Reachable Sets of Homogeneous Polynomial Dynamical Systems using Exact Solutions

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***Abstract*—This paper performs the reachability analysis of odeco-HPDS, which are homogeneous polynomial dynamical systems that can be represented as orthonormally-decomposable supersymmetric tensors. Algorithms for determining the over-approximative reachable sets for these systems with no control and constant control are provided. The simulation results show a significant improvement in the accuracy of the reachable set estimates over the existing frameworks for reachable-set determination of these systems.**

***Index Terms*—Reachable sets, supersymmetric tensors, dynamical systems, homogenous polynomials**

I. Introduction

Homogeneous polynomial dynamical systems represent a class of mathematical models that find widespread applications in scientific and engineering domains. These systems are characterized by polynomial functions where all monomials have the same total degree. We encounter homogeneous polynomial systems that describe complex phenomena in systems biology, chemical reactions, and epidemiological models. For instance, gene regulatory networks can be modeled by a system of homogeneous polynomial equations capturing the interactions among genes. Another example arises in chemical reaction networks, where the concentrations of reactants and products evolve according to homogeneous polynomial kinetics. In neural networks, some architectures can be represented in the homogenous polynomial form. Related work and applicability of these systems in the real world can be found in [1]- [3].

It is often of interest to us to determine whether the dynamical model achieves an unsafe state from an initial state. However, in continuous systems in the real world, the initial state of a system is often probabilistic, having a range of values that it can adopt. In such cases, instead of having a single initial state, we have a set of infinite values called the initial set for the system. Simulation-based techniques [4]- [6] can confirm the lack of safety in the system. Still, they cannot guarantee safety, as an infinite set of initial conditions would require infinite simulations to ensure that safety is not violated in all instances. In such situations, we perform the reachability analysis of these systems, which involves determining the reachable set of the system from its initial set. A reachable set is the set of states a system can reach for given sets of initial states. Safety is guaranteed for the given initial set if no unsafe state belongs to the corresponding reachable set.

Although general methods exist for performing the reachability analysis of systems [7], [8], they are often very conservative and over-approximate the exact reachable set. This leads to a mischaracterization of systems as unsafe in some instances. Through this work, we propose a method for determining the over-approximative reachable sets of certain homogeneous polynomial dynamical systems, which can be represented as orthonormally decomposable supersymmetric tensors, called odeco-HPDS. These reachable sets are seen to be significantly less conservative than the results of the existing tools for reachability analysis.

In this paper, we determine the reachable sets of a special class of systems called odeco-HPDS whose exact solutions can be determined analytically. We exploit certain properties of the solutions that enable us to determine the reachable set effectively. We test the performance of the calculated reachable sets against existing tools for reachability analysis and show significant improvement in the accuracy of the estimated reachable sets of these systems.

The key contributions of this paper are for two classes of polynomial dynamical systems. They can be characterized as follows

1) We provide an algorithm for determining the reachable set of an odeco-HPDS with no control for an axis-aligned and general initial set.
2) We provide an algorithm for determining the reachable set of an odeco-HPDS with constant control for an axis-aligned and general initial set.
3) We compare and show an improvement in performance over CORA (Continuous Reachability Analysis) [7], an existing tool for reachability analysis of dynamical systems

The paper is organized as follows. Section II introduces certain mathematical concepts and previous results that were necessary in our work. In Section III, we prove and present the algorithms for determining the reachable sets of both types of systems. The results of the proposed algorithms are shown in Section IV. We conclude our paper and give directions for future work in Section V.

II. Mathematical Preliminaries

A. Explicit solution of odeco-HPDS

In [9], it was shown that every homogeneous polynomial dynamical system of degree $k-1$ can be written as a tensor-vector multiplication along the first $k-1$ modes:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}^{k-1} \tag{1}$$

Here, $\mathbf{A} \in \mathbb{R}^{n\times n\times n \ldots \times n}$ is a supersymmetric tensor of order $k \geq 3$ and $\mathbf{x} \in \mathbb{R}^n$. $\mathbf{A}$ is said to be orthonormally decomposable (odeco) if it can be written as a sum of the outer products of orthonormal vectors

$$\mathbf{A} = \sum_{p=1}^{n} \lambda_p \mathbf{v}_p \circ \mathbf{v}_p \circ \ldots \circ \mathbf{v}_p \tag{2}$$

Here, λ_p are known as the Z-Eigenvalues and are in descending order. $\mathbf{v}_p$ are the corresponding Z-Eigenvectors of $\mathbf{A}$.

If $\mathbf{A}$ is odeco, then (1) is said to be odeco-HPDS. Given the initial condition $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$, the system has an explicit solution given by

$$\mathbf{x}(t) = \sum_{r=1}^{n} (1-(k-2)\lambda_r \alpha_r^{k-2} t)^{-\frac{1}{k-2}} \alpha_r \mathbf{v}_r \tag{3}$$

B. Implicit solution of odeco-HPDS with constant control

If $\mathbf{b} \in \mathbb{R}^n$, is constant with time, the odeco-HPDS with constant control can be written as

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}^{k-1} + \mathbf{b} \tag{4}$$

This system, with the initial condition $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$ has a solution $\mathbf{x}(t) = \sum_{r=1}^{n} c_r(t) \mathbf{v}_r$ which can be obtained by solving the implicit equations

$$t = -\frac{g(\frac{k-2}{k-1}, -\frac{\tilde{b}_r}{\lambda_r c_r(t)^{k-1}})}{(k-2)\lambda_r c_r(t)^{k-1}} + \frac{g(\frac{k-2}{k-1}, -\frac{\tilde{b}_r}{\lambda_r \alpha_r(t)^{k-1}})}{(k-2)\lambda_r \alpha_r(t)^{k-1}} \tag{5}$$

Here, $\tilde{b}_r$ are the rth entries of $\mathbf{V}^{\intercal}\mathbf{b}$ ($\mathbf{V}$ contains all the vectors $\mathbf{v}_r$) and g(·,·) is the specified Gauss Hypergeometric function given by

$$g(a,z) = {}_2F_1(1,a;a+1;z) = a\sum_{m=0}^{\infty} \frac{z^m}{a+m} \tag{6}$$

C. Outer box approximation of polytopes

In later sections, it will be shown that an elegant method for determining reachable sets of axis-aligned initial sets exists, which can be extended to general initial sets by performing overapproximative axis-aligned decompositions of the general initial sets.

For this purpose, we use the recursive algorithm from [10] for the outer approximation of a polytope, which decomposes it into axis-aligned sets with volumes below a threshold $\mathcal{E}$. An illustrative example is highlighted in Figure 1.

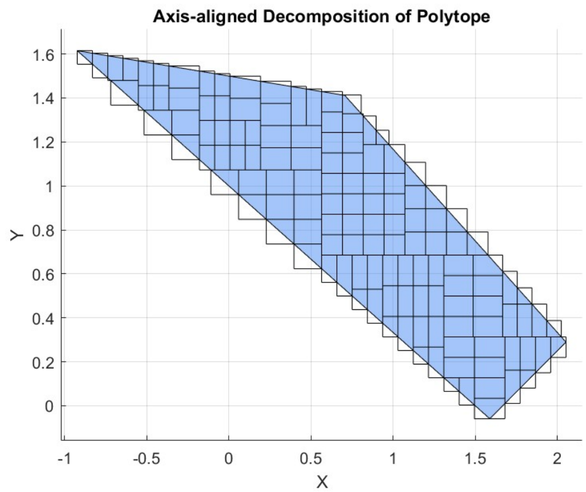


Fig. 1: Outer approximation of a polytope using axis-aligned sets

D. Zonotope representation of sets

Zonotopes provide a convenient method of representation of sets with an ease of performing operations. We will represent our initial and reachable sets as zonotopes in algorithms. A zonotope is defined as a set

$$Z = \{x \in \mathbb{R}^n : x = c + \sum_{i=1}^{p} \beta_i g_i, -1 \leq \beta_i \leq 1\}$$

with $c, g_1, g_2, \ldots, g_p \in \mathbb{R}^n$. c is known as the center of the zonotope and g_i are called the generators

III. Methodologies

A. Reachable Set of odeco-HPDS

Proposition 1. *Let* $\mathbf{x}_1(t) = \sum_{r=1}^{n} a_r(t)\mathbf{v}_r$ *be the solution of (1) for the initial condition* $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$ *and* $\mathbf{x}_2(t) = \sum_{r=1}^{n} b_r(t)\mathbf{v}_r$ *be the solution with* $\mathbf{x}_0 = \sum_{r=1}^{n} \beta_r \mathbf{v}_r$ *as the initial condition. If* $\alpha_p > \beta_p$ *for some* $p \in [1,n]$*, then* $b_p > a_p$

Proof. From (3), we know that

$$a_p = (1-(k-2)\lambda_r \alpha_p^{k-2} t)^{-\frac{1}{k-2}} \alpha_p$$

This can be simplified to

$$a_p = (\alpha_p - (k-2)\lambda_r t)^{-\frac{1}{k-2}}$$

Writing similarly for b_p, and with the same $k \geq 3$ and λ, it follows from $\alpha_p > \beta_p$ that

$$(\alpha_p - (k-2)\lambda_r t)^{-\frac{1}{k-2}} < (\beta_p - (k-2)\lambda_r t)^{-\frac{1}{k-2}}$$

■

The importance of Proposition 1 is seen when we consider an initial set that is axis-aligned to the orthonormal Z-Eigenvectors of $\mathbf{A}$. If this set is represented as a zonotope, its generators would also be along these Z-Eigenvectors. If a generator g_p is along the Z-Eigenvector $\mathbf{v}_p$, and if all points in the zonotope are written in the form $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$, then the maximum and minimum values of α_p over all the points in the zonotope would be found at $x = c + g_p$ and $x = c - g_p$ where c is the center of the initial set because the set is axis-aligned. From Proposition 1, we know that the system's state at time t is ordered according to the values of the initial state. Hence, to determine the reachable set of an initial set with axes aligned to the Z-Eigenvectors, it is sufficient to determine the values of the state for initial points $x_0 = c \pm g_i$ since these values bound all other points. Since the generators are finite in number, we can determine the reachable set.

We display the reachable set calculation for an initial set represented as a zonotope and axis-aligned to the Z-Eigenvectors of $\mathbf{A}$ in Algorithm 1. The algorithm assumes that our reference frame is initially aligned with the axes defined by the Z-Eigenvectors of $\mathbf{A}$ and later rotates this frame back to the standard coordinate axes by multiplying $\mathbf{V}$ to the center and generators of the calculated reachable set.

In the algorithm, c, g_i represents the center and generators of the initial zonotope. $\alpha[r], \beta[r]$ denotes the rth component of vectors α, β respectively. rs_center[i] represents the i-th component of the center, and rs_gen[i] represents the i-th generator of the reachable set at time t. $\mathbf{V}$ is the matrix with the Z-Eigenvectors of $\mathbf{A}$ as the columns.

Algorithm 1 RS of odeco-HPDS for axis-aligned initial set

for each generator g_i **do**
  $\alpha \leftarrow \mathbf{V}^{\intercal}(c + g_i)$
  $\beta \leftarrow \mathbf{V}^{\intercal}(c - g_i)$
  rsbound1 $\leftarrow (1 - (k-2)\lambda_i \alpha[i]^{k-2} t)^{-\frac{1}{k-2}} \alpha[i]$
  rsbound2 $\leftarrow (1 - (k-2)\lambda_i \beta[i]^{k-2} t)^{-\frac{1}{k-2}} \beta[i]$
  rs_center[i] $\leftarrow$ 0.5*(rsbound1 + rsbound2)
  rs_gen[i] $\leftarrow$ 0.5*(rsbound1 - rsbound2)*$\mathbf{V}^{\intercal} g_i$
end for
RS $\leftarrow$ Zonotope{$\mathbf{V}$*rs_center, $\mathbf{V}$*rs_gen}

Using Algorithm 1, we can calculate the reachable set for an axis-aligned initial set. We extend this algorithm to a general initial set by performing an axis-aligned set decomposition of the initial set highlighted earlier and treating each hyperbox obtained from this decomposition as an independent axis-aligned initial set. Algorithm 2 highlights this method. $\mathcal{E}$ represents the volume threshold for the decomposition and m represents the total number of boxes obtained in the decomposition of the general initial set. box_RS[r] represents the reachable set of the r-th hyperbox in the decomposition of the initial set. Note that since we calculate the outer-bound box approximations of sets, the union gives us outer approximations of the reach sets, ensuring safety.

B. Reachable set of odeco-HPDS with constant control

Lemma 1. *The function*

$$f(\alpha) = \frac{g(\frac{k-2}{k-1}, \frac{-\tilde{b}}{\lambda \alpha^{k-2}})}{(k-2)\lambda \alpha^{k-2}} \tag{7}$$

Algorithm 2 RS of odeco-HPDS for general initial set

boxes $\leftarrow$ decomposition(initial set, $\mathcal{E}$)
for each b_i in boxes **do**
  box_RS[i] $\leftarrow$ reachable_set_axis-aligned(b_i)
end for
RS $\leftarrow \cup_{r=1}^{m}$ box_RS[r]

is monotonic for constant $k, \tilde{b}, \lambda$

Proof. Consider $zg(a, z)$ with $0 < a < 1$

$$zg(a, z) = az \sum_{m=0}^{\infty} \frac{z^m}{a + m}$$

Consider

$$\frac{\partial}{\partial z}(zg(a, z)) = a \sum_{m=0}^{\infty} \frac{(m+1)z^m}{a + m}$$

When $z \geq 0$, the partial derivative is greater than 0 since all terms in the summation are positive. When $z < 0$, consider two successive terms in the summation

$$\frac{2k+1}{a+2k} z^{2k} + \frac{2k+2}{a+2k+1} z^{2k+1}$$

We know that since $a > 1$,

$$\frac{2k+1}{a+2k} > 1 \implies \frac{2k+1}{a+2k} > \frac{2k+2}{a+2k+1}$$

Further, $g(a, z)$ is defined for $|z| < 1$, hence, $|z^{2k}| > |z^{2k+1}|$. Hence,

$$|\frac{2k+1}{a+2k} z^{2k}| > |\frac{2k+2}{a+2k+1} z^{2k+1}|$$

This implies that every pair of terms adds to a positive number in the summation. This implies that $zg(a, z)$ increases in z.

Notice that $f(\alpha)$ is $c\alpha z_1 g(a, z_1)$ where c is a constant and $z_1 = \frac{-\tilde{b}}{\lambda \alpha}$. Further, α and $z_1 g(a, z_1)$ are monotonic in α when the other variables are constant. The product of two monotonic functions is monotonic if and only if they have the same sign. Since both α and $z_1 g(a z_1)$ are positive and negative in the left and right half-planes, respectively, their product is monotonic. ∎

Proposition 2. *Let* $\mathbf{x}_1(t) = \sum_{r=1}^{n} a_r(t)\mathbf{v}_r$ *be the solution of (4) for the initial condition* $\mathbf{x}_0 = \sum_{r=1}^{n} \alpha_r \mathbf{v}_r$ *and* $\mathbf{x}_2(t) = \sum_{r=1}^{n} b_r(t)\mathbf{v}_r$ *be the solution with* $\mathbf{x}_0 = \sum_{r=1}^{n} \beta_r \mathbf{v}_r$ *as the initial condition. If* $\alpha_p, \beta_p \neq 0$, $\alpha_p > \beta_p$ *and* $f(\alpha_p) - t, f(\beta_p) - t$ *have the same sign for some* $p \in [1, n]$, *then* $a_p > b_p$

Proof. In Lemma 1, we proved that the function $f(\alpha)$ is monotonic. We can also see that $f(\alpha)$ is undefined at $\alpha = 0$. The solution to (4) can be found by solving for c for each component of the vector, the implicit equation $f(\alpha_i) - t = f(c_i)$. If the function is monotonically decreasing, then

$$\alpha_p > \beta_p \implies f(\alpha_p) - t < f(\beta_p) - t \implies f(a_p) < f(b_p)$$

Hence, $a_p > b_p$ since f is decreasing. If the function is monotonically increasing, then

$$\alpha_p > \beta_p \implies f(\alpha_p) - t > f(\beta_p) - t \implies f(a_p) > f(b_p)$$

Hence, $a_p > b_p$ using the fact that f is monotonically increasing. In both cases, $a_p > b_p$. ■

As in Proposition 1, we establish an order among the solution values based on the initial condition values. We have an additional criterion on $f(\alpha_p) - t, f(\beta_p) - t$ having the same sign to ensure that no point in the reachable set is undefined. We can again exploit the idea of using a rotated frame aligned to the Z-Eigenvectors of $\mathbf{A}$ to evaluate the reachable set of the system followed by a rotation of the reachable set to obtain results in our standard coordinate frame. This leads us to the following algorithm. As before, we take c, g_i, which represents the center and generators of the initial zonotope. $\alpha[r], \beta[r]$ denotes the rth component of vectors α, β respectively. rs_center[i] represents the i-th component of the center, and rs_gen[i] represents the i-th generator of the reachable set at time t. $\mathbf{V}$ is the matrix with the Z-Eigenvectors of $\mathbf{A}$ as the columns. We also define the function

$$f_r(x) = \frac{g(\frac{k-2}{k-1}, -\frac{b_r}{\lambda_r x^{k-1}})}{(k-2)\lambda_r x^{k-1}}$$

Note that we take b_r and not $\tilde{b_r}$ since $\tilde{b_r}$ becomes b_r in the frame with the Z-Eigenvectors as the axes.

Algorithm 3 Reachable set of odeco-HPDS with constant input for axis-aligned initial set

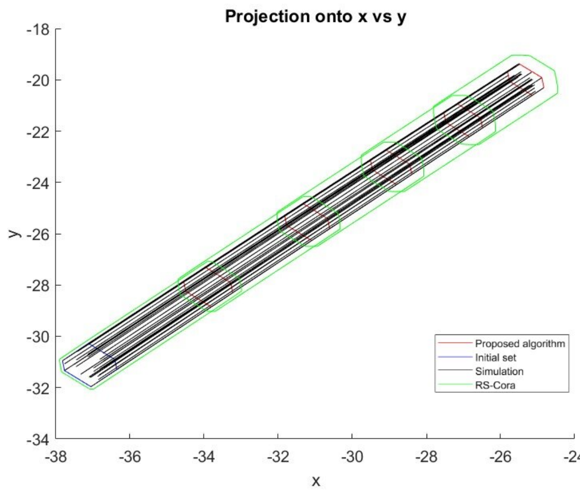
for each generator g_i **do**
  $\alpha \leftarrow \mathbf{V}^\intercal(c + g_i)$
  $\beta \leftarrow \mathbf{V}^\intercal(c - g_i)$
  rsbound1 $\leftarrow$ solve for x in $t = f_i(\alpha[i]) - f_i(x)$
  rsbound2 $\leftarrow$ solve for x in $t = f_i(\beta[i]) - f_i(x)$
  rs_center[i] $\leftarrow$ 0.5*(rsbound1 + rsbound2)
  rs_gen[i] $\leftarrow$ 0.5*(rsbound1 - rsbound2)*$\mathbf{V}^\intercal g_i$
end for
RS $\leftarrow$ Zonotope{$\mathbf{V}$*rs_center, $\mathbf{V}$*rs_gen}

As was done in the no-control odeco-HPDS, we propose using axis-aligned box decomposition to obtain the reachable sets of general initial sets. Using this idea, we propose the following algorithm.

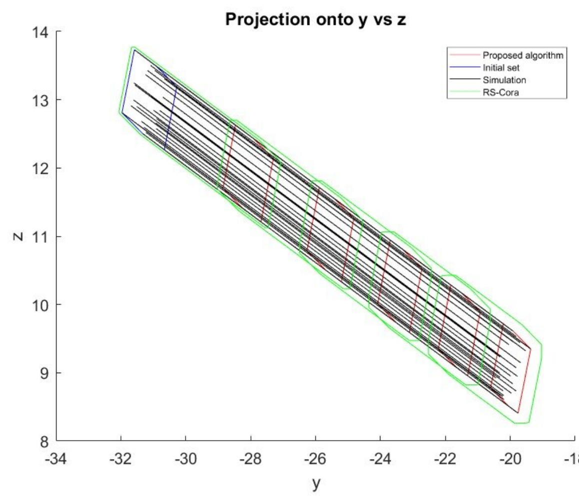
Algorithm 4 Reachable set of odeco-HPDS with constant input for general initial set

boxes $\leftarrow$ decomposition(initial set, $\mathcal{E}$)
for each b_i in boxes **do**
  box_RS[i] $\leftarrow$ rs_axis-aligned_with_control(b_i)
end for
RS $\leftarrow \cup_{r=1}^{m}$ box_RS[r]

These algorithms allow us to overapproximate the reachable sets of odeco-HPDS with and without constant control. The



(a) Projection of the sets on the XY plane



(b) Projection of the sets on the YZ plane

Fig. 2: Comparison of Algorithm 1 vs CORA

extent of overapproximations can be controlled by tuning the value of $\mathcal{E}$ in the box decompositions of non-axis-aligned initial sets since that is the only approximation that we make in our algorithm. This gives us control over the trade-off between the solution's exactness and the desired computational time.

IV. Results

We simulated synthetic examples of odeco-HPDS with and without constant control. It was observed that because the systems with constant control have discontinuities, the simulation would often terminate in the case of CORA because the non-conservative estimates of the reachable sets would often become undefined despite solutions existing in reality. In cases where both methods resulted in a solution, a significant improvement was seen in our methods. As a proxy to the ground truth reachable set, we randomly initialized and simulated points lying within the initial set. We observed that our reachable sets more closely resembled the results of these randomly initialized simulations.

A. Odeco HPDS with no control

We consider the following example for simulating the odeco-HPDS. The orthonormally decomposable tensor $\mathbf{A}$ is of dimensions $3 \times 3 \times 3$ and is as follows

$$\mathbf{A}_{::1}\begin{bmatrix} 0.2507 & -0.0955 & 0.0541 \\ -0.0955 & 0.2048 & -0.0926 \\ 0.0541 & -0.0926 & 0.0363 \end{bmatrix}$$

$$\mathbf{A}_{::2}\begin{bmatrix} -0.0955 & 0.2048 & -0.0926 \\ 0.2048 & -0.0578 & 0.0515 \\ -0.0926 & 0.0515 & 0.0117 \end{bmatrix}$$

$$\mathbf{A}_{::3}\begin{bmatrix} 0.0541 & -0.0926 & 0.0363 \\ -0.0926 & 0.0515 & 0.0117 \\ 0.0363 & 0.0117 & 0.0894 \end{bmatrix}$$

We consider an initial set that is axis-aligned to the Z-Eigenvectors of $\mathbf{A}$. It is easier to represent this initial set as a zonotope, hence it is defined with the center at $c = [-37.09, -31.12, 13.00]^\intercal$ and generators

$$g^1 = \begin{bmatrix} -0.36 \\ 0.32 \\ -0.15 \end{bmatrix}, g^2 = \begin{bmatrix} -0.35 \\ -0.34 \\ 0.12 \end{bmatrix}, g^3 = \begin{bmatrix} -0.03 \\ 0.19 \\ 0.46 \end{bmatrix}$$

Since this set is already aligned with the Z-Eigenvectors of $\mathbf{A}$, we do not need to perform the box decomposition of the initial set and can directly use Algorithm 1. We perform the simulation over 5 timesteps. The projections of the simulation on the XY and YZ planes are shown in Figure 2.

We observe that since the algorithm is computing the exact reachable sets of the system through the exact solutions, the algorithm outperforms CORA. The red lines, which define the boundary of the reachable set determined by our algorithm over various timesteps, more tightly enclose the black lines of the randomly initialized points. The disparity between the two increases over time, displaying the importance of this method when determining reachable sets over longer durations of time.

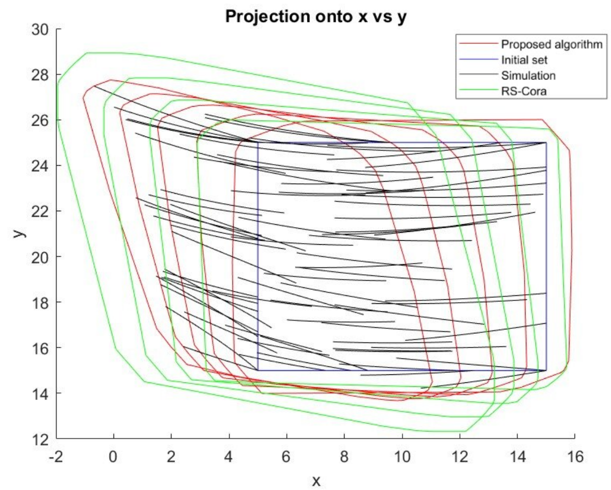
B. Odeco HPDS with constant control

We present an example of an odeco-HPDS with constant control. We take the $3 \times 3 \times 3$ orthonormally decomposable tensor $\mathbf{A}$ and control vector $\mathbf{b} = [1.98, 1.65, -1.34]^\intercal$, where

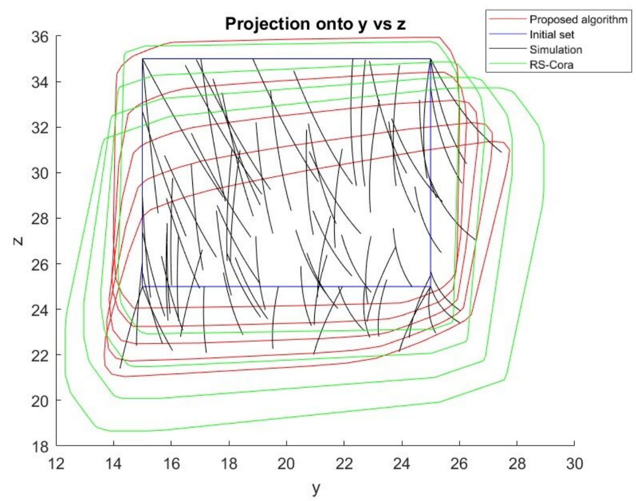
$$\mathbf{A}_{::1}\begin{bmatrix} -0.1169 & -0.0141 & -0.0684 \\ -0.0141 & -0.0256 & -0.0885 \\ -0.0684 & -0.0885 & 0.0349 \end{bmatrix}$$

$$\mathbf{A}_{::2}\begin{bmatrix} -0.0141 & -0.0256 & -0.0885 \\ -0.0256 & 0.1047 & -0.1050 \\ -0.0885 & -0.1050 & 0.1708 \end{bmatrix}$$

$$\mathbf{A}_{::3}\begin{bmatrix} -0.0684 & -0.0885 & 0.0349 \\ -0.0885 & -0.1050 & 0.1708 \\ 0.0349 & 0.1708 & -0.2957 \end{bmatrix}$$



(a) Projection of the sets on the XY plane



(b) Projection of the sets on the YZ plane

Fig. 3: Comparison of Algorithm 4 vs CORA

The initial set we consider is a $5 \times 5 \times 5$ box centered at $(10, 20, 30)$. Note that this set is not aligned to the Z-Eigenvectors of $\mathbf{A}$, and so we use Algorithm 4 to compute the reach set. We set a threshold of $\mathcal{E} = 1$ for the box decomposition of the initial set and simulate over 5 timesteps.

The results are displayed in Figure 3. We project the results on the XY and YZ planes. Algorithm 4 performs better in approximating the reachable set of this system, since the red lines, which represent the reachable sets generated by our algorithm, give a tighter enclosure of the black lines, which are the simulation results of the randomly initialized points. A further improvement can be obtained by decreasing $\mathcal{E}$.

V. Conclusion and Future Work

Through this work, we performed the reachability analysis of a special class of systems called the odeco-HPDS. Our method displayed an improvement in accuracy over the existing method for the reachability analysis of dynamical systems.

Overly conservative estimates may lead to unnecessary design constraints, increased computational complexity, and missed opportunities for system optimization. Our method takes a step toward significantly eliminating these issues.

To expand the applicability of this method, we can explore the possibility of approximating general HPDS and general polynomial systems as odeco-HPDS while ensuring safety guarantees are not violated. Further, we can explore the possibility of applying this method to other systems that have exact solutions and similar ordering properties as shown in Section III of this paper.

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