Probabilistic Reach-Avoid Computation for Partially Degenerate Stochastic Processes

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***Abstract*—This work is concerned with the computation of probabilistic reach-avoid properties over a finite horizon for partially degenerate stochastic (that is, mixed deterministic-stochastic) processes evolving in discrete time over a continuous state-space. The models of interest consist of two fully coupled dynamical parts: the first part is described by deterministic maps (vector fields), whereas the second depends on probabilistic dynamics that are characterized by stochastic kernels. In contrast with a fully probabilistic approach (which is possible since the two dynamical components are coupled), this work shows that the probabilistic reach-avoid problem can be characterized – and thus computed – in two sequential steps: the first is a simple deterministic reachability analysis, which is then followed by a probabilistic reach-avoid problem depending on the outcome of the first step. This characterization leads to implementation advantages over a fully probabilistic approach and allows synthesizing a computational algorithm with explicit error bounds.**

I. Introduction

When working with stochastic processes one has to deal with a probabilistic variant of the known reachability problem, which can be formulated as follows: to evaluate the likelihood that a process, initialized anywhere on the state-space, reaches a given target domain within a finite (or infinite) time horizon. Reachability is the dual of invariance (or safety), which is interested in evaluating the probability that a realization of the process stays within a set of interest (known as invariance domain or safe set) over a given time horizon.

The reach-avoid property generalizes reachability and invariance as follows: given a safe set and a target set defined over the state-space, the probabilistic reach-avoid problem is concerned with quantifying the probability that over a given time horizon a realization of the process, started anywhere on the state-space, reaches the target set while remaining within the safe set (equivalently, while avoiding the complement of the safe set). Probabilistic invariance (or its dual, reachability) has been investigated over various models and with multiple theoretical techniques. Recent work on continuous state-space models has focused on both continuous [6], [16] and discrete time [3]. Probabilistic reach-avoid has been studied in [18] as an extension of [3].

This contribution focuses on autonomous stochastic processes evolving in discrete time over an abstract continuous state-space. With the objective of obtaining computable results (with explicit error bounds), it considers the reach-avoid property over a finite time horizon and extends results developed for the special case of probabilistic invariance [9]. Quite distinctively, this work deals with partially degenerate stochastic models, i.e. models endowed with explicit mixed deterministic-stochastic dynamics. Such models are characterized by heterogeneous dynamics, comprising two sets of coupled variables: the first set of variables has associated dynamics that are described by deterministic maps (vector fields), whereas the complement set is endowed by probabilistic dynamics (characterized by a stochastic kernel). These models can be thought of as special instances of fully stochastic dynamical processes.

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Along with originating from degenerate quantities (variance or volatility) in a probabilistic model, mixed deterministic-stochastic dynamics naturally arise in multi-scale models, where variables take values within ranges that are dimensionally different. Of interest to this work (cf. case study), these heterogeneous dynamics appear in models developed for the simulation of cellular environments endowed with both rare and abundant species [15].

A straightforward (and naïve) approach to the characterization and computation of the probabilistic reach-avoid problem for mixed deterministic-stochastic models is to directly tackle it as a reachability verification instance over a fully stochastic (but degenerate) system. We argue that this approach results in a computationally more expensive solution and leads to the impossibility to leverage computational techniques that apply exclusively to non-degenerate systems [2], [7], [8], [10]. In contrast to the above approach, this contribution originally shows that the probabilistic reach-avoid problem investigated in this modelling framework can be neatly separated into two parts: first a deterministic reachability analysis, then a probabilistic reach-avoid problem that depends on the outcome of the first analysis. This separation is possible despite the explicit coupling between the variables of the two parts of the model. Deterministic reachability analysis is a rather mature field of research [11] with ample software tool support [1], whereas the second problem can harvest recent developments [3], [6], [16]. We argue that this new approach can also lead to practical computational improvements: wherever the first deterministic problem yields a "false" outcome (namely, that no states can be deterministically reached over the given time horizon), then no further probabilistic calculation is necessary – that is, the overall probabilistic reach-avoid probability equals to zero. Besides, the solution of the probabilistic reachability part can be confined within the "reachability domains" resulting from the deterministic computations. The proposed approach furthermore leads to an approximation algorithm for the quantities of interest with explicit error bounds: related approaches derived for fully stochastic models [2], [7], [8], [10] would not be otherwise applicable.

II. Model and Problem Statement

We consider a stochastic process evolving over a continuous state-space $\mathscr{S}$. We assume that $\mathscr{S}$ is a Borel measurable space endowed with a metric, and we denote by $\mathscr{B}$ the associated sigma algebra [12]. In this work for simplicity we refer to a vector space $\mathbb{R}^n$ endowed with the Euclidean distance. The discrete time process is Markovian and driven by the following mixed deterministic-stochastic dynamics:

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

The model in (1) is comprised of

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

Denote by $x(k) = \big(x_1(k), x_2(k)\big) \in \mathbb{R}^n = \mathscr{S}$, $n = n_1 + n_2$, the state variable of the whole model in (1), which can always be considered as a Markov process characterized by a conditional stochastic kernel $T_x : \mathscr{B} \times \mathscr{S} \to [0,1]$ [14]. More precisely, the knowledge of the distribution of the random variable $h(\cdot)$ at a given time k allows us to characterize a conditional stochastic kernel $T_x(\cdot|x)$

that assigns to each point $x \in \mathscr{S}$ a probability measure $T_x(\cdot|x)$, so that for any set $A \in \mathscr{B}, P_x(x(k+1) \in A) = \int_A T_x(d\bar{x}|x(k) = x)$, for any $k \in \mathbb{N}_0$, where P_x denotes the conditional probability $P(\cdot|x)$ and P is a probability measure defined over the space $\mathscr{S}$. We assume that the stochastic kernel T_x admits a density t_x, such that $T_x(d\bar{x}|x) = t_x(\bar{x}|x)d\bar{x}$ [12]. The special structure of model (1) allows the following expression:

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

for $x = (x_1, x_2)$ and where $\delta(x_2 - a)$ is the continuous, n_2-dimensional Dirac delta function shifted at point a. The first term $t_{x_1}(\bar{x}_1|x)$ depends on the stochastic part of the dynamical model, whereas the second term $\delta(\bar{x}_2 - f_2(x))$ hinges on its deterministic vector field.

Consider a compact Borel set $A \subset \mathscr{B}$ as the safe set and a Borel measurable set $B \subseteq A$ as the target set. We study the probabilistic reach-avoid problem over a finite time horizon $[0, N]$: to find the probability that trajectories starting from an initial state $x_0 \in \mathscr{S}$ hit the target set B within time horizon $[0, N]$ while remaining within the safe set A. Quantitatively,

$$p_{x_0}(A, B) = P\{\exists j \in [0, N], x(j) \in B \wedge \forall k < j, x(k) \in A | x(0) = x_0\}, \tag{3}$$

where we have denoted with P the probability measure associated to the canonical sample space $\mathscr{S}^{N+1}$ with associated σ-algebra [4].

A characterization of the problem in (3) is addressed by the following result.

Proposition 1 (Bellman recursion for reach-avoid [18]). *Introduce functions $W_k : \mathscr{S} \to [0, 1], k \in [0, N]$, and define them backward-recursively as follows:*

$$W_k(x) = \mathbb{I}_B(x) + \mathbb{I}_{A\setminus B}(x) \int_{\mathscr{S}} W_{k+1}(x_{k+1}) T_x(dx_{k+1}|x), \tag{4}$$

where $W_N(x)$ is initialized as the indicator function of set B: $W_N(x) = \mathbb{I}_B(x)$, i.e. it is equal to 1 if $x \in B$, else it is equal to 0. Then the solution of problem (3) is $p_{x_0}(A, B) = W_0(x_0)\ \forall x_0 \in \mathscr{S}$.

Notice that probabilistic invariance over a given set A [3] can be related to a special instance of the reach-avoid problem, defined over the same time horizon and where the safe set is taken to be the whole space $\mathscr{S}$ whereas the target set is selected to be $A^c = \mathscr{S} \setminus A$. Furthermore, notice that the reach-avoid formulation $p_{x_0}(A, B)$ can be extended to the instance where $B \not\subset A$ by simply introducing the set $A' = A \cup B$ and solving $p_{x_0}(A', B)$. The solution of $p_{x_0}(A, B)$ is seldom analytic since the recursion in (4) rarely admits a closed form solution. This warrants the development of techniques and algorithms to compute it approximately. With this goal, the work in [2] puts forward a discretization approach – later improved in [7], [8], [10] – with proven error bounds, under continuity conditions of the stochastic kernel T_x. However, such continuity conditions clearly do not hold for mixed deterministic-stochastic models, which are made up of discontinuous densities as in (2).

This leads to the goal of this work: this contribution first tailors problem (3) to the structure of the model in (1) and then provides a technique to compute the solution of (4) by a numerical scheme with associated error bounds. The characterization separates problem (3) into two parts: a deterministic reachability problem and a subsequent stochastic one.

III. Properties and Computation of the Probabilistic Reach-Avoid Problem

A. Characterization of probabilistic reach-avoid via value functions

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

$$\mathscr{D}(W_k) = \{x \in \mathscr{S} | W_k(x) \neq 0\} \quad k \in [0, N),$$

and $\mathscr{D}(W_N) = B$. The support of the value function W_k plays an important role in the problem definition, as elaborated in the following observations:

- $W_k(x) = 1\ \forall x \in B$, while $W_k(x) = 0\ \forall x \notin A$, which leads to $B \subseteq \mathscr{D}(W_k) \subseteq A$, $k \in [0, N]$;
- the value functions are non-decreasing backwards in time: $0 \leq W_{k+1}(x) \leq W_k(x)\ \forall k \in [0, N),\ \forall x \in A$, which leads to conclude that $\mathscr{D}(W_{k+1}) \subseteq \mathscr{D}(W_k)$.

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 the whole state-space $\mathscr{S}$). 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: $\forall x \in A \setminus B$,

$$W_k(x) = \int_{\mathscr{D}(W_{k+1})} W_{k+1}(\bar{x}_1, \bar{x}_2) t_{x_1}(\bar{x}_1|x) \delta(\bar{x}_2 - f_2(x)) d\bar{x}_2 d\bar{x}_1, \tag{5}$$

where we have used the expression in (2). Characterizing the sets $\mathscr{D}(W_k), k \in [0, N)$, becomes thus critical for the optimization of the original recursion in (4). However, in general the exact computation of the sets $\mathscr{D}(W_k)$ is problematic, in particular due to the characterization of $\mathscr{D}(t_{x_1}(\cdot|x))$ as a function of x. In order to mitigate this complication, let us introduce two projection maps as follows: $\Pi_1 : \mathbb{R}^n \to \mathbb{R}^{n_1}$, $\Pi_1(x_1, x_2) = x_1$; $\Pi_2 : \mathbb{R}^n \to \mathbb{R}^{n_2}$, $\Pi_2(x_1, x_2) = x_2$. Exploiting the special structure of the conditional density function, an over-approximation of the sets $\mathscr{D}(W_k)$ can be determined as follows:

$$\mathscr{D}(W_k) \subseteq B \cup \left\{x \in A \setminus B | f_2(x) \in \Pi_2\left(\mathscr{D}(W_{k+1})\right)\right\}.$$

Because $\mathscr{D}(W_{k+1}) \subseteq \mathscr{D}(W_k)$ and in general the above inclusion is strict, we can over-approximate the sets $\mathscr{D}(W_k)$ by Γ_k, as defined by the following recursive procedure:

$$\Gamma_k = B \cup \left\{x \in A \setminus B | f_2(x) \in \Pi_2\left(\Gamma_{k+1}\right)\right\}, \qquad \Gamma_N = B. \tag{6}$$

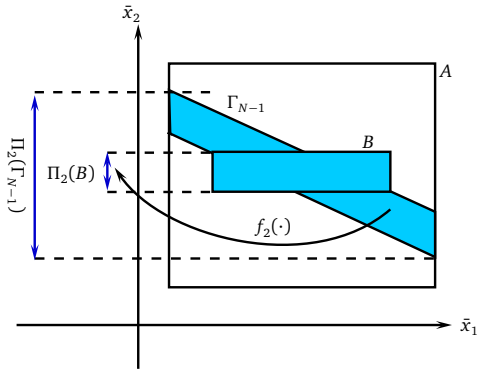
The sequence $\{\Gamma_k\}_{k=0}^N$ is endowed with the following properties:

- $B = \Gamma_N \subseteq \Gamma_{N-1} \subseteq \Gamma_{N-2} \subseteq \cdots \subseteq \Gamma_0 \subseteq A$;
- because $\mathscr{D}(W_k) \subseteq \Gamma_k$, then $p_{x_0}(A, B) = 0\ \forall x_0 \notin \Gamma_0$;
- if $\exists k_0 \leq N, \Pi_2\left(\Gamma_{k_0+1}\right) = \Pi_2\left(\Gamma_{k_0}\right)$, then $\Gamma_k = \Gamma_{k_0}\ \forall 0 \leq k \leq k_0$;
- in particular, if $\exists k_0 \leq N, \Pi_2\left(\Gamma_{k_0+1}\right) = \Pi_2(A)$, then $\Gamma_k = \Gamma_{k_0}$ $\forall 0 \leq k \leq k_0$.

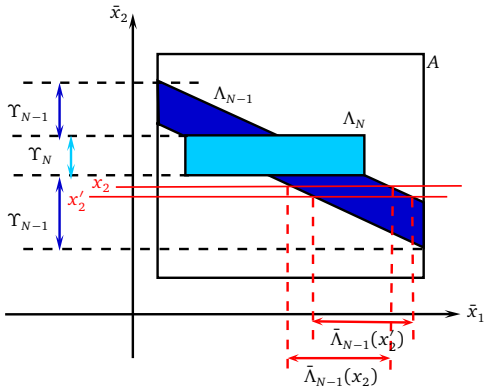
These properties highlight the dependence of the sets Γ_k (in the sequel we will denote them simply as *support sets*) on the deterministic vector field f_2 and in particular on the points that are mapped by f_2 inside such sets. Notice that since in the above definition $\Gamma_k \supseteq B$, the domain $A \setminus B$ can be practically replaced by set A. This observation leads to an advantage in the numerical computation of Γ_k, as will be discussed later (cf. Theorem 3). Let us define two sequences of disjoint sets $\{\Lambda_k\}_{k=0}^N$ and $\{\Upsilon_k\}_{k=0}^N$ (they will be needed in the sequel to establish continuity properties of the value functions $W_k(\cdot)$) as follows:

$$\begin{aligned} &\Lambda_k = \Gamma_k \setminus \Gamma_{k+1}, && \Lambda_N = \Gamma_N = B; \\ &\Upsilon_k = \Pi_2(\Gamma_k) \setminus \Pi_2(\Gamma_{k+1}), && \Upsilon_N = \Pi_2(\Gamma_N) = \Pi_2(B). \end{aligned}$$

The two sequences are related by the inclusion $\Lambda_k \subseteq f_2^{-1}(\Upsilon_{k+1})$, namely, $f_2(x) \in \Upsilon_{k+1}\ \forall x \in \Lambda_k$. In other words, $\Lambda_k = \emptyset$ if $\Upsilon_{k+1} = \emptyset$.



(a) Visualization of the sets Γ_k.



(b) Visualization of the sets Λ_k, Υ_k and of the map $\bar{\Lambda}_k(\cdot)$.

Fig. 1. Visualization of the sets Γ_k, Λ_k, and Υ_k, and of the backward recursion over them (cf. case study in Section IV).

Let us introduce the set-valued functions $\bar{\Lambda}_k : \Pi_2(\Gamma_{k+1}) \to 2^{\Pi_1(\Lambda_k)}$, $k = [0, N)$, as

$$\bar{\Lambda}_k(x_2) = \{x_1 \in \Pi_1(\Lambda_k) | (x_1, x_2) \in \Lambda_k\} \quad \forall x_2 \in \Pi_2(\Gamma_{k+1}).$$

Recall the recursive formula in (5) for W_k. By definition of Γ_k, we know that W_k is equal to zero outside of the set Γ_k and equal to one inside the set B, which allows us to express (5) as follows: $\forall x \in \Gamma_k \backslash B = \bigcup_{j=k}^{N-1} \Lambda_j$,

$$\begin{aligned} W_k(x) &= \int_{\Gamma_{k+1}} W_{k+1}(\bar{x}) T_x(d\bar{x}|x) \\ &= \sum_{i=k+1}^{N} \int_{\bar{\Lambda}_i(f_2(x))} W_{k+1}(\bar{x}_1, f_2(x)) t_{x_1}(\bar{x}_1|x) d\bar{x}_1. \end{aligned} \tag{7}$$

This formulation fully characterizes the value functions W_k in terms of the sets Γ_k. The computation of sets Γ_k based on (6) is a known deterministic backward reachability procedure over the map f_2. Deterministic reachability analysis is a mature topic of research [11], supported by software tools [1]. Sets Λ_k, Υ_k are illustrated in Figure 1, along with the backward recursion in (6), for a two dimensional system (cf. case study in Section IV).

B. Continuity of the value functions for probabilistic reach-avoid

Continuity properties of the value functions over their support are key for the computational schemes that will be introduced later. 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_1}, the vector field f_2, and the parametrized sets $\bar{\Lambda}_k$ satisfy the following conditions with finite constants $h_{kj}, \bar{h}_j, \theta_{kj}$:*

1) $\left|t_{x_1}(\bar{x}_1|x) - t_{x_1}(\bar{x}_1|x')\right| \le h_{kj}\|x - x'\|$, *for all* $\bar{x}_1 \in \Pi_1(\Gamma_{k+1})$, $x, x' \in \Lambda_j$, $k, j \in [0, N), k \le j$;
2) $\left\|f_2(x) - f_2(x')\right\| \le \bar{h}_j\|x - x'\|$, *for all* $x, x' \in \Lambda_j$, $j \in [0, N)$;
3) $\mathscr{L}(\bar{\Lambda}_k(x_2) \triangle \bar{\Lambda}_k(x_2')) \le \theta_{kj}\|x_2 - x_2'\|$, *for all* $x_2, x_2' \in \Upsilon_j$, $k, j \in [1, N]$.

Here $\mathscr{L}$ is the Lebesgue measure over $\mathbb{R}^{n_1}$, whereas $\triangle$ denotes the symmetric difference between two sets ($A \triangle B = (A \backslash B) \cup (B \backslash A)$). The first two are continuity assumptions on the probabilistic density and on the vector field, whereas the third is a regularity requirement on the variation of the (projection along the x_1 variables of the) sets Λ_k as a function of x_2. The last assumption depends on the shape of the sets Λ_k and on f_2, as in Figure 1.

Theorem 1. *If Assumption 1 is valid, then the value functions W_k are piecewise Lipschitz continuous on $\Gamma_k = \cup_{j=k}^{N} \Lambda_j$, namely for all $k \in [0, N], j \in [k, N]$, and $x, x' \in \Lambda_j$,*

$$\left|W_k(x) - W_k(x')\right| \le \lambda_{kj}\|x - x'\|,$$

where the finite Lipschitz constant λ_{kj} satisfies the recursive formula

$$\lambda_{kj} = L_{k+1}h_{kj} + \bar{h}_j \sum_{i=k+1}^{N} \left(\lambda_{(k+1)i} M_{ij}^\star + \theta_{i(j+1)} M_{ij}\right),$$

for all $k, j \in [0, N)$, $k \le j$, initialized with $\lambda_{kN} = 0$ for $k \in [0, N]$, and where for $i, k \in [1, N]$, $j \in [0, N)$, $L_k = \mathscr{L}\left(\Pi_1(\Gamma_k)\right)$, $M_{ij} = \sup\left\{t_{x_1}(\bar{x}_1|x) | \bar{x}_1 \in \Pi_1(\Lambda_i), x = (x_1, x_2) \in \Lambda_j\right\}$, $M_{ij}^\star = \sup_{x \in \Lambda_j} \int_{\Pi_1(\Lambda_i)} t_{x_1}(\bar{x}_1|x) d\bar{x}_1$.

Proof. Since $W_N(x) = \mathbb{I}_B(x)$, it follows that $\lambda_{NN} = 0$ and that the statement holds for $k = N$. Now suppose that the statement holds at step $k+1$, namely for all $j \in [k+1, N]$ and $x, x' \in \Lambda_j$,

$$\left|W_{k+1}(x) - W_{k+1}(x')\right| \le \lambda_{(k+1)j}\|x - x'\|.$$

We show that it holds as well at step k and for all $j \in [k, N]$. Since $W_k(x) = 1 \ \forall x \in \Lambda_N = B$, it follows that $\lambda_{kN} = 0$ and that the statement holds for $j = N$. Recall the simplified recursion in (7): for a fixed $j \in [k, N)$ select any two states $x, x' \in \Lambda_j$ and let us temporarily introduce sets $A_i^\star = \bar{\Lambda}_i(f_2(x))$ and $B_i^\star = \bar{\Lambda}_i(f_2(x'))$ to simplify the notations. Then

$$\begin{aligned} |W_k(x) - W_k(x')| \le & \left| \sum_{i=k+1}^{N} \int_{A_i^\star \cap B_i^\star} \Big(W_{k+1}(\bar{x}_1, f_2(x)) t_{x_1}(\bar{x}_1|x) - \right. \\ & \left. W_{k+1}(\bar{x}_1, f_2(x')) t_{x_1}(\bar{x}_1|x')\Big) d\bar{x}_1 \right| \\ & + \sum_{i=k+1}^{N} \int_{A_i^\star \backslash B_i^\star} W_{k+1}(\bar{x}_1, f_2(x)) t_{x_1}(\bar{x}_1|x) d\bar{x}_1 \\ & + \sum_{i=k+1}^{N} \int_{B_i^\star \backslash A_i^\star} W_{k+1}(\bar{x}_1, f_2(x')) t_{x_1}(\bar{x}_1|x') d\bar{x}_1 \\ \le & \left| \sum_{i=k+1}^{N} \int_{A_i^\star \cap B_i^\star} W_{k+1}(\bar{x}_1, f_2(x)) \left[t_{x_1}(\bar{x}_1|x) - t_{x_1}(\bar{x}_1|x')\right] d\bar{x}_1 \right| \\ & + \left| \sum_{i=k+1}^{N} \int_{A_i^\star \cap B_i^\star} t_{x_1}(\bar{x}_1|x') \left[W_{k+1}(\bar{x}_1, f_2(x)) - W_{k+1}(\bar{x}_1, f_2(x'))\right] d\bar{x}_1 \right| \\ & + \sum_{i=k+1}^{N} M_{ij} \mathscr{L}(A_i^\star \triangle B_i^\star). \end{aligned}$$

This inequality is made up of three terms, of which the first can be upper bounded by

$$h_{kj}\|x - x'\| \int_{\Pi_1(\Gamma_{k+1})} W_{k+1}(\bar{x}_1, f_2(x)) d\bar{x}_1 \le L_{k+1}h_{kj}\|x - x'\|.$$

Notice that if $\bar{x}_1 \in A_i^\star \cap B_i^\star$, then $(\bar{x}_1, f_2(x)), (\bar{x}_1, f_2(x')) \in \Lambda_i$. Using the induction hypothesis, the second term can be upper bounded as follows:

$$\begin{aligned}\sum_{i=k+1}^{N} \lambda_{(k+1)i} \|f_2(x) - f_2(x')\| \int_{A_i^\star \cap B_i^\star} t_{x_1}(\bar{x}_1|x') d\bar{x}_1 \\ \leq \sum_{i=k+1}^{N} \lambda_{(k+1)i} \bar{h}_j \|x - x'\| \int_{\Pi_1(\Lambda_i)} t_{x_1}(\bar{x}_1|x') d\bar{x}_1 \\ \leq \bar{h}_j \|x - x'\| \sum_{i=k+1}^{N} \lambda_{(k+1)i} M_{ij}^\star.\end{aligned}$$

Because $x, x' \in \Lambda_j$, then $f_2(x), f_2(x') \in \Upsilon_{j+1}$, and the last term can be upper bounded by

$$\begin{aligned}\sum_{i=k+1}^{N} \mathscr{L}(\bar{\Lambda}_i(f_2(x)) \triangle \bar{\Lambda}_i(f_2(x'))) M_{ij} \\ \leq \sum_{i=k+1}^{N} \theta_{i(j+1)} \|f_2(x) - f_2(x')\| M_{ij} \leq \sum_{i=k+1}^{N} \theta_{i(j+1)} \bar{h}_j \|x - x'\| M_{ij}.\end{aligned}$$

Collecting the three bounds, we obtain

$$\begin{aligned}\left|W_{k+1}(x) - W_{k+1}(x')\right| \leq \\ \left(L_{k+1} h_{kj} + \bar{h}_j \sum_{i=k+1}^{N} \left(\lambda_{(k+1)i} M_{ij}^\star + \theta_{i(j+1)} M_{ij} \right) \right) \|x - x'\|,\end{aligned}$$

for all $x, x' \in \Lambda_j$, which completes the proof. □

The previous result can be stated in a notationally simplified manner as discussed in [9].

C. Approximation scheme for computation, quantification of the corresponding error

The established piecewise Lipschitz continuity of the value functions allows computing the solution of the probabilistic reach-avoid problem by considering approximations that are piecewise constant within the domains of continuity. We propose an approximation scheme to perform the computations in (7). In order to keep the notations light, we replace the generic integration domain $\cup_{i=k+1}^{N} \bar{\Lambda}_i(f_2(x)), k \in [0, N)$, by $\Pi_1(A)$, and later comment on how the procedure applies similarly to the other case.

Select two arbitrary partitions of the sets $B, A\backslash B$. The union of these partitions constructs a partition of the safe 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 of the partition. A partition of the whole state-space $\mathscr{S}$ is obtained by adding the complement set $A_{p+1} = \mathscr{S}\backslash A$. Pick any point $x^i = (x_1^i, x_2^i) \in A_i, i = 1, \ldots, p+1$. Since the collection of the sets $\Pi_1(A_i)$ produce in general a cover (not necessarily a partition) of the set $\Pi_1(A)$, let us additionally select an arbitrary (q dimensional) partition $\Pi_1(A) = \cup_{j=1}^{q} X_j$ for the projection of the safe set along the first variable. This allows us to express

$$\begin{aligned}W_k(x) = \int_{\Pi_1(A)} W_{k+1}(\bar{x}_1, f_2(x)) t_{x_1}(\bar{x}_1|x) d\bar{x}_1 \\ = \sum_{j=1}^{q} \int_{X_j} W_{k+1}(\bar{x}_1, f_2(x)) t_{x_1}(\bar{x}_1|x) d\bar{x}_1 \quad \forall x \in A\backslash B.\end{aligned}$$

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

$$\bar{W}_k(x) = \sum_{i=1}^{p+1} \bar{W}_k(x^i) \mathbb{I}_{A_i}(x) \quad \forall x \in A\backslash B,$$

for $k \in [0, N)$, and initialized as $\bar{W}_N(x^i) = 1 \ \forall x^i \in B$, and $\bar{W}_N(x^i) = 0 \ \forall x^i \in A\backslash B$. Introduce the simplified notation $W_k^i = \bar{W}_k(x^i)$. These functions are recursively computed as follows:

$$W_k^i = \sum_{j=1}^{q} \int_{X_j} \bar{W}_{k+1}(\bar{x}_1, f_2(x^i)) t_{x_1}(\bar{x}_1|x^i) d\bar{x}_1 \quad \forall x^i \in A\backslash B. \tag{8}$$

In this formulation the values of $\bar{W}_{k+1}$ over the hyperplane $X_j \times \{f_2(x^i)\}$ are needed. Thus, in order to implement the procedure discretely, the function $\bar{W}_{k+1}$ should be constant over this hyperplane. This feature is achieved by raising the following assumption on the partition sets X_j of $\Pi_1(A)$: $\forall i \in [1, p], j \in [1, q], \exists i' \in [1, p] : \ X_j \times \{f_2(x^i)\} \subseteq A_{i'}$. Notice that this assumption does not depend on step k and is immediately satisfiable by selecting two partitions $\Pi_1(A) = \cup_j X_j$ and $\Pi_2(A) = \cup_r Y_r$, and then constructing the partition for A as a subset of the cross product of these two partitions: $A \subseteq \Pi_1(A) \times \Pi_2(A) = \cup_{j,r} X_j \times Y_r$.

Consider a map $i' = R(i, j)$ which assigns to each partition set X_j and value $f_2^i = f_2(x^i)$ the corresponding partition set $A_{i'}$ containing $X_j \times f_2^i$. Finally, starting from the recursive procedure (7), the discrete version of the (continuous) operation in (8) can be formulated as

$$W_k^i = \sum_{j=1}^{q} W_{k+1}^{i'} \int_{X_j} t_{x_1}(\bar{x}_1|x^i) d\bar{x}_1. \tag{9}$$

Let us again emphasize that the steps above, developed for the fixed set A, can be tailored to the integration domains based on Γ_k. Furthermore, notice that in the procedure above we allow for an additional approximation error, since there may exist partition sets that cross the boundaries of the support sets, and which are contained neither in Γ_k, nor in $\mathscr{S}\backslash\Gamma_k$. In order to avoid this error, we select a partition for the smallest support set Γ_N and, iteratively, extend the partition of set $\Gamma_{k+1} \subseteq \Gamma_k$ to obtain a proper partition of Γ_k.

The scheme is summarized in Algorithm 1 and its error is explicitly quantified as follows.

Algorithm 1 Approximation scheme for probabilistic reach-avoid

Require: mixed deterministic-stochastic system $(T_x, \mathscr{S})$, safe set $A \in \mathscr{B}$, target set $B \in \mathscr{B}$, finite time horizon N; sequence of support sets $\Gamma_k, k \in [0, N], \Gamma_N = B$

1: Select partitions $\cup_j X_j$ of $\Pi_1(\Gamma_k)$ and associated partitions $\cup_i A_i$ of set Γ_k, $k = N, \ldots, 0$
2: Compute the map $i' = R(i, j)$ based on the chosen partition sets
3: Compute marginalization matrix P, with entries $P_{ij} = \int_{X_j} t_{x_1}(\bar{x}_1|x^i) d\bar{x}_1$
4: At $k \in [0, N]$, use Γ_k to set entries equal to zero: $W_k^i = 0, \forall i : A_i \subset \mathscr{S}\backslash\Gamma_k$
5: Recursively compute value functions $W_k^i = \sum_{j=1}^{q} P_{ij} W_{k+1}^{i'}$ as in (9) and put $W_k^i = 1 \ \forall x^i \in B$, where $W_N^i = 1 \ \forall x^i \in B$, and $W_N^i = 0 \ \forall x^i \in A\backslash B$

Ensure: $W_0^i, i \in [1, p+1]$, approximate solution of reach-avoid problem defined over sets A and B

Theorem 2. *Suppose that the value functions W_k are approximated by piecewise constant functions $\bar{W}_k$, as described above. Then the approximation error is upper bounded by the quantity*

$$|W_k(x) - \bar{W}_k(x)| \leq E_k \quad \forall x \in \Gamma_k,$$

where $E_k = \max_{j \in [k,N]} \lambda_{kj} \delta + M_k^\star E_{k+1}$, initialized by $E_N = 0$, and where δ is the partition size of the (largest) support set Γ_0 (namely,

$\delta = \max_i \delta_i$, where δ_i is the diameter of the partition set indexed by i), λ_{kj} is the Lipschitz constant of the value function W_k over Λ_j, and $M_k^\star$ is defined as $M_k^\star = \sup_{x\in\Gamma_k\setminus B}\int_{\Pi_1(\Gamma_{k+1})} t_{x_1}(\bar{x}_1|x)d\bar{x}_1$.

Proof. The proof is based on induction, using the direct definition of the value functions (7),(8), while employing a chain of triangular inequalities. □

D. Affine deterministic dynamics on polytopic safe and target sets

It is in general difficult to find an explicit bound for Condition 3) in Assumption 1, which depends on the shape of the sets Λ_k and on the map f_2. However, such a bound can be derived in the relevant instance of models in (1) with affine deterministic dynamics and of invariant and target sets A, B that are bounded convex polytopes [5]. The following results provide a procedure to compute sets $\Gamma_k, \Lambda_k, \Upsilon_k$, which are later used to derive error bounds. The sets $\Gamma_k, k \in [0, N)$, can be expressed as $\Gamma_k = \Gamma_{k+1} \cup \tilde{\Gamma}_k$, where $\tilde{\Gamma}_k$ is defined by

$$\tilde{\Gamma}_k = \left\{(x_1, x_2) \in A | f_2(x_1, x_2) \in \Pi_2(\tilde{\Gamma}_{k+1})\right\}, \quad \tilde{\Gamma}_N = B. \tag{10}$$

This observation leads to the following characterization of the sets $\Gamma_k, \Lambda_k, \Upsilon_k$.

Theorem 3. *Suppose that the deterministic dynamics in (1) are characterized by affine functions, namely $f_2(x_1, x_2) = F_1 x_1 + F_2 x_2 + F_3$, where $F_1 \in \mathbb{R}^{n_2\times n_1}, F_2 \in \mathbb{R}^{n_2\times n_2}, F_3 \in \mathbb{R}^{n_2\times 1}$. Assume that sets A, B are bounded convex polytopes, described by the following linear inequalities:*

$$A = \left\{(x_1, x_2) \in \mathbb{R}^n | \bar{A}_1 x_1 + \bar{A}_2 x_2 \le \bar{B}\right\},$$
$$B = \left\{(x_1, x_2) \in \mathbb{R}^n | A_N^1 x_1 + A_N^2 x_2 \le B_N\right\}.$$

Then the sets $\tilde{\Gamma}_k, k \in [0, N)$, are also bounded convex polytopes, as described in (11). This means that sets Γ_k are unions of at most $(N-k+1)$ convex polytopes, whereas sets Λ_k, Υ_k can be expressed as the intersection of at most $(N-k)$ (possibly non-convex) polytopes.

Proof. Based on Equation (10), we can compute the sets $\tilde{\Gamma}_k, k = N-1, \dots, 0$, as

$$\tilde{\Gamma}_k = f_2^{-1}(\Pi_2(\tilde{\Gamma}_{k+1})) \cap A.$$

Suppose $\tilde{\Gamma}_{k+1}$ is compact and convex, then $\Pi_2(\tilde{\Gamma}_{k+1})$ is also a compact and convex set since the operator Π_2 is linear, and $f_2^{-1}(\Pi_2(\tilde{\Gamma}_{k+1}))$ is compact and convex since the function f_2 is affine. Suppose now that set $\tilde{\Gamma}_{k+1}$ is a polytope in $\mathbb{R}^n$, characterized by the linear inequalities

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

Then $\Pi_2(\tilde{\Gamma}_{k+1})$ is also a polytope in $\mathbb{R}^{n_2}$ characterized by

$$\Pi_2(\tilde{\Gamma}_{k+1}) = \left\{x_2 \in \mathbb{R}^{n_2} | C_{k+1} x_2 \le D_{k+1}\right\}.$$

The matrices C_{k+1}, D_{k+1} in the definition of $\Pi_2(\tilde{\Gamma}_{k+1})$ can be directly obtained from $\tilde{\Gamma}_{k+1}$ by taking the perpendicular projection of bounded polytopes: [13] proved that the polyhedral projection is equivalent to the feasibility of a parametric linear programming problem. Computationally, the MPT toolbox [17] performs this operation by first constructing a vertex representation of $\tilde{\Gamma}_{k+1}$, 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 $\Pi_2(\tilde{\Gamma}_{k+1})$ from its vertex representation (facet enumeration problem).

Having matrices C_{k+1}, D_{k+1} from the expression of $\Pi_2(\tilde{\Gamma}_{k+1})$, set $\tilde{\Gamma}_k$ can be found as

$$\tilde{\Gamma}_k = \{(x_1, x_2) \in A | C_{k+1}(F_1 x_1 + F_2 x_2 + F_3) \le D_{k+1}\}.$$

Then $\tilde{\Gamma}_k$ is a convex and bounded polytope with the half-space representation

$$\tilde{\Gamma}_k = \left\{(x_1, x_2) \in \mathbb{R}^n | A_k^1 x_1 + A_k^2 x_2 \le B_k\right\}, \tag{11}$$

where

$$A_k^1 = \begin{bmatrix} \bar{A}_1 \\ C_{k+1}F_1 \end{bmatrix}, A_k^2 = \begin{bmatrix} \bar{A}_2 \\ C_{k+1}F_2 \end{bmatrix}, B_k = \begin{bmatrix} \bar{B} \\ D_{k+1} - C_{k+1}F_3 \end{bmatrix}.$$

Note that this representation is not unique: it is in particular possible to eliminate redundant half-spaces in the representation of $\tilde{\Gamma}_k$ at each step k. The relation of the sets $\tilde{\Gamma}_k$ and Γ_k provides $\Gamma_k = \Gamma_{k+1} \cup \tilde{\Gamma}_k = \bigcup_{i=k}^N \tilde{\Gamma}_i$, which leads to $\Lambda_k = \Gamma_k \setminus \Gamma_{k+1} = \bigcap_{i=k+1}^N (\tilde{\Gamma}_k \setminus \tilde{\Gamma}_i)$, and to

$$\Upsilon_k = \Pi_2(\Gamma_k) \setminus \Pi_2(\Gamma_{k+1}) = \bigcup_{i=k}^N \Pi_2(\tilde{\Gamma}_i) \setminus \bigcup_{i=k+1}^N \Pi_2(\tilde{\Gamma}_i) = \bigcap_{i=k+1}^N (\Pi_2(\tilde{\Gamma}_k) \setminus \Pi_2(\tilde{\Gamma}_i)).$$

□

This leads to the following bound for Condition 3) in Assumption 1, which can be proved by direct calculation as in [9]. For completeness sake, let us mention that the Lipschitz constant for an affine map f_2 can be derived explicitly [9].

Theorem 4. *For a fixed $k, j \in [1, N]$, suppose facets of the polytope $\Lambda_k \cap (\mathbb{R}^{n_1} \times \Upsilon_j)$ lie on the hyperplanes $G_k(i)x_1 + H_k(i)x_2 = I_k(i), i = 1, 2\cdots, m_k$, where m_k is the number of facets. Then the sets $\tilde{\Gamma}_k(x_2)$ are polytopes in $\mathbb{R}^{n_1}$, for all $x_2 \in \Upsilon_j$, which satisfy Condition 3) in Assumption 1 with the constant*

$$\theta_{kj} = \sum_{i=1, G_k(i)\neq 0}^{m_k} c_{kj}(i) \frac{\|H_k(i)\|}{\|G_k(i)\|}.$$

The constant $c_{kj}(i)$ is computed as follows:

1) *if $n_1 = 1$ then $c_{kj}(i) = 1$ for any $i = 1, \dots, m_k$;*
2) *if $n_1 \ge 2$, project $\Pi_1(\Lambda_k)$ along the normal to the vector $G_k(i)$, resulting in $\Pi^\perp(\Pi_1(\Lambda_k))$, a polytope in $\mathbb{R}^{n_1-1}$. Then $c_{kj}(i) = \mathscr{L}(\Pi^\perp(\Pi_1(\Lambda_k)))$ (or any upper bound).*

IV. Case study: model of a chemical reaction network

We consider the model of a chemical reaction network, describing the dynamics of the concentration of cellular components involved in DNA transcription and characterized by species with heterogeneous concentrations. In this context, [15] has investigated an approach that is based on the use of both first and second order approximations, namely, species that are abundant in the environment are associated with deterministic dynamics (ordinary differential equations), whereas species present in small numbers are assigned probabilistic dynamics (stochastic differential equations).

The stoichiometry (set of chemical reactions) underlying the system is the following: $D \xrightarrow{k_a} D^\star$, $D^\star \xrightarrow{k_d} D$, $D^\star \xrightarrow{k_r} M + D^\star$, $M \xrightarrow{\gamma_r} \emptyset$. The reactants represent the number of inactive and active genes (D and $D^\star$ respectively) and of m-RNA species (M). There are three kinds of reactions: conversion (between inactive and active state of a gene), transcription of m-RNA, and degradation of m-RNA. The reaction and degradation rates (appearing above the arrows) are $k_a = k_d = 0.1$, $k_r = 0.8$, $\gamma_r = 0.4$, and expressed in $[s^{-1}]$. Notice that the dynamics of D and $D^\star$ are coupled via the first two reactions, which allows focusing exclusively on $D^\star$. Let us introduce a vector $s = \begin{bmatrix} s_1 & s_2 \end{bmatrix}^T = \begin{bmatrix} D^\star & M \end{bmatrix}^T$, describing the (low) concentration of the active genes ($D^\star$), as well as the (relatively abundant) concentration of m-RNA (M).

The continuous dynamics are described by the stochastic differential equation

$$s_1(k+1) = (1-k_d-k_a)s_1(k) + 2k_a D^\star_{ss} + \sqrt{2k_a D^\star_{ss}}\omega(k),$$
$$s_2(k+1) = k_r s_1(k) + (1-\gamma_r)s_2(k),$$

where $\omega(k), k \in \mathbb{N}\cup\{0\}$, are independent standard normal random variables and $D^\star_{ss}$ is the steady state, estimated based on the above parameters as done in [15].

Notice that the model dynamics are deterministic over s_2 (concentration of m-RNA M) and stochastic for s_1 (active genes $D^\star$), and that in (1) we would consider variables $x_1 = s_1$ and $x_2 = s_2$. Further, to connect the model with the representation in (2), the kernel for the dynamics in s_1 is normal and admits a density $t_{x_1}(\bar{s}_1|s_1) \sim \mathcal{N}(\mu,\sigma)$, where the mean is an affine function of the conditional variable s_1, whereas the variance is a constant: $\mu = (1-k_d-k_a)s_1 + 2k_a D^\star_{ss}$, $\sigma = \sqrt{2k_a D^\star_{ss}}$.

Consider sets A, B to be rectangles centred around the steady-state equilibria $(D^\star_{ss}, M_{ss})$ as follows:

$$S = \left\{(s_1,s_2)\in\mathbb{R}^2 : \left|\frac{s_1 - D^\star_{ss}}{D^\star_{ss}}\right| \le r_{1S}, \left|\frac{s_2 - M_{ss}}{M_{ss}}\right| \le r_{2S}\right\},$$

where $S = A \vee B$, and select the following parameters determining the size of the two sets: $r_{1A} = 0.3, r_{2A} = 0.6, r_{1B} = 0.2, r_{2B} = 0.05$. The support sets and the numerical values for the probabilistic reach-avoid problem have been computed over a horizon $N = 10$. Figure 2 displays the value functions W_9, W_8, W_7, and finally W_0 whereby $p_x(A,B) = W_0(x)$. With focus on W_0, as expected the reach-avoid specification is maximal (that is, equal to one) within the reach set $\Gamma_N = B$, which can be spotted as the (dark) red rectangle aligned with the axes. Likewise, its value is close to zero at the boundary of the safe set A (bounding box). Recall that the size of the sets Γ_k grows backwards in time, and notice that at the first iterations the value of W_k on the complement of Γ_k is equal to zero – in particular, $W_{10}(x) = \mathbb{I}_B(x)$. In this study the sets Γ_k are unions of at most two convex polytopes. As expected, the sets Λ_k are given as the union of (non-convex) sets, whereas the sets Υ_k are obtained from the subtraction between two intervals. Notice that the plots confirm the piecewise continuity of the value functions within the domains Λ_k. The Lipschitz constants h_k are computed based on the maximum norm of the partial derivative of the density function with respect to the conditional variable x_1 and are upper bounded by the constant 1.83. The following constants have been derived from Theorem 1: $M = 1.22$, $M^\star = 0.59$, $\bar{h} = 1$, $L_N = 0.4D^\star_{ss}$, $L_k = 0.6D^\star_{ss}$, and $\theta_{99} = \theta_{89} = 3/4$, $\theta_{88} = \theta_{78} = 3/2$. This leads to a global error $E_0 = 1.22\cdot 10^3\delta$, which can be tuned by choice of the discretization parameter δ (the diameter of the partitioning sets, which have been introduced as a uniform grid aligned with the main axes). Selecting a $\delta = 9\cdot 10^{-5}$ ($E_0 \approx 0.1$), the CPU time required for the deterministic reachability problem (computation of sets Γ_k) has amounted to 52 ms, whereas that for the reach-avoid probabilities to 2.46 s. The latter figure can be decreased to 0.29 s for a choice of $\delta = 9\cdot 10^{-4}$ (for a max allowable error $E_0 \approx 1$). The experiments have been run on a 12-core Intel Xeon 3.47 GHz PC with 24 GB of memory.

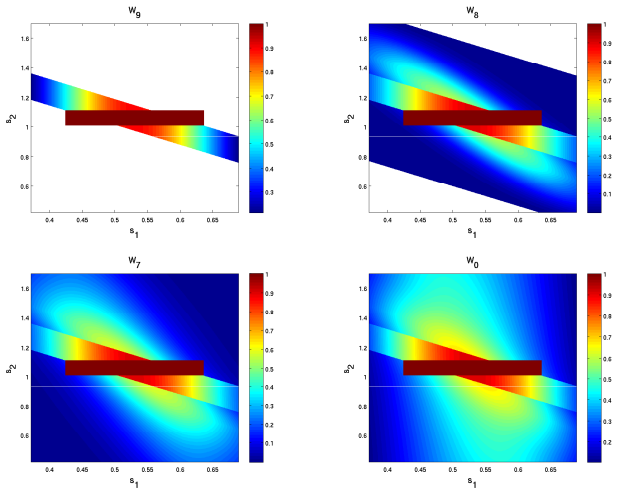


Fig. 2. Value functions W_k at time steps $k = 9, 8, 7$, and solution of the probabilistic reach-avoid problem $p_x(A,B) = W_0(x)$.

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