(t)$, $v_i(t)$ and $\Theta(t)$ which is bi-linear in $P(t)$ and $\tau(x)$), with

- $\tau(x(t)) = \chi(t)^\top \Omega \chi(t)$, a polynomial in $x(t)$ of degree $2m_x - 2$,
- $\Sigma(t)$, a polynomial matrix in t of degree $2m$ such that $\chi(t)^\top \Sigma(t) \chi(t) = (x(t)^\top \dot{P}(t) x(t)) d(x(t))$
- $\Theta(t)$, a polynomial matrix in t of degree $2m$ such that $\chi(t)^\top \Theta(t) \chi(t) = (1 - x(t)^\top P(t) x(t)) \tau(x(t))$,
- $v_i(t) = \sum_{j=0}^{2m} v_{i,j} t^j$, with arbitrary $v_{i,j}$,
- $P(t) = \sum_{i=0}^{2m} P_i t^i, (P_i = P_i^\top, i = 0, \cdots, 2m)$,

and 2) if

$$d(x(t)) > 0, \ \forall x(t) \mid x(t)^\top P(t) x(t) \leqslant 1 \ \forall t \in [0, t_f], \tag{35}$$

then

$$\forall x(0) \mid x(0)^\top P(0) x(0) \leq 1 \Rightarrow \tilde{V}(x(t), t) = x(t)^\top P(t) x(t) \leq 1, \quad \forall t \in [0, t_f]. \tag{36}$$

Proof

The application of Lemma 4 to inequalities (30) and (31) implies that (33) is negative definite and that (34) is negative semi-definite. To have (33) negative definite implies that $\tilde{V}(x(t), t) = x(t)^\top P(t) x(t) > 0$ as required in (11). For what concerns the negative semi-definiteness of (31), we multiply both sides by $\chi(t)$ and then we get

$$\chi(t)^\top \left(F^\top P(t)\Gamma + \Gamma^\top P(t) F + \Theta(t) + \Sigma(t) + \sum_{i=1}^{\iota} v_i(t) Q_i \right) \chi(t) \leqslant 0 \tag{37}$$

In (37), the term $\chi(t)^\top (\sum_{i=1}^{\iota} v_i(t) Q_i) \chi(t)$ is a slack term that equals 0. Then, thanks to the S-procedure (with an x-varying multiplier [27]), if $(1 - x(t)^\top P(t) x(t)) \geq 0$, which is what we demand, and $\tau(x(t)) \geq 0$, which is implied by (32), then

$$N(x(t))^\top P(t) x(t) + x(t)^\top P(t) N(x(t)) + (x(t)^\top \dot{P}(t) x(t)) d(x(t)) \leqslant 0. \tag{38}$$

Dividing by $d(x(t))$, which is possible due to the condition in (35), we have

$$\dot{x}(t)^\top P(t) x(t) + x(t)^\top P(t) \dot{x}(t) + x(t)^\top \dot{P}(t) x(t) \leqslant 0 \tag{39}$$

which means $\dot{V}(x(t), t) \leqslant 0$, i.e. the value of $\tilde{V}$ will not grow, implying (36). □

Algorithm 9

Problem 2 can be solved by maximizing the trace of $P(t_f)$ with respect to the three inequalities (30), (31) and (32), for the unknowns ($P_1, \ldots, P_{2m}$, $\mathcal{D}_1, \mathcal{D}_2, \mathcal{G}_1$and $\mathcal{G}_2$), Ω (not a full matrix, but structured in order to limit the degree of $\tau(x(t))$ to $2m_x - 2$), α_i, $v_{i,j}$. Such a maximization

is unfortunately not a convex optimisation problem, due to the bi-linearity of the term $(1 - \Gamma^\top P(t)\Gamma)\tau(x(t))$. Nevertheless, the theorem can be used as in the previous case either by deleting the disturbing term (it is an arbitrary, conservative choice of $\tau(x(t)) = 0$), or by replacing the $P(t)$ inside it with a guessed term $H(t)$ that overestimates the span of the state, i.e. such that $\left\{x(t)|x(t)^\top P(t)x(t) \leqslant 1\right\} \subset \left\{x(t)|x(t)^\top H(t)x(t) \leqslant 1\right\}$. This guess can subsequently be refined by iterating the solution. In both these cases the problem becomes a convex optimization problem under LMI constraints. Another possible approach, not explored in this paper, is of course to try and solve directly the bilinear matrix inequality with an appropriate solver.

The condition for $d(x(t)) > 0$, if needed, can be verified with a sum of squares kind of condition, i.e. by testing $d(x(t)) - \eta(x(t))(1 - x(t)^\top P(t)x(t)^\top) > 0$ for $t \in [0, t_f]$, with $\eta(x(t)) \geqslant 0$ a polynomial.

7. EXAMPLE OF APPLICATION

In order to show the effectiveness of this method, we consider a very simple nonlinear dynamical system from biology, namely the Lotka-Volterra model for predator-prey populations [28]. According to this model, the evolution of the population x_1 of a species which is prey for a second species (the predator) whose population is x_2, both interacting in a closed environment, is described by

$$\begin{cases} \dot{x_1} = \alpha x_1 - \beta x_1 x_2 \\ \dot{x_2} = \delta x_1 x_2 - \gamma x_2 \end{cases} \tag{40}$$

with α, β, γ, δ specific constants. This model is of course quite simple, with several approximations including the fact that the populations are considered real numbers whereas they are obviously integer.

We pick an arbitrary model with $\alpha = 0.13$ year^{-1}, $\beta = 0.0066$ year^{-1}, $\gamma = 0.20$ year^{-1}, $\delta = 0.0002$ year^{-1}, with an initial population of 1000 ± 100 prey and 40 ± 4 predators, (which we adapt into an ellipsoidal description). We try and use Algorithm 9 and Theorem 8 to simulate the system for a span of 15 years, using Matlab with Yalmip [25] and SeDuMi [26]. We have chosen $m = 4$, and we have verified that it is not possible to simulate the whole 15-year interval in one single go (i.e., solving the optimisation in Algorithm 9 for $t_f = 15$ years), so we have cut the interval into smaller intervals of one year each, and propagated the simulation at the end of each interval by using the final result of each step as initial value for the following. Moreover, for each time step we have solved two optimisation problems, as explained in Algorithm 9; the first optimisation problem uses a time-constant guessed H term "wide" enough to encompass the evolution of the state for all $t \in [0, t_f]$, and subsequently we use the $P(t)$ result of the first optimisation in order to run a second one, using this first $P(t)$ as $H(t)$ and refining the result (see Figure 1). Further iterations would improve the result even more, but we have decided to stop at just two. The choice of m and the length of each sub-interval has to be considered as a compromise between computational complexity and accuracy: bigger values m and smaller time spans lead to more precision, at the cost of slower computations. A value of m too small, or a span which is too long might even lead the optimization to fail finding a solution, as it is the case for us if we try and compute the solution over the 15 years.

Figure 2 shows the results of the complete simulation, compared with points from a Monte Carlo simulation. We can see that the method effectively bounds all such points, confirming that it is "safe", on the other hand we can also see that the bounding ellipses are not tight, which is a drawback of the method but which could be partially eased by running more iterations at each time step.

8. CONCLUSIONS

In this paper we have shown a method which can be employed in order to validate the properties of a continuous-dynamical systems through a robust simulation. The method offers hard mathematical

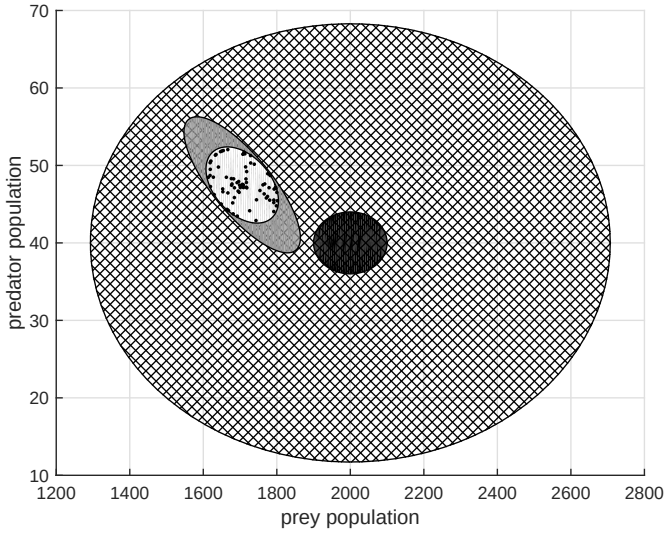

Figure 1. Lotka-Volterra model, one iteration. The blue ellipse in the center is the set of initial conditions, the black ellipse is the set enclosed by the guessed time-constant term H, the dark red ellipse shows the result of the first optimisation for $t = t_f$, whereas the bright red one shows the result of the second again for $t = t_f$. The black dots represent the values of some simulations at $t = t_f$ for states which were in the initial set at $t = 0$.

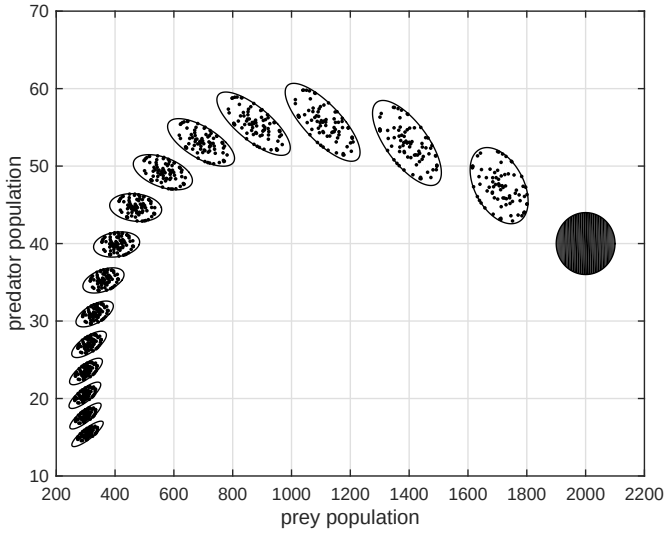

Figure 2. Lotka-Volterra model, evolution of the state-bounding ellipsoid over several times steps, covering a period of 15 years. The blue ellipse (first on the right) is the set of initial conditions, the bright red ellipses are the bounding sets at the end of each year, and the black dots show the values of some Monte Carlo simulations.

bounds but it requires solving a convex optimisation for each simulated time interval, which can be computationally intensive. In any case, we believe that this method can be helpful in relevant application, proposing a different and complementary approach with respect to the usual Monte Carlo approach.

Future research will focus on introducing robustness with respect to uncertainties in the model parameters, which should be possible by using the LMI-based theory on robust control. We are

also interested in applying the methods to the simulation of real-life systems, and specifically to aerospace systems. Another interesting approach which will be explored is the use of Koopman operators and their eigenfunctions [17, 29], which might allow the search for a state transformation that can linearise a system in the large [30], simplifying the simulation problem.

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