Reachability Analysis of Nonlinear Systems Using Matrix Measures

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***Abstract*—Matrix measures, also known as logarithmic norms, have historically been used to provide bounds on the divergence of trajectories of a system of ordinary differential equations. In this technical note we use them to compute guaranteed over-approximations of reachable sets for nonlinear continuous-time systems using numerically simulated trajectories and to bound the accumulation of numerical simulation errors along simulation traces. Our method employs a user-supplied bound on the matrix measure of the system's Jacobian matrix to compute bounds on the behavior of nearby trajectories, leading to efficient computation of reachable sets when such bounds are available. We demonstrate that the proposed technique scales well to systems with a large number of states.**

***Index Terms*—Differential equations, nonlinear dynamical system.**

I. Introduction

Given a nonlinear dynamical system

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

with $f : [0, \infty) \times \mathbb{R}^n \to \mathbb{R}^n$ continuous in t and C^1 in x, and a bounded set of initial states, we consider the problem of computing an overapproximation of the set of states reachable from these initial states in finite time. Computing such sets allows finite-time safety specifications to be verified by demonstrating that no trajectory of the system originating from a given set of initial conditions can reach a set of states labeled "unsafe." Existing approaches to this problem include level set methods [1], generating linear or piecewise linear models approximating the nonlinear dynamics for which linear reachability techniques can be applied [2], [3], methods based on simulation relations [4], [5], interval Taylor series methods [6], [7], differential inequality methods [8], [9], and numerical simulation-based approaches [10]–[13]. Simulation-based approaches have the advantage that numerical simulation is a relatively inexpensive operation, even for systems with a large number of states. Thus unlike the more computationally expensive approaches, they have the potential to scale well with state dimension.

Simulation-based methods have further advantages: first, if the method fails to compute a reachable set accurate enough to verify a given safety property, they provide information about the regions of the state space that require additional simulations to be performed before safety can be verified or an unsafe trajectory generated. Therefore these approaches can lead to iterative schemes for safety verification, such as the one presented in [10]. In addition, simulation-based approaches are naturally parallelizable due to the fact that simulations and expansion bounds for each initial condition considered can be computed independently. Finally, numerical simulation is a common method used in industrial practice to search for undesirable behaviors of a modelled system. Thus formal verification methods that leverage simulation have the potential for wide adoption.

We consider a simulation-based approach where we first sample a number of trajectories of the system and next establish a bound on the divergence between the samples and neighbouring trajectories. In particular we use a user-supplied bound on the matrix measure to generate a bound on this divergence. Unlike [10] which also takes a simulation-based approach but is not able to guarantee that the computed approximation contains the true reachable set, here we provide a guaranteed overapproximation of the set of reachable states. Thus our technique can be used to provide formal guarantees of safety. Another related method is [13] which uses finite-time invariant sets computed using sum-of-squares methods to bound the divergence of trajectories. We provide a comparison of our method with this approach in Section V.

We begin by surveying existing results related to matrix measures in Section II. In Section III we demonstrate that our matrix measure approach to nonlinear reachability analysis provides a guaranteed overapproximation of the set of reachable states of the system. The approximation can be made arbitrarily accurate by choosing a sufficiently fine mesh of initial states. We then provide a method of improving the accuracy of the approximation by weighting matrix measures in an optimal manner. In Section IV we use the matrix measure for analysing the accumulation of numerical errors along simulated trajectories of the system. Finally, in Section V we demonstrate our method on a model of a relaxation oscillator taken from [14] and a model of a biological transcription cascade from [15].

II. Overview of Matrix Measures and Contraction

Let $|\cdot|$ be a norm on $\mathbb{R}^n$ and $\|\cdot\|$ be its induced norm on the set of real matrices of dimension $n \times n$. The measure $\mu(A)$ of a matrix $A \in \mathbb{R}^{n\times n}$ is the one-sided derivative of $\|\cdot\|$ at $I \in \mathbb{R}^{n\times n}$ in the direction A

$$\mu(A) = \lim_{t\to 0^+} \frac{\|I + tA\| - \|I\|}{t}. \tag{2}$$

This limit is guaranteed to exist for any norm $|\cdot|$ and $A \in \mathbb{R}^{n\times n}$ (see [16]). The following properties of μ are of interest to us [16], [17].

1) For all eigenvalues $\lambda_i(A)$ of A we have $-\|A\| \le -\mu(-A) \le \Re(\lambda_i(A)) \le \mu(A) \le \|A\|$.
2) $\mu(cA) = c\mu(A)$ for all $c \ge 0$.
3) $\mu(A + B) \le \mu(A) + \mu(B)$.
4) If $P \in \mathbb{R}^{n\times n}$ is nonsingular then the measure μ_P of the norm $|x|_P = |Px|$ is given in terms of μ by $\mu_P(A) = \mu(PAP^{-1})$.

Some familiar vector norms as well as their corresponding induced matrix norms and measures are given in Table I.

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TABLE I
COMMONLY USED VECTOR NORMS AND THEIR CORRESPONDING MATRIX NORMS AND MEASURES

Vector norm	Induced matrix norm	Induced matrix measure
$\|x\|_1 = \sum_j \|x_j\|$	$\|A\|_1 = \max_j \sum_i \|a_{ij}\|$	$\mu_1(A) = \max_j \left(a_{jj} + \sum_{i\neq j} \|a_{ij}\|\right)$
$\|x\|_2 = \sqrt{\sum_j x_j^2}$	$\|A\|_2 = \sqrt{\max_j \lambda_j(A^T A)}$	$\mu_2(A) = \max_j \frac{1}{2}\left(\lambda_j(A + A^T)\right)$
$\|x\|_\infty = \max_j \|x_j\|$	$\|A\|_\infty = \max_i \sum_j \|a_{ij}\|$	$\mu_\infty(A) = \max_i \left(a_{ii} + \sum_{j\neq i} \|a_{ij}\|\right)$

The matrix measure has long been used to provide estimates on solutions of systems of ordinary differential equations [16]–[20]. The following proposition allows us to bound the distance between trajectories in terms of their initial distance and the rate of expansion of the system given by the measure of the Jacobian matrix $J(t,x)$ with respect to x.

Proposition 1: Let $\mathcal{D} \subseteq \mathbb{R}^n$ and let the Jacobian $J(t,x) = (\partial f/\partial x)(t,x)$ satisfy $\mu(J(t,x)) \leq c$ for all $(t,x) \in [0,T] \times \mathcal{D}$. If every trajectory of (1) with initial conditions in the line segment $\{hx_0 + (1-h)z_0 : h \in [0,1]\}$ remains in $\mathcal{D}$ until time T then the solutions $\xi(t)$ and $\zeta(t)$ with $\xi(0) = x_0$ and $\zeta(0) = z_0$ satisfy

$$|\xi(t) - \zeta(t)| \leq |\xi(0) - \zeta(0)| e^{ct} \tag{3}$$

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

The proof of Proposition 1 is given in [20] emphasizing the case that $c < 0$. It holds for any $c \in \mathbb{R}$ following the same argument. The proposition provides global results about the divergence between trajectories of (1) using only information about the system's Jacobian at each point.

If there exists $c < 0$ such that for all $(t,x) \in [0,\infty) \times \mathcal{D}$ we have $\mu(J(t,x)) \leq c$ then the system (1) or the vector field $f(t,x)$ is said to be contracting with respect to $|\cdot|$. From (3) it follows that for such systems any two trajectories converge asymptotically. Unlike the literature on contractive or incrementally stable systems [20]–[22] which deals primarily with the case where $c < 0$, our results allow the expansion rate c to be positive.

III. OVERAPPROXIMATION OF REACHABLE SETS

Given a compact initial set K and final time T we wish to find a set R such that all trajectories $\xi(\cdot, x_0)$ of (1) with initial condition $\xi(0,x_0) = x_0 \in K$ satisfy $\xi(T,x_0) \in R$. To simplify the presentation, we assume throughout Section III that trajectories of (1) can be computed exactly. In Section IV we will extend the results presented here to ensure that numerical inaccuracies due to floating point arithmetic and discretization of the continuous dynamics are accounted for.

Before continuing, we introduce the required notation. The ball with radius ϵ and centre x_0 is given by $\{x : |x - x_0| \leq \epsilon\}$ and is denoted $\mathcal{B}_\epsilon(x_0)$. Throughout, we denote the solution to the differential equation (1) with initial condition x_0 as $\xi(t,x_0)$, or when it is clear that we have fixed a particular initial condition x_0, simply as $\xi(t)$. The set reachable at time t from initial set S is denoted $Reach_t(S)$ and is defined as $\{\xi(t,x) : x \in S\}$. The tube reachable from the initial set S over an interval $[0,t]$ is denoted $Reach_{[0,t]}(S) = \{\xi(s,x) : s \in [0,t], x \in S\}$. For symmetric matrices A and B, the inequality $A \preceq B$ means that $B - A$ is positive semidefinite and $A \prec B$ means that $B - A$ is positive definite. For a set $X \subseteq Y$, the error with which Y overapproximates X can be quantified via the Hausdorff distance $d(X,Y) = \sup_{y\in Y} \inf_{x\in X} |x - y|$.

A. Basic Algorithm

We begin by covering the initial set K by a finite number of norm balls $\mathcal{B}_{\epsilon_k}(x_k)$. The set reachable from K is contained in the union of the sets reachable from these norm balls. The number of balls can be chosen so as to achieve the required accuracy in the approximation of the reachable set; a larger number of balls provides a more accurate approximation, while covering K by a single ball reduces computation time at the cost of reduced accuracy. The computation of the set reachable from each norm ball can be performed in parallel, thus we assume without loss of generality that the initial set is given by a single norm ball $K = \mathcal{B}_\epsilon(x_0)$.

In light of Proposition 1, given a global bound c on $\mu(J(t,x))$, we know that all trajectories of (1) with initial conditions in $\mathcal{B}_\epsilon(x_0)$ lie in $\mathcal{B}_{\epsilon e^{cT}}(\xi(T,x_0))$. Since a global bound c on the expansion rate is far too conservative, we provide an iterative method for computing a more accurate approximation based on a local bound on the expansion rate. We begin with the following corollary of Proposition 1.

Corollary 1: Let the Jacobian $J(t,x)$ of $f(t,x)$ with respect to x satisfy $\mu(J(t,x)) \leq c_i$ for all $(t,x) \in [t_i, t_{i+1}] Reach_{[t_i,t_{i+1}]} \times (\mathcal{B}_{\delta_i}(\xi(t_i)))$. Then any solution ζ of (1) with $\zeta(t_i) \in \mathcal{B}_{\delta_i}(\xi(t_i))$ satisfies

$$|\xi(t_{i+1}) - \zeta(t_{i+1})| \leq |\xi(t_i) - \zeta(t_i)|\, e^{c_i(t_{i+1}-t_i)}. \tag{4}$$

Thus given a sequence of local bounds c_i we can compute a guaranteed overapproximation of $Reach_T(\mathcal{B}_\epsilon(x_0))$ as $\mathcal{B}_\delta(\xi(T,x_0))$ where

$$\delta = \left(\prod_{i=0}^{N-1} e^{c_i(t_{i+1}-t_i)}\right)\epsilon.$$

The set $Reach_{[t_i,t_{i+1}]}(\mathcal{B}_{\delta_i}(\xi(t_i)))$ is generally not known, but a crude overapproximation will suffice for the purpose of computing the constant c_i. For example if we can find some crude bound S on $Reach_{[0,T]}(K)$ (for example an invariant set containing K) such that $|f(t,x)| \leq M$ for all $t \in [0,T]$ and all $x \in S$ then we have the containment

$$Reach_{[t_i,t_{i+1}]}\left(\mathcal{B}_{\delta_i}\left(\xi(t_i)\right)\right) \subseteq \mathcal{B}_{\delta_i + M(t_{i+1}-t_i)}\left(\xi(t_i)\right).$$

Note that once an overapproximation of the reach set is computed using our method, this bound can then be used to recompute a smaller M and the method reapplied to generate an even tighter approximation. Our method is described in Algorithm 1.

Algorithm 1 Basic algorithm for bounding $Reach_T(K)$

Require: Initial ball size $\epsilon > 0$, bound M on magnitude of vector field f, sequence of simulation points $x_i := \xi(t_i)$ for $i = 0, \ldots, N$

1: Set $\delta_0 = \epsilon$
2: **for** i from 0 to $N-1$ **do**
3: Compute upper bound c_i on expansion rate $\mu(J(t,x))$ within the set with
4: $t_i \leq t \leq t_{i+1}$ and $|x - x_i| \leq \delta_i + M(t_{i+1} - t_i)$.
5: Set $\delta_{i+1} = e^{c_i(t_{i+1}-t_i)}\delta_i$
6: **end for**
7: **return** $\mathcal{B}_{\delta_N}(x_N)$

Corollary 1 ensures that Algorithm 1 yields an overapproximation of the set of reachable states. The following additional corollaries of Proposition 1 provide information about the tightness of this approximation. Corollary 2 establishes that the approximation can be made arbitrarily accurate by covering the initial set K by a collection of balls of sufficiently small radius. Corollary 3 establishes that for contractive systems, a single ball overapproximating the initial set K is sufficient to generate an approximation that becomes arbitrarily tight as $T \to \infty$.

Corollary 2 (Tightness as a Function of Mesh Size): Let $\mathcal{D} \subseteq \mathbb{R}^n$ and let the Jacobian $J(t,x)$ of f with respect to x satisfy $\mu(J(t,x)) \leq c$ for all $(t,x) \in [0,\infty) \times \mathcal{D}$. Then the approximation error $d(Reach_t(\mathcal{B}_\epsilon(x_0)), \mathcal{B}_{e^{ct}\epsilon}(\xi(t,x_0)) \to 0$ linearly as $\epsilon \to 0$.

Corollary 3 (Asymptotic Tightness for Contractive Systems): Let $\mathcal{D} \subseteq \mathbb{R}^n$ and let f satisfy $\mu(J(t,x)) \leq c < 0$ for all $(t,x) \in [0,\infty) \times \mathcal{D}$. Then the approximation error $d(Reach_T(\mathcal{B}_\epsilon(x_0)), \mathcal{B}_{e^{cT}\epsilon}(\xi(T,x_0))) \to 0$ exponentially as $T \to \infty$.

Note that covering a set $S \subseteq \mathbb{R}^n$ by a uniform mesh of radius ϵ requires $\Theta(\epsilon^{-n})$ mesh points and hence the practical applicability of these tightness results is limited. However, methods exist in the literature for choosing non-uniform meshes of trajectories to simulate (e.g. Section 3 of [10]) which help alleviate this problem.

B. Algorithm With Norm Updating

We now provide a modified scheme that allows us to optimize the norm in which the expansion is measured at a given time and state (t,x). We consider a family of weighted norms $\{|\cdot|_\Gamma\}$ parametrized by weights Γ from some set of real $n \times n$ matrices. Given an initial set B_i described as a norm ball of $|\cdot|_{\Gamma_i}$ we

- overapproximate the initial ball B_i by a ball $\bar{B}_i$ in some new norm $|\cdot|_{\Gamma_{i+1}}$
- compute an expansion rate c_{i+1} at the point (t_i, x_i) satisfying $c_{i+1} \geq \mu_{\Gamma_{i+1}}(J(t_i,x_i))$ where $\mu_{\Gamma_{i+1}}$ is the matrix measure induced by $|\cdot|_{\Gamma_{i+1}}$ (Recall that μ_Γ can be computed in terms of μ via Property 4 from Section II.)
- compute an overapproximation of the set reachable form $\bar{B}_i$ using the expansion rate c_{i+1}. This gives the new set B_{i+1}.

It may appear that Γ_{i+1} should be selected to minimize c_{i+1}. However there is a tradeoff between how small we can make c_{i+1} and how tightly $\bar{B}_i$ approximates B_i. Thus, at each step we choose Γ_{i+1} such that the volume $\mathrm{vol}(B_{i+1})$ is minimized

$$\begin{aligned} \textbf{minimize} \quad & \mathrm{vol}(B_{i+1}) \\ \textbf{subject to} \quad & B_i \subseteq \bar{B}_i \\ & \mu_{\Gamma_{i+1}}(J(t_i,x_i)) \leq c_{i+1}. \end{aligned} \tag{5}$$

For certain families of norms, this can be formulated as an optimization problem that is convex in the weighting Γ. We now describe three such cases.

1) Euclidean Norms Weighted by Positive Definite Matrices: We consider the family of weighted Euclidean norms of the form $x \mapsto |Px|_2$ where P is a positive definite matrix. There is a one-to-one correspondence between such norms and their unit balls, described by the nondegenerate ellipsoid $\{x : x^T \Gamma x \leq 1\}$ and parametrized by $\Gamma = P^2$ from the set of positive definite matrices.

The following proposition relates Γ with the expansion rate of (1) at (t,x).

Proposition 2 (Lemma 2 of [23]): If $\Gamma J(t,x) + J(t,x)^T \Gamma \leq 2c\Gamma$ where Γ is a positive definite matrix then $\mu(J(t,x)) \leq c$ in the norm $x \mapsto |Px|_2$ where $P = \Gamma^{1/2} \succ 0$.

If $B_i = \{x : x^T \Gamma_i x \leq 1\}$ and $\bar{B}_i = \{x : x^T \Gamma_{i+1} x \leq 1\}$ then the constraint $B_i \subseteq \bar{B}_i$ can be expressed in terms of the parameters as $\Gamma_{i+1} \preceq \Gamma_i$.

The set reachable from $\{x_i + x : x^T \Gamma_{i+1} x \leq 1\}$ is approximated by $\{x_{i+1} + x : x^T \Gamma_{i+1} x \leq e^{2c(t_{i+1}-t_i)}\}$ where c_{i+1} satisfies $\Gamma_{i+1} J(t_i,x_i) + J(t_i,x_i)^T \Gamma_{i+1} \leq 2c\Gamma_{i+1}$. We wish to choose Γ_{i+1} so as to minimize the volume of the computed reach set $B_{i+1} = \{x_{i+1} + x : x^T \Gamma_{i+1} x \leq e^{2c(t_{i+1}-t_i)}\}$. As the volume of the ellipsoid $\{x : x^T \Gamma x \leq 1\}$ is proportional to $\det(P^{-1})$, the volume $\mathrm{vol}(B_{i+1})$ is proportional to $1/\sqrt{\det(e^{-2c(t_{i+1}-t_i)}\Gamma_{i+1})}$. Problem (5) can now be cast as the following convex problem:

$$\begin{aligned} \textbf{minimize} \quad & -e^{-2c(t_{i+1}-t_i)} \det(\Gamma_{i+1})^{\frac{1}{n}} \\ \textbf{subject to} \quad & \Gamma_{i+1} \preceq \Gamma_i \\ & \Gamma_{i+1} J(t_i,x_i) + J(t_i,x_i)^T \Gamma_{i+1} \preceq 2c\Gamma_{i+1}. \end{aligned} \tag{6}$$

For fixed $c \in \mathbb{R}$ this is a convex problem in the variable Γ_{i+1}. Thus a solution can be found via a line search over c where each evaluation involves solving this convex problem.

Once we have chosen Γ_{i+1}, we proceed as in Section III-A. This leads to Algorithm 2 below for computing an overapproximation of the reachable set using weighted norms, with the weights adjusted at each step.

Algorithm 2 Bounding of reachable set from norm ball based on weighted Euclidean norms

Require: Initial ball shape matrix Γ_0, sequence of simulation points $x_i := \xi(t_i)$ for $i = 0, \ldots, N$.

1: **for** i from 0 to $N-1$ **do**
2: Find (c, Γ_{i+1}) to solve optimization problem (6)
3: Compute bound M on magnitude of vector field f in norm defined by Γ_{i+1}
4: Compute upper bound c_i on expansion rate $\mu(J(t,x))$ within the set with
5: $t_i \leq t \leq t_{i+1}$ and $\{x_i + x : x^T \Gamma_{i+1} x \leq 1 + M(t_{i+1} - t_i)\}$.
6: Set $\Gamma_{i+1} = e^{-2c_i(t_{i+1}-t_i)}\Gamma_{i+1}$
7:
8: **end for**
9: **return** $\{x_N + x : x^T \Gamma_N x \leq 1\}$

2) 1-Norms Weighted by Positive Diagonal Matrices: We now show that using norms $|x|_{1,D} = |Dx|_1$ parametrized by positive diagonal matrices $D \succ 0$ also leads to a convex optimization problem. The corresponding induced matrix measure $\mu_{1,D}$ is given by

$$\mu_{1,D}(A) = \mu_1(DAD^{-1}) = \max_j \left(a_{jj} + \sum_{i \neq j} \frac{d_i}{d_j} |a_{ij}| \right)$$

hence the condition $\mu_{1,D}(A) \leq c$ can be expressed as $a_{jj}d_j + \sum_{i \neq j} |a_{ij}| d_i \leq c d_j$ for $j = 1, \ldots, n$ which is linear in the d_i for fixed c. The condition $\{x : |x|_{1,P} \leq 1\} \subseteq \{x : |x|_{1,D} \leq 1\}$ requires that $d_j \leq p_j$ for all $j = 1, \ldots, n$. Finally, the volume of the set $\{x : |x|_{1,D} \leq e^{ct}\}$ is proportional to $e^{nct} \prod_{i=1}^n (1/d_i)$ which is convex in d. Thus if D is a solution to the problem

$$\begin{aligned} \textbf{minimize} \quad & \left(e^{nct} \prod_{i=1}^n \frac{1}{d_i} \right)^{\frac{1}{n}} \\ \textbf{subject to} \quad & D \preceq P \\ & a_{jj}d_j + \sum_{i \neq j} |a_{ij}| d_i \leq c d_j \quad j = 1, \ldots, n \end{aligned} \tag{7}$$

where $A = J(t,x)$ then $|\cdot|_{1,D}$ is a good norm in which to overapproximate the reachable set in a neighbourhood of the point (t,x) in order to minimize the accumulation in volume. As with problem (6) in

the Euclidean case, the problem (7) is convex in D for fixed c. Hence it can be readily solved via a line search over c.

3) ∞-Norms Weighted by Positive Diagonal Matrices: For norms of the form $|x|_{\infty,D} = |Dx|_\infty$ where $D \succ 0$ is a positive diagonal matrix, a similar procedure yields the problem

$$\begin{aligned} \textbf{minimize} \quad & e^{nct} \prod_{i=1}^{n} \frac{1}{d_i} \\ \textbf{subject to} \quad & \frac{d_i}{p_i} \leq 1 \quad i = 1, \ldots, n \\ & \frac{1}{c - a_{ii}} \sum_{j \neq i} |a_{ij}| \frac{d_i}{d_j} \leq 1 \quad i = 1, \ldots, n. \end{aligned} \tag{8}$$

which is a geometric program in posynomial form. This problem is not necessarily convex in the d_i, but can be transformed to an equivalent convex problem (see Section 4.5.3 of [24]).

IV. Bounding Error Due to Numerical Integration

Numerical solvers for ordinary differential equations suffer from errors inherent in the discretization of continuous-time systems. Performing simulation-based verification of a continuous-time model thus requires a bound on the accumulated numerical error over subsequent time steps. The matrix measure has been used for the analysis of numerical algorithms for ordinary differential equations [17]–[19]. We extend these results to provide reachability algorithms that are robust against numerical error.

We again consider the system (1) with $f : [0, T] \times \mathbb{R}^n \to \mathbb{R}^n$ continuous in t and C^1 in x. We are given a simulation trace $(t_0, x_0), (t_1, x_1), \ldots, (t_l, x_l)$ of this system with initial condition x_0 and an accuracy constant $K_a > 0$ such that $|\xi(t_{i+1} - t_i, x_i) - x_{i+1}| \leq K_a$ for all $i = 0, \ldots, l-1$. We wish to compute a set guaranteed to contain the true system trajectory $\xi(\cdot, x_0)$.

Reference [11] provides a solution to this problem using a Lipschitz constant. We demonstrate here an alternative procedure using the matrix measure. As a consequence of property 1 of the matrix measure: $\mu(A) \leq \|A\|$, our method provides at least as good a bound on the accumulated error as a similar method using the Lipschitz constant. Unlike the Lipschitz constant which is always positive, leading to bounds on the reachable set that necessarily diverge exponentially as the time horizon increases, the matrix measure is negative for contractive systems and thus can provide bounds on the reachable set that improve with time.

We now extend our results from Section III to develop a verification method that provides guarantees robust against numerical error.

Proposition 3: Define $\epsilon_0 = 0$. For each $i = 0, \ldots, l-1$ suppose that we can find $c_i \in \mathbb{R}$ such that $\mu(J(t, x)) \leq c_i$ for all $(t, x) \in [t_i, t_{i+1}] \times Reach_{[t_i . t_{i+1}]}(\mathcal{B}_{\epsilon_i}(x_i))$. Define $\epsilon_{i+1} = \epsilon_i e^{c_i(t_{i+1} - t_i)} + K_a$. We have the following bounds on the accumulated numerical error:

$$|\xi(t_i, x_0) - x_i| \leq \epsilon_i \quad i = 0, \ldots, l \tag{9}$$

In light of Proposition 3 we can account for numerical error in Algorithm 1 by modifying line 5 as

5: $\delta_{i+1} = e^{c_i(t_{i+1} - t_i)} \delta_i + K_a$.

The extension of Algorithm 2 to be robust to numerical error is less straightforward, as we need a bound K_a' on the numerical error in the weighted Euclidean norm $|x|_{\Gamma_i} = x^T \Gamma_i x$ being used at each step. If we have $|\xi(t_{i+1} - t_i, x_i) - x_{i+1}| \leq K_a$ in the initial norm $|x| = x^T \Gamma_0 x$ then the bound K_a' can be computed as $K_a' = \sqrt{s}$ where s is the solution to the optimization problem

$$\begin{aligned} \textbf{minimize} \quad & s \\ \textbf{subject to} \quad & K_a^2 \Gamma_i \preceq s \Gamma_0 \end{aligned} \tag{10}$$

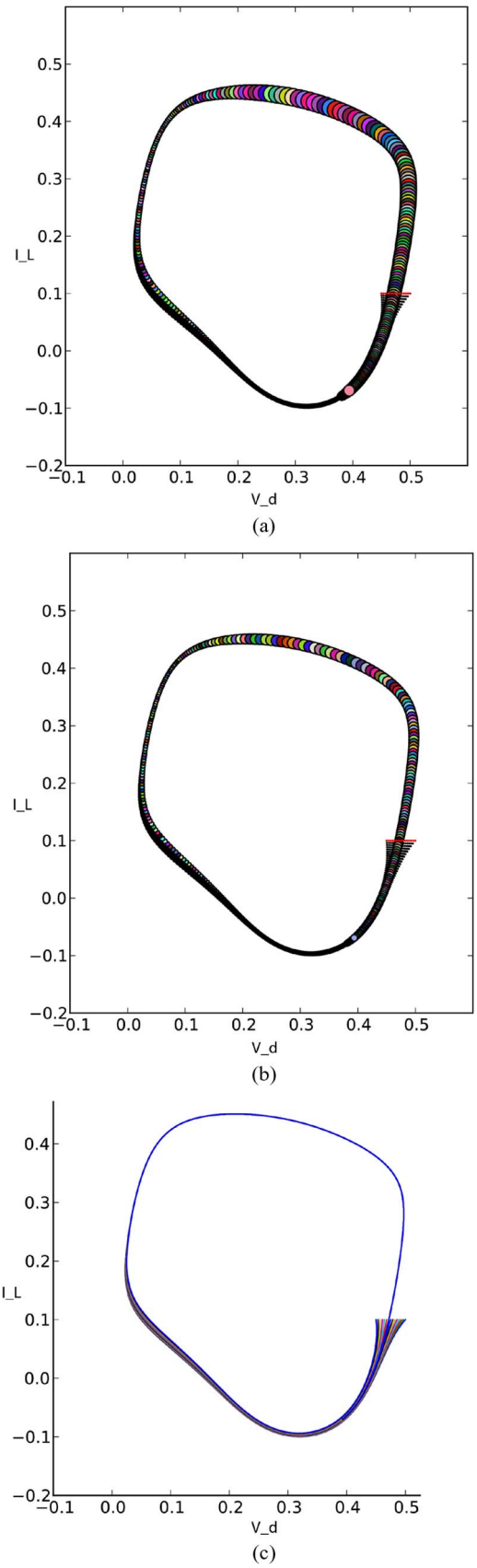

Fig. 1. Approximated reachable sets for the tunnel-diode oscillator with initial set K in red. (a) Overapproximation of the reachable set in Euclidean norm (Algorithm 1). Figure generated in 158 s. (b) Overapproximation of the reachable set using weighted Euclidean norms (Algorithm 2). Figure generated in 7979 s. (c) Approximation of the reachable set by brute force simulation.

TABLE II
COMPARISON OF TIME TO COMPUTE REACHABLE SET FOR SYSTEMS OF VARYING DIMENSION USING ALGORITHM 1 AND THE SUM-OF-SQUARES METHOD DESCRIBED IN [13]. THE SYMBOL $*$ INDICATES THAT THE COMPUTATION DID NOT RETURN WITHIN 10 000 s

state dimension	4	10	20	50	100	150	200
matrix measure computation time (s)	0.022	0.030	0.051	0.161	0.504	1.045	1.786
SOS computation time (s)	12.221	2527.851	*	*	*	*	*

The solution to this problem can then be incorporated to the update of Γ_{i+1} in Algorithm 2 by modifying lines 6 and 7 as

6: Find solution s to optimization problem (10)
7: Set $\Gamma_{i+1} = (1/e^{2c_i(t_{i+1}-t_i)} + s)\Gamma_i$.

V. APPLICATIONS

A. Tunnel Diode Oscillator

We consider a 2-dimensional model of a tunnel-diode oscillator which has been analysed by several authors for safety verification in [10], [14], [25]. The state equations are given by

$$\dot{V}_d = \frac{1}{C}\left(-I_d(V_d) + I_L\right) \quad \dot{I}_L = \frac{1}{L}(-V_d - R \cdot I_L + V_{in})$$

where $C = 1$ pF, $L = 1$ μH, $R = 200$ Ω, $V_{in} = 0.3$ V. The diode characteristic is approximated by a fifth degree polynomial $I_d(V_d) = 803.712(V_d)^5 - 1086.288(V_d)^4 + 551.088(V_d)^3 - 124.548(V_d)^2 + 10.656(V_d)$. We consider the initial set $K = \{(V_d, I_L) : V_d \in [0.45, 0.50], I_L = 0.1\}$ over a horizon of $T = 9$ ns with an absolute tolerance $k = 10^{-8}$. For this problem, the measure of the Jacobian can be computed explicitly as a function of the state V_d as seen in the equation shown at the bottom of the page. This function is quasiconvcave with a maximum at V_d^* and hence a bound on the matrix measure over an interval $[a, b]$ can be computed as

$$\max_{V_d \in [a,b]} \mu_2\left(J(V_d)\right) = \begin{cases} \mu_2\left(J\left(V_d^*\right)\right) & \text{if } V_d^* \in [a,b] \\ \max\left\{\mu_2\left(J(a)\right), \mu_2\left(J(b)\right)\right\} & \text{otherwise.} \end{cases}$$

We compute overapproximations of the reachable set at 400 evenly-spaced times using Algorithms 1 and 2. The matrix measure reachability computations are performed using Python 2.7.1 running on a machine with a 2.3 GHz Intel Core i7 processor and 8.0 GB RAM. CVXPY is used to solve the semidefinite programs required for Algorithm 2. For comparison, we also provide an underapproximation of the reachable set computed by simulating a finite number of trajectories of the system. For this low-dimensional system, this provides a good approximation of the true reachable set. These approximations are shown in Fig. 1.

We see that using Algorithm 1 [Fig. 1(a)] generates an overapproximation that is somewhat conservative compared with the brute force simulations in Fig. 1(c). We see in Fig. 1(b) that the approximation can be improved by updating the norm weights as in Algorithm 2 at the expense of a significant increase in CPU time. Note that this example demonstrates that reasonably tight bounds on the reachable set can be generated even for systems in which the matrix measure of the Jacobian is positive in some regions of the state space. This leads to the expansion of the norm balls in the region where V_d is approximately 0.1, but does not lead to undue expansion globally since bounds on the matrix measure are computed within a local region.

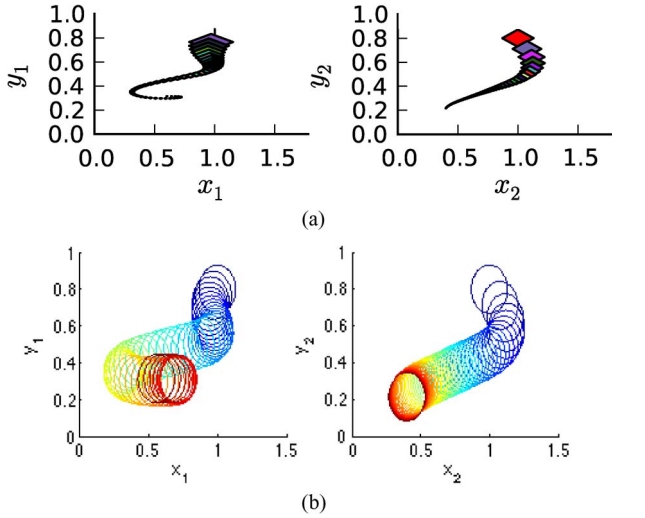

Fig. 2. Overapproximation of reachable sets projected onto (x_i, y_i) coordinate planes. (a) Overapproximation of the reachable set computed using Algorithm 1 with weighted 1-norm. (b) Overapproximation of the reachable set computed using the algorithm of [13] corresponding to the solution of (12) with (ϵ, ϕ, k) given as below.

B. Cascade of Contractive Transcription Modules

To demonstrate that our method scales well to large systems, we consider a model of a protein transcription cascade consisting of n subsystems S_i each with two states governed by the dynamics

$$\begin{aligned} \dot{x}_i &= u_i(t) - \delta_i x_i + k_{1i} y_i - k_{2i}(1 - y_i)x_i \\ \dot{y}_i &= -k_{1i} y_i + k_{2i}(1 - y_i)x_i. \end{aligned} \tag{11}$$

When the inputs u_i are constrained to be nonnegative, it is easily seen that the set $[0, \infty) \times [0, 1]$ is positively invariant. It is shown in [15] that cascades of systems of the form (11) are globally contracting in a diagonally weighted 1-norm $|\cdot|_{1,D}$ for any values of the parameters δ_i, k_{1i} and k_{2i} and a global bound on the contraction rate is given in terms of the parameter values.

For a given problem size n, we generate random values for the parameters δ_i, k_{1i} and k_{2i} and compute a norm in which the corresponding $2n$-dimensional system with state $z = [x^T y^T]^T$ and interconnection $u_i(t) = 3\sin(10t)$ for $i = 1$ and $u_i(t) = 10y_{i-1}(t)$ for $i > 1$ is contractive. We then compute an overapproximation of the set of states reachable from the ball $K = \{z : |D(z - \bar{z})|_1 \leq 0.2\}$ with centre $\bar{x}_i = 1$, $\bar{y}_i = 0.8$. System trajectories are computed at 50 evenly-spaced time points over a horizon of $T = 1$. The time required to compute the trajectory along with corresponding norm ball diameters is given as a function of the state dimension in Table II.

For comparison, we also perform the trajectory-based reachability method described in [13]. For an autonomous system $\dot{x} = f(x)$, the

$$\mu_2\left(J(V_d)\right) = \begin{cases} -\frac{R}{2L} - \frac{1}{2C} I_d'(V_d) & \text{if } \left(\frac{R}{L} + \frac{1}{C} I_d'(V_d)\right)^2 < 4\left(\frac{1}{LC} + \frac{R}{LC} I_d'(V_d)\right) \\ -\frac{R}{2L} - \frac{1}{2C} I_d'(V_d) + \frac{1}{2}\sqrt{\left(\frac{R}{L} + \frac{1}{C} I_d'(V_d)\right)^2 - 4\left(\frac{1}{LC} + \frac{R}{LC} I_d'(V_d)\right)} & \text{otherwise.} \end{cases}$$

authors of [13] prove that if there exist functions $\epsilon, \phi : \mathbb{R}^n \times \mathbb{R}^n \to R$ and a constant $k \in \mathbb{R}$ satisfying

$$\nabla_x \phi(x,y) f(x) + \nabla_y \phi(x,y) f(y) \leq \epsilon(x,y)\gamma(x,y) + k\epsilon(x,y) \geq 0 \quad (12)$$

then within the region $\gamma(x,y) \leq 0$ trajectories satisfy $\phi(x,y) \leq \beta \Longrightarrow \phi(\xi(t,x),\xi(t,y)) \leq \beta + kt$. For polynomial f, if the inequalities (12) are relaxed to sum-of-squares (SOS) constraints, the search for (ϵ, ϕ, k) can be formulated as a semidefinite program. In Table II we provide times taken to find a solution to the SOS relaxation of (12) in MATLAB using SOSTOOLS 3.00 [26] for systems of the form (11) of varying dimension with input $u_1(t) = 0$. The matrix measure method performs favourably in comparison with determining the solution to this sum of squares program in terms of computation time.

To illustrate our method, we plot reachable sets for a cascade of length 2 (state dimension 4) with randomly-generated parameter values $\delta_1 = 6.61,\ \delta_2 = 8.18,\ k_{11} = 2.70,\ k_{12} = 7.64,\ k_{21} = 1.94,\ k_{22} = 5.04$. Projections of the overapproximation onto the (x_i, y_i) planes are shown in Fig. 2. Since the system is contractive in the norm considered, we see that the diameter of the reachable sets computed using Algorithm 1 decreases exponentially as time increases. Note that the reachable sets computed using [13] do not shrink with time as it is not possible to find a negative k such that $\phi(\xi(t,x),\xi(t,y)) \leq \beta + kt$ for all t.

VI. Conclusion

We provided a method of overapproximating reachable sets of nonlinear dynamical systems using matrix measures. The examples illustrate that our method can be used to compute guaranteed overapproximations of reachable sets for nonlinear systems with as many as two hundred states. This comes at the cost of a guarantee on the accuracy of the approximation; we can only guarantee convergence to the true reachable set asymptotically as the size of the mesh from which initial conditions are chosen tends to zero. However, we show that reachable sets can be computed to reasonable accuracy in a number of practically-motivated problems.

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