Probabilistic Invariance of Mixed Deterministic-Stochastic Dynamical Systems *

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ABSTRACT

This work is concerned with the computation of probabilistic invariance (or safety) over a finite horizon for mixed deterministic-stochastic, discrete-time processes over a continuous state space. The models of interest are made up of two sets of (possibly coupled) variables: the first set of variables has associated dynamics that are described by deterministic maps (vector fields), whereas the complement has dynamics that are characterized by a stochastic kernel. The contribution shows that the probabilistic invariance problem can be separated into two parts: a deterministic reachability analysis, and a probabilistic invariance problem that depends on the outcome of the first. This technique shows advantages over a fully probabilistic approach, and allows putting forward an approximation algorithm with explicit error bounds. The technique is tested on a case study modeling a chemical reaction network.

Categories and Subject Descriptors

G.3 [**Probability and Statistics**]: Markov processes, Stochastic processes; G.4 [**Mathematical Software**]: Algorithm design and analysis, Verification

General Terms

Algorithms, Verification

Keywords

Invariance and safety, Mixed deterministic-stochastic dynamics, Finite approximations, Chemical reaction networks

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1. INTRODUCTION

Given a stochastic process evolving over a state space and a set of interest (known as invariance domain, or safe set) that is a subset of the state space, the probabilistic invariance problem is concerned with the computation of the probability that a realization of the process, started anywhere on the state space, remains within the invariance set over a given time horizon.

Probabilistic invariance (or its dual, reachability) has been investigated for various models and with multiple techniques. Classical results on models with discrete state spaces are recapitulated in [3], whereas recent work deals with hybrid models in continuous- [5, 11] and discrete-time [2], respectively.

In this contribution, we are interested in working with processes that evolve in discrete time over a continuous state space (we shall consider an Euclidean vector space for the sake of simplicity, however the results are susceptible of being extended to hybrid spaces). Furthermore, we deal with models with explicit mixed deterministic-stochastic dynamics. With regards to the probabilistic invariance problem, we shall focus on the finite horizon case.

Mixed deterministic-stochastic dynamics naturally arise in a number of situations or application domains. For instance, this feature is expected in models with variables that take values within ranges that are dimensionally different. Of interest to this study, one such case is represented by a chemically reacting network in an environment with both rare and abundant species [8]. Mixed deterministic-stochastic models are composed of two complementary sets of variables, possibly coupled between each other. The first set of variables has associated dynamics that depend on deterministic maps, namely vector fields. The complement set has dynamics characterized by a stochastic kernel.

A naïve approach to the probabilistic invariance problem for mixed deterministic-stochastic models would merely tackle it as a safety verification instance over degenerate systems (by degenerate systems we refer to probabilistic laws that are concentrated deterministically, i.e. whose support consists of a single point). This would not only be a computationally expensive solution, but also lead to the inability to leverage computational techniques that apply exclusively to non-degenerate systems [1].

The contribution originally shows that the probabilistic invariance problem can be separated into two parts: a deterministic reachability analysis, and a probabilistic invariance problem that depends on the outcome of the first. Deterministic reachability analysis is a rather mature field of research with ample software tool support, whereas the second problem can harvest recent developments [2, 5, 11]. We argue that this decomposition approach can lead to computational improvements – for instance, whenever the first deterministic problem yields a “false” outcome (i.e., no states are deterministically safe over the given time horizon), no further probabilistic invariance calculation is necessary. This advantage of the proposed approach also leads to an approximation algorithm to compute the quantity of interest with explicit error bounds.

The contribution is structured as follows. Section 2 introduces the model class and the problem statement. Section 3 focuses on the properties of the value functions that characterize probabilistic invariance. Section 4 puts forward an approximation scheme for the computation of the desired quantities based on the discretization of the state space, and explicitly characterizes its error. Section 6 presents a case study from Systems Biology.

2. PRELIMINARIES

2.1 Model

We consider a stochastic process over a continuous state-space $\mathcal{S}$. We assume that $\mathcal{S}$ is endowed with a metric and is Borel measurable. We denote by $\mathcal{B}(\mathcal{S})$ the associated sigma algebra. The process is Markovian and driven in discrete time by the following mixed deterministic-stochastic dynamics:

$$\begin{cases} x_1(k+1) = f_1(x_1(k), x_2(k), h(k)) \\ x_2(k+1) = f_2(x_1(k), x_2(k)). \end{cases} \tag{1}$$

In model (1),

- $h(\cdot)$ is an i.i.d. random sequence with known distribution;
- $x_1(k) \in \mathbb{R}^{n_1}$ is a vector-valued random sequence with dynamics that are directly affected by the random variable $h(\cdot)$ at a given time;
- $x_2(k) \in \mathbb{R}^{n_2}$ is a vector-valued random sequence with dynamics characterized by a given deterministic vector field f_2.

Denote by

$$x(k) = \begin{bmatrix} x_1(k) \\ x_2(k) \end{bmatrix} \in \mathbb{R}^n = \mathcal{S}, \quad n = n_1 + n_2,$$

the state variable of the whole model in (1). The knowledge of the distribution of random variable $h(\cdot)$ at a given time allows to characterize a conditional stochastic kernel $T_x(\cdot|x)$ that assigns to each point $x \in \mathcal{S}$ a probability measure $T_x(\cdot|x)$, so that for any set $A \in \mathcal{B}(\mathcal{S}), P_x(x(k+1) \in A) = \int_A T_x(d\bar{x}|x(k) = x)$, where P_x denotes the conditional probability $P(\cdot|x)$ and P is a probability measure defined over the canonical sample space (with associated σ-algebra) for the above stochastic process [4].

The special structure of model (1) allows expressing the density function of the stochastic kernel T_x as follows:

$$t_x(\bar{x}|x) = t_x(\bar{x}_1|x_1, x_2)\delta(\bar{x}_2 - f_2(x_1, x_2)), \tag{2}$$

for $x = (x_1, x_2)^T$ and where $\delta(x - a)$ is the continuous Dirac delta function shifted at point a. The first term $t_x(\bar{x}_1|x_1, x_2)$ depends on the stochastic part of the dynamical model, whereas the second term $\delta(\bar{x}_2 - f_2(x_1, x_2))$ hinges on the deterministic vector field.

2.2 Problem statement

Consider a compact Borel set $A \subset \mathcal{B}(\mathcal{S})$. We are interested to solve the following probabilistic invariance problem over a finite time horizon $[0, N]$: to characterize and compute the probability that an execution with an initial condition $x_0 \in \mathcal{S}$ remains within set A during the whole time horizon, namely

$$p_{x_0}(A) \doteq P\{x(k) \in A, \forall k \in [0, N] | x(0) = x_0\}. \tag{3}$$

A characterization of the problem in (3) is addressed in the following result [2].

Proposition 1 (Bellman recursion). *Introduce functions $V_k : \mathcal{S} \to [0, 1], k \in [0, N]$, and define them backward-recursively as follows:*

$$V_k(x) = \mathbb{I}_A(x) \int_{\mathcal{S}} V_{k+1}(x_{k+1}) T_x(dx_{k+1}|x), \tag{4}$$

where $V_N(x)$ is initialized as the indicator function of set A: $V_N(x) = \mathbb{I}_A(x)$. Then the solution of problem (3) is $p_{x_0}(A) = V_0(x_0)$, for any $x_0 \in \mathcal{S}$.

A solution of $p_{x_0}(A)$ is seldom analytic, which warrants the development of techniques and algorithms to compute an approximation of it. The work in [1] puts forward a discretization approach with proven error bounds, under continuity conditions of the stochastic kernel T_x. Such bounds are refined in [7], by leveraging an adaptive partitioning approach with improved (local) error computations.

The goal of this contribution is first to tailor problem (3) to the structure of model (1), then to provide a technique to compute the solution of (3) by a numerical scheme with associated errors.

3. PROPERTIES OF THE VALUE FUNCTIONS

3.1 On the support of the value functions

With focus on the recursion step in Equation (4), let us define the support of function V_k as:

$$supp(V_k) = \{x \in \mathcal{S} | V_k(x) \neq 0\}, \quad k \in [0, N-1],$$

and $supp(V_N) = A$. The support of the value functions V_k plays an important role in the problem definition, as elaborated in the following observations:

- since $\forall x \notin A, V_k(x) = 0$, then
$$\forall k \in [0, N], \quad supp(V_k) \subseteq A;$$
- by direct inductive argument, it can be shown that
$$\forall k \in [0, N-1], \forall x \in A, \quad 0 \leq V_k(x) \leq V_{k+1}(x),$$
which leads to conclude that
$$supp(V_k) \subseteq supp(V_{k+1}).$$

Notice that, because of the constant value of the cost function on the complement of the set A, the integral in (4) is effectively computed only over A (rather than on $\mathcal{S}$). Furthermore, the observations above suggest that it is possible to adapt the integration domain in (4) to the actual support of the value functions, as follows:

$$V_k(x) = V_k(x_1, x_2) = \tag{5}$$
$$\int_{supp(V_{k+1})} V_{k+1}(\bar{x}_1, \bar{x}_2) t_x(\bar{x}_1|x_1, x_2)\delta(\bar{x}_2 - f_2(x_1, x_2)) d\bar{x}_2 d\bar{x}_1,$$

where we have used the expression in (2). Characterizing the sets $supp(V_k), k \in [0, N-1)$, becomes thus critical for the optimization of the original recursion in (4). However, in general it is complicated to exactly determine the sets $supp(V_k)$, in particular due to the need to characterize $supp(t_x(\cdot|x))$ as a function of x.

To mitigate this complication, let us introduce two projection maps as follows:

$$\Pi_1 : \mathbb{R}^n \to \mathbb{R}^{n_1} \qquad \Pi_2 : \mathbb{R}^n \to \mathbb{R}^{n_2}$$
$$\Pi_1\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = x_1, \qquad \Pi_2\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = x_2.$$

We can determine an over-approximation of the sets $supp(V_k)$ as follows:

$$supp(V_k) \subseteq$$
$$\{(x_1, x_2) \in supp(V_{k+1}) | f_2(x_1, x_2) \in \Pi_2(supp(V_{k+1}))\}.$$

Notice that in general the above inclusion is strict. This suggests to over-approximate the sets $supp(V_k)$ by Γ_k, as defined by the following recursive procedure:

$$\begin{cases} \Gamma_N = A, \\ \Gamma_k = \{(x_1, x_2) \in \Gamma_{k+1} | f_2(x_1, x_2) \in \Pi_2(\Gamma_{k+1})\}. \end{cases} \tag{6}$$

The sequence $\{\Gamma_k\}_{k=0}^N$ is endowed with the following facts:

- $supp(V_k) \subseteq \Gamma_k$, then $\forall x_0 \notin \Gamma_0, p_{x_0}(A) = 0$;
- $A = \Gamma_N \supseteq \Gamma_{N-1} \supseteq \Gamma_{N-2} \supseteq ... \supseteq \Gamma_0$;
- if there exists a positive integer $k_0 \leq N$ such that $\Gamma_{k_0} = \Gamma_{k_0+1}$, then for all $0 \leq k \leq k_0, \Gamma_k = \Gamma_{k_0+1}$;
- if there exists a positive integer $k_0 \leq N$ such that $\Pi_2(\Gamma_{k_0}) = \Pi_2(\Gamma_{k_0+1})$, then for all $0 \leq k \leq k_0, \Gamma_k = \Gamma_{k_0}$.

These properties highlight the dependence of the sets Γ_k (we will denote them simply as *support sets*) on the deterministic vector field f_2, particularly over the points that are mapped by f_2 outside of the support sets.

3.2 Simplifying the Bellman recursion

With focus on the support sets introduced in (6), define additionally the following quantities: for any $x_2 \in \Pi_2(\Gamma_k)$,

$$\Gamma_k^1(x_2) = \{x_1 \in \Pi_1(\Gamma_k) | (x_1, x_2) \in \Gamma_k\}.$$

Recall the recursive formula in (5) for V_k. By definition of Γ_k, we know that V_k is equal to zero outside of the set Γ_k. We can then simplify the recursive formula to the following:

$$V_k(x_1, x_2) = \int_{\Gamma_{k+1}^1(f_2(x_1,x_2))} V_{k+1}(\bar{x}_1, f_2(x_1, x_2)) t_x(\bar{x}_1|x_1, x_2) d\bar{x}_1, \tag{7}$$

for any $(x_1, x_2) \in \Gamma_k$. This formulation characterizes the value functions V_k in terms of the sets Γ_k.

3.3 Continuity of the value functions

We are interested in establishing the continuity of the value functions over their support. To achieve this, the following set of assumptions is needed.

ASSUMPTION 1. *Suppose that the kernel T_x admits a density function t_x as in (2). Furthermore, suppose that the density function t_x, the vector field f_2, and the parametrized sets $\Gamma_k^1(x_2)$ satisfy the following conditions:*

1. $|t_x(\bar{x}_1|x_1, x_2) - t_x(\bar{x}_1|x_1', x_2')| \leq h_1\|(x_1, x_2) - (x_1', x_2')\|$, *for any* $\bar{x}_1 \in \Pi_1(A)$ *and* $(x_1, x_2), (x_1', x_2') \in A$;
2. $\|f_2(x_1, x_2) - f_2(x_1', x_2')\| \leq h_2\|(x_1, x_2) - (x_1', x_2')\|$, *for any* $(x_1, x_2), (x_1', x_2') \in A$;
3. $\mathcal{L}(\Gamma_k^1(x_2) \triangle \Gamma_k^1(x_2')) \leq \theta_k\|x_2 - x_2'\|$, *for any* $x_2, x_2' \in \Pi_2(\Gamma_k), k \in [0, N]$,

where h_1, h_2, θ_k are finite constants. Here $\mathcal{L}$ is the Lebesgue measure over $\mathbb{R}^{n_1}$, whereas $\triangle$ denotes the symmetric difference of two sets.

The first two are continuity assumptions on the density and on the vector field. The third assumption is a regularity requirement on the variation of the (projection along the x_1 variables of the) support sets, as a function of the x_2 coordinates. Intuitively, this last assumption depends on the actual shape of the support sets Γ_k and on f_2 – as such, it has to hold over the entire time horizon $[0, N]$.

THEOREM 1. *If Assumption 1 is valid, then the value functions V_k are Lipschitz continuous on Γ_k, namely $\forall (x_1, x_2)$, $(x_1', x_2') \in \Gamma_k$,*

$$\left|V_k(x_1, x_2) - V_k(x_1', x_2')\right| \leq \lambda_k\|(x_1, x_2) - (x_1', x_2')\|,$$

where the finite Lipschitz constant λ_k satisfies the recursive formula:

$$\lambda_k = (h_1 L_{k+1} + M h_2 \theta_{k+1}) + h_2 M^\star \lambda_{k+1}, \quad 0 \leq k < N,$$

initialized with $\lambda_N = 0$, and where:

$$L_k = \mathcal{L}(\Pi_1(\Gamma_k)),$$
$$M = \sup\{t_x(\bar{x}_1|x_1, x_2) | x_1, x_2 \in A, \bar{x}_1 \in \Pi_1(A)\},$$
$$M^\star = \sup_{(x_1,x_2)\in A} \int_{\Pi_1(A)} t_x(\bar{x}_1|x_1, x_2) d\bar{x}_1.$$

PROOF. Since $V_N(x) = \mathbb{I}_A(x)$, it follows that $\lambda_N = 0$. Now suppose that the statement holds at step $k+1$: $\forall (x_1, x_2)$, $(x_1', x_2') \in \Gamma_{k+1}$,

$$\left|V_{k+1}(x_1, x_2) - V_{k+1}(x_1', x_2')\right| \leq \lambda_{k+1}\|(x_1, x_2) - (x_1', x_2')\|.$$

Select any two states $(x_1, x_2), (x_1', x_2') \in \Gamma_k$ and express the inequality via (7) as:

$$|V_k(x_1, x_2) - V_k(x_1', x_2')| =$$
$$\left|\int_{\Gamma_{k+1}^1(f_2(x_1,x_2))} V_{k+1}(\bar{x}_1, f_2(x_1, x_2)) t_x(\bar{x}_1|x_1, x_2) d\bar{x}_1 - \right.$$
$$\left.\int_{\Gamma_{k+1}^1(f_2(x_1',x_2'))} V_{k+1}(\bar{x}_1, f_2(x_1', x_2')) t_x(\bar{x}_1|x_1', x_2') d\bar{x}_1\right|.$$

To ease the notational burden, let us introduce sets $A^\star \doteq \Gamma^1_{k+1}(f_2(x_1,x_2))$ and $B^\star \doteq \Gamma^1_{k+1}(f_2(x_1',x_2'))$. Then:

$$\begin{aligned}
&|V_k(x_1,x_2) - V_k(x_1',x_2')| = \\
&\quad = \Big| \int_{A^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&\qquad - \int_{B^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| \\
&\quad \le \Big| \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&\qquad - \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| \\
&\quad + \Big| \int_{A^\star \setminus B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&\qquad - \int_{B^\star \setminus A^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| .
\end{aligned}$$

The above inequality is made up of two main terms, of which the first can be upper bounded as follows:

$$\begin{aligned}
&\Big| \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&\quad - \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| \\
&\le \Big| \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) \left[t_x(\bar{x}_1|x_1,x_2) - t_x(\bar{x}_1|x_1',x_2') \right] d\bar{x}_1 \\
&\quad + \int_{A^\star \cap B^\star} t_x(\bar{x}_1|x_1',x_2') \cdot \\
&\qquad \left[V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) - V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) \right] d\bar{x}_1 \Big| \\
&\le \int_{A^\star \cap B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) \left| t_x(\bar{x}_1|x_1,x_2) - t_x(\bar{x}_1|x_1',x_2') \right| d\bar{x}_1 \\
&\quad + \int_{A^\star \cap B^\star} t_x(\bar{x}_1|x_1',x_2') \cdot \\
&\qquad \left| V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) - V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) \right| d\bar{x}_1 \\
&\le h_1 \|(x_1,x_2) - (x_1',x_2')\| \mathcal{L}\left(A^\star \cap B^\star\right) \\
&\quad + \lambda_{k+1} \int_{A^\star \cap B^\star} \|(\bar{x}_1, f_2(x_1,x_2)) - (\bar{x}_1, f_2(x_1',x_2'))\| t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \\
&\le h_1 \|(x_1,x_2) - (x_1',x_2')\| \mathcal{L}\left(\Pi_1(\Gamma_{k+1})\right) \\
&\quad + \lambda_{k+1} \, h_2 \|(x_1,x_2) - (x_1',x_2')\| \int_{A^\star \cap B^\star} t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \\
&\le \left(h_1 L_{k+1} + h_2 M^\star \lambda_{k+1}\right) \|(x_1,x_2) - (x_1',x_2')\|.
\end{aligned}$$

Recalling that the value functions take values in the interval $[0,1]$, the second term is upper bounded as follows:

$$\begin{aligned}
&\Big| \int_{A^\star \setminus B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&\quad - \int_{B^\star \setminus A^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| \\
&\le \Big| \int_{A^\star \setminus B^\star} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \Big| \\
&\quad + \Big| \int_{B^\star \setminus A^\star} V_{k+1}(\bar{x}_1, f_2(x_1',x_2')) t_x(\bar{x}_1|x_1',x_2') d\bar{x}_1 \Big| \\
&\le M\mathcal{L}(A^\star \setminus B^\star) + M\mathcal{L}(B^\star \setminus A^\star) = M\mathcal{L}(A^\star \triangle B^\star) \\
&= M\mathcal{L}\left(\Gamma^1_{k+1}(f_2(x_1,x_2)) \triangle \Gamma^1_{k+1}(f_2(x_1',x_2'))\right) \\
&\le M\theta_{k+1} \|f_2(x_1,x_2) - f_2(x_1',x_2')\| \\
&\le M\theta_{k+1} h_2 \|(x_1,x_2) - (x_1',x_2')\|.
\end{aligned}$$

Collecting the two bounds, we obtain:

$$\begin{aligned}
&|V_k(x_1,x_2) - V_k(x_1',x_2')| \\
&\le \left(h_1 L_{k+1} + h_2 M^\star \lambda_{k+1}\right) \|(x_1,x_2) - (x_1',x_2')\| \\
&\quad + M\theta_{k+1} h_2 \|(x_1,x_2) - (x_1^\star,x_2^\star)\| \\
&= \left(h_1 L_{k+1} + h_2 M^\star \lambda_{k+1} + M\theta_{k+1} h_2\right) \|(x_1,x_2) - (x_1',x_2')\| \\
&= \lambda_k \|(x_1,x_2) - (x_1',x_2')\|,
\end{aligned}$$

which completes the proof. $\square$

Notice that $0 \le M^\star \le 1$ and that the quantities M and M* (hence, the overall bound) can be further refined to functions of the time step k.

4. APPROXIMATION SCHEME AND QUANTIFICATION OF THE ERROR

In this section we propose an approximation scheme to perform the computations in (7), and furthermore explicitly quantify its error. To keep the notations light, in (7) we replace the generic integration domain $\Gamma^1_{k+1}(f_2(x_1,x_2))$ by $\Pi_1(A)$ – however, the procedure applies similarly to the general case.

4.1 Approximation scheme for computation

Select an arbitrary partition of the invariant set $A = \cup_{i=1}^p A_i$, $A_{i_1} \cap A_{i_2} = \emptyset$, $i_1, i_2 = 1, \ldots, p$, $i_1 \neq i_2$, where p represents the cardinality. The whole state space $\mathcal{S}$ can be also partitioned by adding the complement set $A_{p+1} = \mathcal{S} \setminus A$. Pick any point $x^i = (x_1^i, x_2^i) \in A_i, i = 1, \ldots, p+1$. Notice that $\Pi_1(A) = \Pi_1\left(\cup_{i=1}^p A_i\right) = \cup_{i=1}^p \Pi_1(A_i)$, however the sets $\Pi_1(A_i)$ produce a cover (in general not a partition) of the set $\Pi_1(A)$. To make up for this, we can additionally select an arbitrary partition $\Pi_1(A) = \cup_{j=1}^q X_j$ for the projection of the safe set along the first variable. This allows to express, $\forall (x_1,x_2) \in A$:

$$\begin{aligned}
V_k(x_1,x_2) &= \int_{\Pi_1(A)} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1 \\
&= \sum_{j=1}^q \int_{X_j} V_{k+1}(\bar{x}_1, f_2(x_1,x_2)) t_x(\bar{x}_1|x_1,x_2) d\bar{x}_1.
\end{aligned}$$

Let us now approximate the value functions V_k by piecewise constant ones $\bar{V}_k$, which are computed over the selected points $\{x^i \in A_i\}_{i=1}^{p+1}$, as follows:

$$\bar{V}_k(x_1,x_2) = \sum_{i=1}^{p+1} \bar{V}_k(x_1^i, x_2^i) \mathbb{I}_{A_i}(x_1,x_2),$$

$\forall (x_1,x_2) \in A$. Denote $V_k^i \doteq \bar{V}_k(x_1^i,x_2^i)$. These functions are initialized as $V_N^i = 1$, $i = 1, \ldots, p$, $V_N^{p+1} = 0$, and recursively computed as follows:

$$V_k^i = \sum_{j=1}^q \int_{X_j} \bar{V}_{k+1}(\bar{x}_1, f_2(x_1^i,x_2^i)) t_x(\bar{x}_1|x_1^i,x_2^i) d\bar{x}_1.$$

In this formulation the values of $\bar{V}_{k+1}$ over the hyperplane $X_j \times \{f_2(x_1^i,x_2^i)\}$ are needed. In order to implement the procedure in a discrete manner, the function $\bar{V}_{k+1}$ should be constant over this hyperplane. This feature is achieved by raising the following assumption on the partition sets X_j of $\Pi_1(A)$:

$$\forall i, j\ \exists i' :\ X_j \times \{f_2(x_1^i, x_2^i)\} \subseteq A_{i'}.$$

Notice that this assumption does not depend on the step k, and is immediately satisfiable by selecting a partition for A uniformly along the first variable x_1, while considering non-redundant sets of $\Pi_1(A_i)$ as a partition for $\Pi_1(A)$.

Consider a map $i' = R(i, j)$, which assigns to each partition set X_j and value $f_2^i \doteq f_2(x_1^i, x_2^i)$ the corresponding partition set $A_{i'}$ containing $X_j \times f_2^i$. Having this map, we are able to formulate the discrete version of our continuous recursive procedure (7) as:

$$V_k^i = \sum_{j=1}^{q} V_{k+1}^{i'} \int_{X_j} t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1. \tag{8}$$

To recapitulate, the following steps are required to implement the algorithm:

- Select a partition $\cup_i A_i$ of the invariant set A and the associated partition $\cup_j X_j$ of $\Pi_1(A)$;
- Compute the map $i' = R(i, j)$ based on the selected partitions;
- Compute the marginal matrix P with the entries: $P_{ij} = \int_{X_j} t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1$;
- Compute recursively: $V_k^i = \sum_{j=1}^{q} P_{ij} V_{k+1}^{i'}$ as in (8), initialized by $V_N^i = 1$;
- Use the support set Γ_k at step k to set the required entries equal to zero, namely $V_k^i = 0$ for all i such that $A_i \subset \mathcal{S} \backslash \Gamma_k$.

Note that in the above steps we allow for additional approximation error, since there exist partition sets that may cross the boundaries of the support sets, and which are not contained in neither Γ_k nor $\mathcal{S} \backslash \Gamma_k$. In order to avoid this error, we should further adapt the selected partition to the boundaries of support sets.

4.2 Bound on the approximation error

THEOREM 2. *Suppose we approximate the value functions V_k by the piecewise constant functions $\bar{V}_k$, as described in the previous section. Then the approximation error is upper bounded, $\forall (x_1, x_2) \in \Gamma_k$, by*

$$|V_k(x_1, x_2) - \bar{V}_k(x_1, x_2)| \le E_k,$$

where

$$E_k = \lambda_k \delta + M^\star E_{k+1},$$

initialized by $E_N = 0$, and where δ is the partition size of $\cup_{i=1}^p A_i$ (namely, $\delta = \max_{i=1}^p \delta_i$, where δ_i is the diameter of A_i), λ_k is the Lipschitz constant of the value function V_k, and $M^\star$ is defined as in Theorem 1.

PROOF. We reason again by induction. The statement holds for $k = N$, since $V_N = \bar{V}_N = \mathbb{I}_A$. Suppose now that it is valid for step $k + 1$. Noting that $\forall (x_1, x_2) \in A, \exists i : (x_1, x_2) \in A_i$, then:

$$\begin{aligned}
&|V_k(x_1, x_2) - \bar{V}_k(x_1, x_2)| = |V_k(x_1, x_2) - \bar{V}_k(x_1^i, x_2^i)| \\
&\le |V_k(x_1, x_2) - V_k(x_1^i, x_2^i)| + |V_k(x_1^i, x_2^i) - \bar{V}_k(x_1^i, x_2^i)| \\
&\le \lambda_k \delta + \Bigg| \sum_{j=1}^{p} \int_{X_j} V_{k+1}(\bar{x}_1, f_2(x_1^i, x_2^i)) t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1 \\
&\qquad - \sum_{j=1}^{p} \int_{X_j} \bar{V}_{k+1}(\bar{x}_1, f_2(x_1^i, x_2^i)) t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1 \Bigg| \\
&\le \lambda_k \delta + \sum_{j=1}^{p} \int_{X_j} \left| V_{k+1}(\bar{x}_1, f_2(x_1^i, x_2^i)) - \bar{V}_{k+1}(\bar{x}_1, f_2(x_1^i, x_2^i)) \right| \cdot \\
&\qquad\qquad t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1 \\
&\le \lambda_k \delta + \sum_{j=1}^{p} \int_{X_j} E_{k+1} t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1 \\
&\le \lambda_k \delta + E_{k+1} \int_{\Pi_1(A)} t_x(\bar{x}_1 | x_1^i, x_2^i) d\bar{x}_1 \\
&\le \lambda_k \delta + M^\star E_{k+1},
\end{aligned}$$

which equals to E_k. □

Note that the constant M^* can be replaced by a decreasing finite sequence $\{M_k^*\}_{k=N}^1$, which yields a lower abstraction error.

5. AFFINE DETERMINISTIC DYNAMICS ON POLYTOPIC INVARIANT SET

It is in general difficult to find an explicit and computable bound for Condition 3 in Assumption 1. Such a bound depends directly on the shape of the sets Γ_k. However, a bound can be derived for models with deterministic dynamics that are affine and when the invariant set is a convex polytope. Under these conditions, the following lemma gives an explicit representation for the invariant sets Γ_k.

LEMMA 1. *Suppose that the deterministic dynamics in* (1) *are characterized by affine functions, namely:*

$$f_2(x_1, x_2) = A_1 x_1 + A_2 x_2 + A_3,$$

where $A_1 \in \mathbb{R}^{n_2 \times n_1}, A_2 \in \mathbb{R}^{n_2 \times n_2}, A_3 \in \mathbb{R}^{n_2 \times 1}$. Furthermore, suppose that the invariant set A is a (bounded) convex polytope, characterized by the following set of linear inequalities:

$$A = \left\{ (x_1, x_2) \in \mathbb{R}^n | A_N^1 x_1 + A_N^2 x_2 \le B_N \right\}.$$

Then the support sets $\Gamma_k, k = N-1, \ldots, 0$, are also bounded convex polytopes.

PROOF. Based on Equation (6), we can compute the sets $\Gamma_k, k = 0, \ldots, N-1$, as:

$$\Gamma_k = f_2^{-1}(\Pi_2(\Gamma_{k+1})) \cap \Gamma_{k+1}.$$

Suppose Γ_{k+1} is compact and convex then $\Pi_2(\Gamma_{k+1})$ is also a compact and convex set since the operator Π_2 is linear. Additionally, as the function f_2 is linear (and continuous), then $f_2^{-1}(\Pi_2(\Gamma_{k+1}))$ is also compact and convex.

Suppose now that set Γ_{k+1} is a polytope in $\mathbb{R}^n$, characterized by the following set of linear inequalities:

$$\Gamma_{k+1} = \left\{ (x_1, x_2) \in \mathbb{R}^n | A_{k+1}^1 x_1 + A_{k+1}^2 x_2 \le B_{k+1} \right\}.$$

Then $\Pi_2(\Gamma_{k+1})$ is also a polytope in n_2 dimensions, characterized by:

$$\Pi_2(\Gamma_{k+1}) = \{x_2 \in \mathbb{R}^{n_2} | C_{k+1}x_2 \leq D_{k+1}\}.$$

Techniques to perform a perpendicular projection of bounded polytopes allow to obtain $\Pi_2(\Gamma_{k+1})$ from Γ_{k+1}. [9] proved that the polyhedral projection is equivalent to the feasibility of a parametric linear programming problem. The MPT toolbox [12] constructs a vertex representation of Γ_{k+1}, having its half-space representation (vertex enumeration problem); it then projects these vertices based on the Π_2 operator; and finally it obtains a half-space representation of $\Pi_2(\Gamma_{k+1})$ from its vertex representation (facet enumeration problem).

Having obtained matrices C_{k+1}, D_{k+1} expressing $\Pi_2(\Gamma_{k+1})$, we can find Γ_k as follows:

$$\begin{aligned}\Gamma_k &= \{(x_1,x_2) \in \Gamma_{k+1} | f_2(x_1,x_2) \in \Pi_2(\Gamma_{k+1})\} \\ &= \{(x_1,x_2) \in \Gamma_{k+1} | C_{k+1} f_2(x_1,x_2) \leq D_{k+1}\} \\ &= \{(x_1,x_2) \in \Gamma_{k+1} | C_{k+1}(A_1x_1 + A_2x_2 + A_3) \leq D_{k+1}\} \\ &= \{(x_1,x_2) \in \Gamma_{k+1} | C_{k+1}A_1x_1 + C_{k+1}A_2x_2 \leq \\ &\qquad\qquad\qquad\qquad (D_{k+1} - C_{k+1}A_3)\}.\end{aligned}$$

Then Γ_k is a convex and bounded polytope with the following half-space representation:

$$\Gamma_k = \left\{(x_1,x_2) \in \mathbb{R}^n | A_k^1 x_1 + A_k^2 x_2 \leq B_k\right\}, \qquad (9)$$

where:

$$A_k^1 = \begin{bmatrix} C_{k+1}A_1 \\ A_{k+1}^1 \end{bmatrix}, A_k^2 = \begin{bmatrix} C_{k+1}A_2 \\ A_{k+1}^2 \end{bmatrix},$$
$$B_k = \begin{bmatrix} D_{k+1} - C_{k+1}A_3 \\ B_{k+1} \end{bmatrix}.$$

Note that this representation is not unique: it is possible to eliminate redundant half-spaces in the representation of Γ_k in each step. □

The following theorem derives the bound for Condition 3 in Assumption 1.

THEOREM 3. *Suppose Γ_k is a bounded convex polytope with the representation in* (9). *Then the sets $\Gamma_k^1(x_2)$ are polytopes in $\mathbb{R}^{n_1}$, which satisfy the Condition 3 in Assumption 1 with the following constant:*

$$\theta_k = \sum_{i=1, A_k^1(i)\neq 0}^{m_k} s_k(i) \frac{\|A_k^2(i)\|}{\|A_k^1(i)\|}.$$

The vectors $A_k^1(i)$ and $A_k^2(i)$ represent the i^{th} row of A_k^1 and A_k^2, respectively. The constant m_k accounts for the number of inequalities in the half-space representation of Γ_k, i.e. m_k is equal to the number of rows of A_k^1 (we do not account for the rows of A_k^1 that are equal to the zero vector). The constant $s_k(i)$ is computed as follows:

1. *if $n_1 = 1$ then $s_k(i) = 1$.*
2. *if $n_1 \geq 2$, project $\Pi_1(\Gamma_k)$ along the normal to the i^{th} hyperplane, i.e. along vector $A_k^1(i)$. The result is a polytope in $\mathbb{R}^{n_1-1}$, namely $\Pi^\perp(\Pi_1(\Gamma_k))$. Then $s_k(i) = \mathcal{L}(\Pi^\perp(\Pi_1(\Gamma_k)))$ or any upper bound for this Lebesgue measure.*

PROOF. Recall the definition of $\Gamma_k^1(x_2)$: for any $x_2 \in \Pi_2(\Gamma_k)$

$$\begin{aligned}\Gamma_k^1(x_2) &= \{x_1 \in \Pi_1(\Gamma_k) | (x_1,x_2) \in \Gamma_k\} \\ &= \left\{x_1 \in \mathbb{R}^{n_1} | A_1^k x_1 \leq B_k - A_k^2 x_2\right\}.\end{aligned}$$

For any fixed x_2 the set $\Gamma_k^1(x_2)$ is represented by a set of linear inequalities, which again characterizes a polytope. Each facet of the polytope is represented by one row of the above half-space representation:

$$A_1^k(i)x_1 \leq B_k(i) - A_k^2(i)x_2, \quad i = 1,\ldots,m_k.$$

The normal vector to this hyperplane in $\mathbb{R}^{n_1}$ is independent of parameter x_2. Varying x_2 to x_2', we obtain two parallel hyperplanes in $\mathbb{R}^{n_1}$. The volume bounded within the two hyperplanes is proportional to their distance d:

$$\begin{aligned}d &= \frac{|(B_k(i) - A_k^2(i)x_2) - (B_k(i) - A_k^2(i)x_2')|}{\|A_k^1(i)\|} \\ &= \frac{|A_k^2(i)(x_2 - x_2')|}{\|A_k^1(i)\|}.\end{aligned}$$

Suppose the values of $s_k(i)$ are defined as in the statement. Then:

$$\begin{aligned}&\mathcal{L}(\Gamma_k^1(x_2) \triangle \Gamma_k^1(x_2')) \\ &\qquad \leq \sum_{i=1}^{m_k} s_k(i) \frac{|A_2^k(i)(x_2 - x_2')|}{\|A_1^k(i)\|} \\ &\qquad = \sum_{i=1}^{m_k} s_k(i) \frac{\|A_2^k(i)\|}{\|A_1^k(i)\|} \|(x_2 - x_2')\| \\ &\qquad = \theta_k \|(x_2 - x_2')\|,\end{aligned}$$

which completes the proof. □

For the sake of completeness, let us explicitly derive the Lipschitz constant required for Condition 2 in Assumption 1, given affine deterministic dynamics.

PROPOSITION 2. *The Lipschitz constant of the affine function $f_2(x_1,x_2) = A_1x_1 + A_2x_2 + A_3$ is equal to:*

$$h_2 = \|[A_1, A_2]\|_2.$$

PROOF.

$$\begin{aligned}\|f_2(x_1,x_2) - f_2(x_1',x_2')\| &= \|A_1(x_1 - x_1') + A_2(x_2 - x_2')\| \\ &= \|[A_1, A_2][x_1 - x_1', x_2 - x_2']^T\| \\ &\leq \|[A_1, A_2]\|_2 \|(x_1,x_2) - (x_1',x_2')\|.\end{aligned}$$

□

6. CASE STUDY

This section applies the probabilistic invariance problem and the results derived above to a chemical reaction network characterized by species with heterogeneous concentrations. The dynamics of chemically reacting environments can be described by the general Chemical Master Equation (CME) [8], which unfortunately has seldom an analytical solution and is usually quite hard to integrate. Alternatively, species dynamics in time are studied via the Stochastic Simulation Algorithm (SSA) [8], which is a computational scheme that has attracted much research. Among the various approaches to approximate and speed up the SSA, the work in [10] has investigated one that is based on the use of first- and second-order approximations: species that are abundant in the environment are associated with deterministic dynamics (ordinary differential equations), whereas species with negligible numbers are given probabilistic dynamics (stochastic differential equations).

The underlying stoichiometry, reaction and degradation rates are directly taken from [6] and summarized in Table 1. Let us introduce the following vector:

$$x = \left[\begin{array}{cccc} D & D^\star & M & P \end{array}\right]^T,$$

describing the (low) concentration of an inactive and active gene (D and $D^\star$ respectively), as well as the (relatively abundant) concentration of m-RNA (M) and of a protein (P). The continuous dynamics are described by the following stochastic differential equation:

$$dx = f(x)dt + \sigma(x)dW.$$

Time is discretized with sampling interval Δ, according to an Euler-Maruyama, first-order scheme, obtaining:

$$x(k+1) = x(k) + f(x(k))\Delta + \sigma(x(k))\sqrt{\Delta}W(k),$$

where $f(x) = Ax$ and

$$A = \left[\begin{array}{cccc} -k_a & k_d & 0 & 0 \\ k_a & -k_d & 0 & 0 \\ 0 & k_r & -\gamma_r & 0 \\ 0 & 0 & k_p & -\gamma_p \end{array}\right],$$

and

$$\sigma(x) = \left[\begin{array}{cc} -\sqrt{k_a D} & \sqrt{k_d D^\star} \\ \sqrt{k_a D} & -\sqrt{k_d D^\star} \\ 0 & 0 \\ 0 & 0 \end{array}\right],$$

and finally $W(k) = [W_1(k), W_2(k)]^T$, and $W_i(k), i = 1,2, k \in \mathbb{N}\cup\{0\}$, are independent standard Normal random variables, which are also independent of the initial condition of the process. The steady-state values for the dynamics are estimated as in [10]:

- $P_{ss} = 65\,[nM] \Rightarrow M_{ss} = \frac{\gamma_p}{k_p}P_{ss}$,
- $D_{ss} = D^\star_{ss} = \frac{\gamma_r}{k_r}M_{ss} = \frac{\gamma_r}{k_r}\frac{\gamma_p}{k_p}P_{ss} = \frac{\gamma_p}{bk_r}P_{ss}$.

Since the dynamics of D and $D^\star$ are coupled, it is possible to eliminate the variable D, which leads to the following dynamical system:

$$\begin{aligned} x_1(k+1) &= (1 - k_d\Delta - k_a\Delta)x_1(k) + 2k_a\Delta D^\star_{ss} \\ &\qquad + \sqrt{2k_a\Delta D^\star_{ss}}W(k) \\ x_2(k+1) &= k_r\Delta x_1(k) + (1-\gamma_r\Delta)x_2(k) \\ x_3(k+1) &= k_p\Delta x_2(k) + (1-\gamma_p\Delta)x_3(k), \end{aligned}$$

where we have denoted

$$\left[\begin{array}{ccc} D^\star & M & P \end{array}\right]^T = \left[\begin{array}{ccc} x_1 & x_2 & x_3 \end{array}\right]^T,$$

and $W(k), k \in \mathbb{N}\cup\{0\}$, are again independent standard Normal random variables. Notice that the model is mixed deterministic-stochastic: namely, deterministic over the dynamics of $x_2\,(M), x_3\,(P)$, whereas stochastic for $x_1\,(D^\star)$.

We select a hyper-box A around the steady state values defined above, and compute probabilistic invariance over this region, for a given time horizon. The hyper-box is characterized by the parameters r_1, r_2, and r_3 as:

$k_a = k_d$	k_r	γ_r	k_p	γ_p
0.001	0.0078	0.0039	$b\gamma_r, b = 11$	0.0007

Table 1: Parameters for the case study, taken from [6], and expressed in $[s^{-1}]$.

$$\left|\frac{x_1 - D^\star_{ss}}{D^\star_{ss}}\right| \le r_1, \quad \left|\frac{x_2 - M_{ss}}{M_{ss}}\right| \le r_2, \quad \left|\frac{x_3 - P_{ss}}{P_{ss}}\right| \le r_3.$$

The kernel for the x_1 dynamics is Normal and admits a density $t_x(\bar{x}_1|x_1) \sim \mathcal{N}(\mu, \sigma)$, where the mean is an affine function of the conditional variable x_1 and the variance is constant:

$$\mu = (1 - k_d\Delta - k_a\Delta)x_1 + 2k_a\Delta D^\star_{ss}, \quad \sigma = \sqrt{2k_a\Delta D^\star_{ss}}.$$

The Lipschitz constant h_1 is computed based on the maximum norm of the partial derivative of the density function with respect to the conditional variable x_1:

$$\begin{aligned} h_1 &= \max\left\{\left|\frac{\partial t_x}{\partial x_1}(\bar{x}_1|x_1)\right| \Big| x_1, \bar{x}_1 \in \Pi_1(A)\right\} \\ &= (1 - k_d\Delta - k_a\Delta)\frac{\exp(-0.5)}{\sigma^2\sqrt{2\pi}}. \end{aligned}$$

The constants M and M^* have been considered independent of the step k and take the following values:

$$\begin{aligned} M &= \frac{1}{\sigma\sqrt{2\pi}}, \\ M^* &= 2\int_0^{\frac{r_1}{\sigma}D^\star_{ss}} \frac{1}{\sqrt{2\pi}}\exp\left[-\frac{u^2}{2}\right]du = \operatorname{erf}\left(\frac{r_1}{\sigma\sqrt{2}}D^\star_{ss}\right), \end{aligned}$$

where erf is the error function.

6.1 First Experiment (original parameters)

Suppose we select equal rates for the hyper-box that defines the invariance set: $r_i = r,\ i = 1,2,3$. It can be explicitly shown that in this case the invariance set does not shrink backwards, namely since

$$\forall (x_1, x_2, x_3) \in A, \qquad f_2(x_1, x_2, x_3) \in \Pi_2(A),$$

then the support sets are such that

$$\Gamma_{N-1} = A \Rightarrow \Gamma_k = A \quad \forall k \in \{0, 1, ..., N\}.$$

This fact also means that, with regards to Assumption 1,

$$\Gamma^1_k(x_2, x_3) = \Pi_1(A) = [(1-r)D^\star_{ss}, (1+r)D^\star_{ss}],$$

which leads to $\theta_k = 0$. The parameters L_k required for the error bounds are:

$$\begin{aligned} L = L_k &= \mathcal{L}(\Pi_1(\Gamma_k)) = \mathcal{L}(\Pi_1(A)) \\ &= (1+r)D^\star_{ss} - (1-r)D^\star_{ss} = 2rD^\star_{ss}. \end{aligned}$$

We have selected a time horizon $N = 10$, a time discretization step $\Delta = 1$, and a parameter $r = 0.05$. Recall that $n_1 = 1, n_2 = 2$. This has lead to a variance $\sigma = 0.03$ and to constants

$$h_1 = 227.7, h_2 = 1.02, L = 0.05, M = 12.25, M^\star = 0.58.$$

Finally, the abstraction error can be computed as $E_0 = 70.01\delta$. A partition size $\delta = 0.03$ has been selected for the experiment. Figure 1 shows the level set $V_8 = 0.12$ together with the invariant set (transparent bounding box).

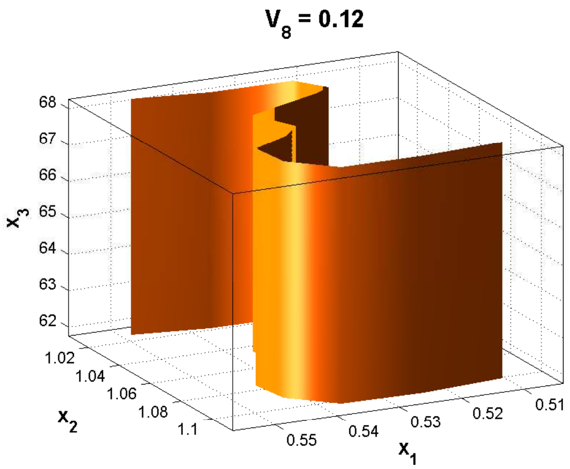

Figure 1: Representation of the level set $V_8 = 0.12$ for the value function of the first experiment.

6.2 Second Experiment (rescaled parameters)

It is easily seen that Γ_k are all equal by selecting the rates for the invariance hyper-box such that $r_1 \leq r_2 \leq r_3$. In order to show the efficiency of the proposed algorithm, the following rates have been thus selected:

$$r_1 = 0.20, \quad r_2 = 0.10, \quad r_3 = 0.05.$$

Furthermore, we have rescaled the constants $k_r, k_p, \gamma_r, \gamma_p$ by a factor of 100. The equilibrium point of the dynamics is not affected by this choice, and we obtain a variance $\sigma = 0.32$ and the following constants:

$$h_1 = 1.82, h_2 = 4.43, M = 12.25, M^\star = 0.99.$$

The algorithm results in time varying support sets Γ_k, however it turns out that $\Pi_1(\Gamma_k) = \Pi_1(A)$ for any k. This leads to constants $L = L_k = \mathcal{L}(\Pi_1(A)) = 0.21$. We have selected again a time horizon $N = 10$, a time discretization step $\Delta = 1$, and a partition size $\delta = 0.03$.

Figure 2 displays the support sets Γ_N, Γ_{N-1}, and Γ_0. Notice that the sets shrink as time decreases.

Over the support sets Γ_k, the probabilistic invariance is computed. Figure 3 displays the level sets of $V_0(x) = p_x(A)$, for varying invariance levels: $0, 0.02, 0.04, 0.06, 0.08, 0.1$. Notice that the set of points $V_0 = 0$ cover a region that is the complement of in Γ_0 in A (cfr. the top left plot in Figure 3 with the bottom plot in Figure 2).

Figure 4 displays the level set $V_k(x) = 0.1$, for varying time instants $k = 2, 4, 6, 8$. Additionally, for $k = 0$ we obtain the last (bottom-right) plot of Figure 3.

7. CONCLUSIONS

This work has presented an approach to compute probabilistic invariance (or safety) over a finite horizon for mixed deterministic-stochastic, discrete time processes. The computational technique, based on state-space discretization, has been associated to an explicit error bound. On the theoretical side, the contribution has shown that the problem under study can be separated into a deterministic reachability problem, and a probabilistic invariance one that depends

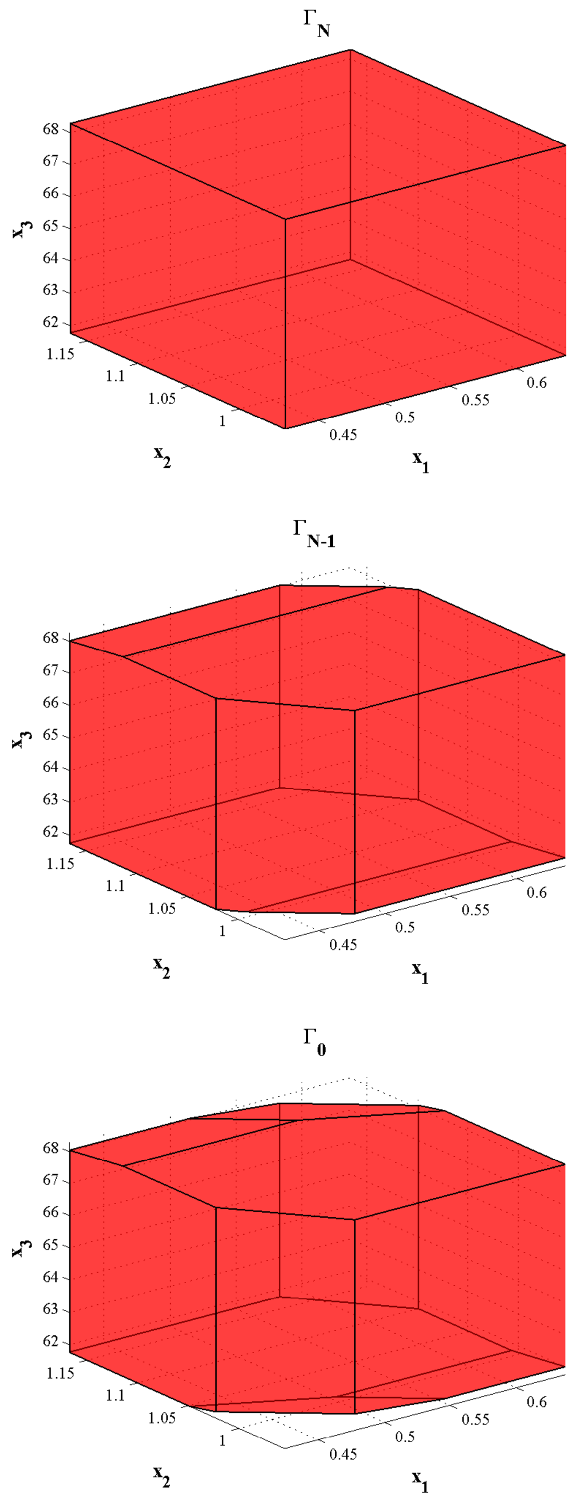

Figure 2: Representation of the support sets Γ_N, Γ_{N-1}, and Γ_0 for the second experiment.

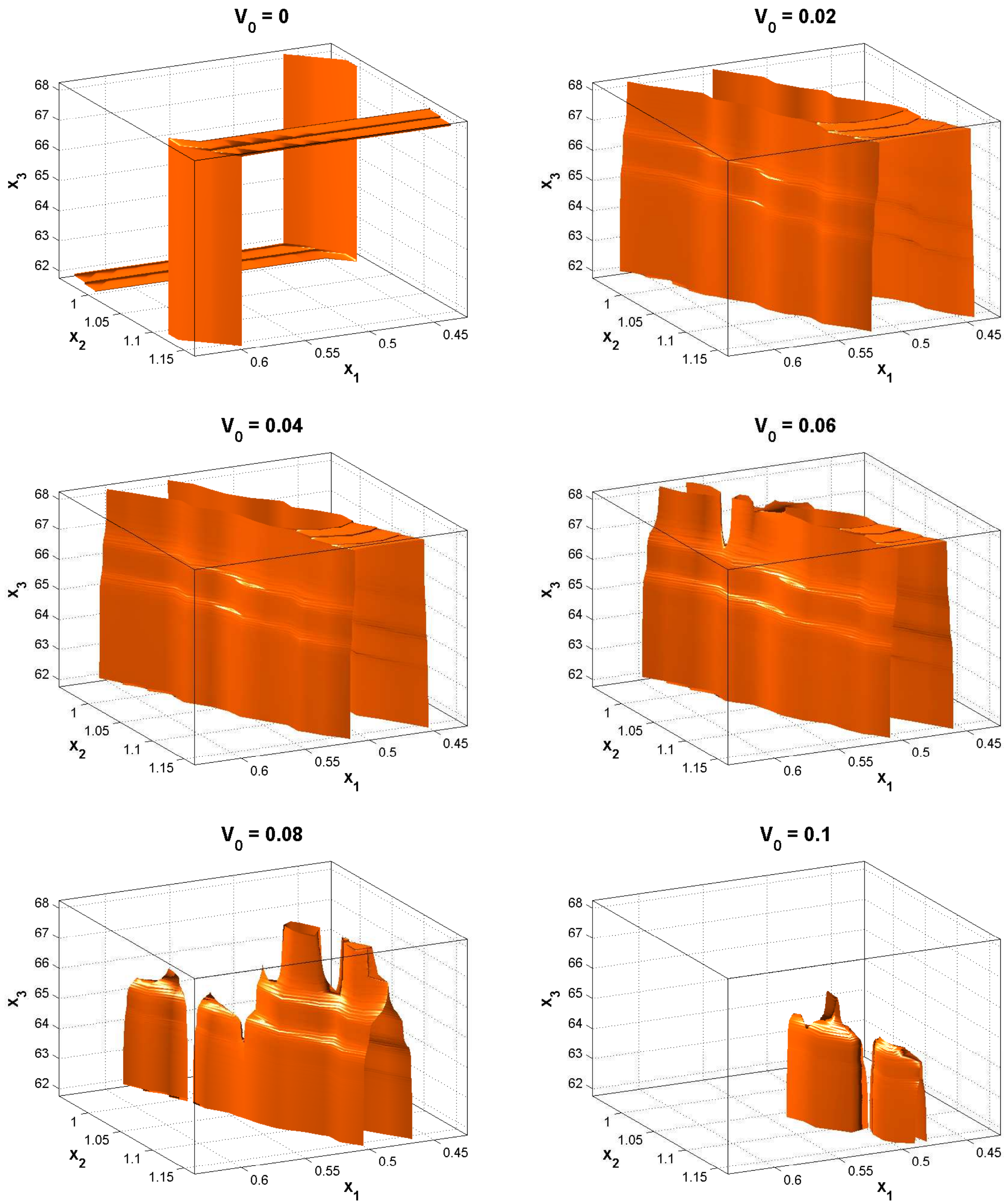

Figure 3: Representation of the level sets of $V_0(x) = p_x(A)$, for varying levels $(0, 0.02, 0.04, 0.06, 0.08, 0.1)$, for the second experiment.

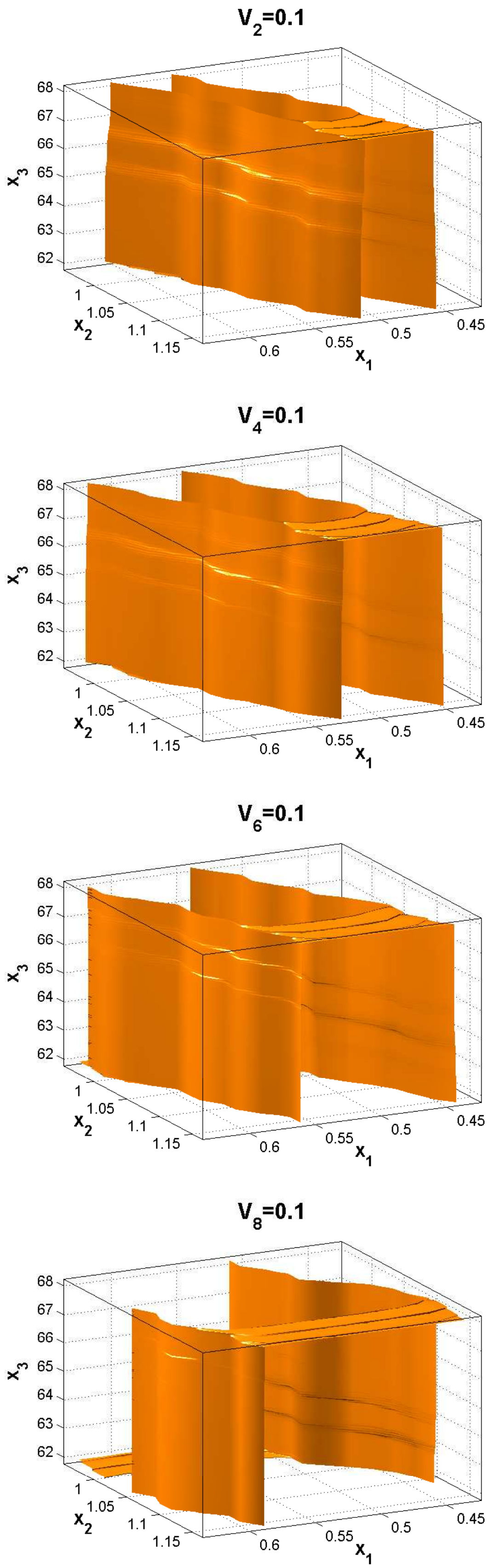

Figure 4: Representation of the level set $V_k(x) = 0.1$, for varying time instants $k = 2, 4, 6, 8$, for the second experiment.

on the outcome of the first. The technique has been tested on a case study modeling a chemical reaction network.

The authors are interested in extensions and further computational improvements of the proposed method.

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