Higher-Order Approximations for Verification of Stochastic Hybrid Systems

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Abstract. This work investigates the approximate verification of probabilistic specifications expressed as any non-nested PCTL formula over Markov processes on general state spaces. The contribution puts forward new algorithms, based on higher-order function approximation, for the efficient computation of approximate solutions with explicit bounds on the error. Approximation error related to higher-order approximations can be substantially lower than those for piece-wise constant (zeroth-order) approximations known in the literature and, unlike the latter, can display convergence in time to a finite value. Furthermore, higher-order approximation procedures, which depend on the partitioning of the state space, can lead to lower partition cardinality than the related piece-wise constant ones. The work is first presented for Markov processes over Euclidean spaces and thereafter extended to hybrid spaces characterizing models known as Stochastic Hybrid Systems.

Keywords: General State-Space Markov Processes, Stochastic Hybrid Systems, PCTL Verification, Bounded-Until and Reach-Avoid, Interpolation Theory.

1 Introduction and background

This work addresses the investigation of complex properties over Markov processes evolving in discrete time over continuous (uncountable) state spaces [10,14]. We are in particular interested in Markov models with state spaces displaying a *hybrid* structure, namely characterized by a finite collection of bounded continuous domains (typically taken to be subsets of Euclidean spaces). These models are known in the literature as Stochastic Hybrid Systems (SHS) [6,7].

With regards to the probabilistic properties under investigation in this work, we focus on formulae expressed via a modal logic known as PCTL [4]. PCTL encodes probabilistic specifications that can be equivalently expressed via value functions [15] and computed by recursive application of known operators or by solving integral equations, as typical in dynamic programming problems over continuous spaces [5]. This work zooms in on autonomous models (namely, on models admitting no controller, nor scheduler, nor non-determinism), on non-nested PCTL specifications, and mostly on finite-horizon properties that admit

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a finite recursive expression. Extensions to non-autonomous models have been explored in [3], whereas to infinite-horizon specifications in [17].

With focus on a particular PCTL specification expressing probabilistic invariance, the work in [1] has put forward a formal connection between the study of probabilistic invariance over SHS and the computation of a related property over a discretized version of the model, namely a Markov chain (MC) – the latter property can be computed with a probabilistic model checker, such as PRISM [11] or MRMC [12]. The work in [2] has extended the approach to automata-based properties. Both contributions are formal in that they allow an exact computation of a bound on the formula-dependent approximation error. Recent contributions in [8,9] have investigated the development of enhanced computational approaches with tightened bounds on the error, to translate a SHS into a MC with the end goal of model checking PCTL formulae. In approximating SHS as MC, the surveyed results [1,2,8,9] have leveraged piece-wise constant interpolations of the kernels characterizing the SHS models under study, which has direct consequences on the derived error bounds. In contrast, this work provides approximation methods via higher-order interpolations of the value functions that are aimed at requiring less computational effort. More precisely, drawing on the expression of non-nested PCTL formulae as value functions [1,15], this work builds on the premises in [1,2,8,9] and puts forward higher-order approximation methods, obtained via interpolation procedures, in order to express the value functions under study as compactly as possible. The claim is that using higher-order interpolations (versus piece-wise constant ones) can be beneficial in terms of obtaining tighter bounds on the approximation error. Furthermore, since the approximation procedures depend on the partitioning of the state space, higher-order schemes display an interesting tradeoff between more parsimonious representations versus more complex local computation – this work explores the computational compromise between partition size and local interpolation. In assessing the computability of the results, an underlying tenet is that the total number of integrations required in the interpolation is a proxy for total computational time. An additional advantage of the present study over previous work is that in some cases the approximation error converges in time, which allows the applicability of the method to the approximate solution of infinite-horizon PCTL properties.

The article is structured as follows: Section 2 introduces a general state-space Markov process and zooms in on a specific PCTL formula – finite-time *bounded-until* – equivalently expressing it, via value functions, as a bounded-horizon *reach-avoid* problem. Section 3 considers higher-order approximation schemes over the value functions of interest, and quantifies explicitly the introduced approximation error over the formula (or problem). Section 4 tailors the results to a well studied case in the literature, and specializes the proposed approach to explicit schemes for low-dimensional models and known interpolation bases. Section 5 extends the results to SHS models. Finally, Section 6 develops a few numerical case studies to test and benchmark the proposed schemes. Due to length limitations, the statements are presented without proofs.

2 PCTL *bounded-until* Formula as a *reach-avoid* Problem

Consider a discrete-time, homogeneous Markov process $X = (X_n)_{n\in\mathbb{N}}$, taking values on a general (namely, uncountable) state space $\mathscr{S}$, with $\mathscr{B}(\mathscr{S})$ representing the associated σ-algebra. The evolution of the Markov process is fully characterized by a transition kernel $T(dy|x)$ as:

$$T(\mathcal{A}|x) = P_x\{X_{n+1} \in \mathcal{A}|X_n = x\}, \quad \forall \mathcal{A} \in \mathscr{B}(\mathscr{S}), \quad n \geq 0.$$

In this work we suppose that the transition kernel $T(dy|x)$ of the Markov process admits a density function $t(y|x)$, such that $T(dy|x) = t(y|x)dy$. We consider a bounded-until PCTL formula over a finite time horizon $[0, N]$ and express it as a reach-avoid problem over that time horizon. Given two Borel measurable bounded sets $\mathcal{A} \in \mathscr{B}(\mathscr{S})$ and $\mathcal{B} \subset \mathcal{A}$, we are interested in computing the probability that executions of the Markov process reach the target set $\mathcal{B}$, while never leaving the safe set $\mathcal{A}$ (that is, while avoiding $\mathcal{A}^c$) during the time horizon $[0, N]$, namely [16]:

$$P_x(\mathcal{A}, \mathcal{B}) \doteq P\{\exists k \in [0, N], X_k \in \mathcal{B} \wedge \forall l \in [0, k-1], X_l \in \mathcal{A}|X_0 = x\}. \tag{1}$$

(Notice that the expression above holds also for $k = 0$ since $\mathcal{B} \subset \mathcal{A}$, and can easily be extended to the case where $\mathcal{B} \cap \mathcal{A} = \emptyset$.) Given a probability level $\epsilon \in [0, 1]$ and the inequality operator $\sim \in \{>, \geq, <, \leq\}$, the quantity in (1) can be employed to perform a satisfiability check over the corresponding bounded-until PCTL formula, namely:

$$P_x(\mathcal{A}, \mathcal{B}) \sim \epsilon \quad \Leftrightarrow \quad x \models \mathbb{P}_{\sim\epsilon}\{\mathcal{A}\, \mathcal{U}^{\leq N} \mathcal{B}\}.$$

Next, we show that the quantity in (1), characterizing the satisfiability set of the bounded-until PCTL formula, can be equivalently expressed by introducing time-dependent value functions $W_k : \mathscr{S} \to [0, 1], k \in [0, N]$, which lead to the alternative expression $P_x(\mathcal{A}, \mathcal{B}) = W_N(x)$. The value functions W_k are obtained recursively according to the following Bellman scheme, which characterizes the reach-avoid problem in (1) [16]:

$$W_{k+1}(x) = \mathbb{1}_{\mathcal{B}}(x) + \mathbb{1}_{\mathcal{A}\setminus\mathcal{B}}(x) \int_{\mathscr{S}} W_k(y) T(dy|x), \quad k \in [0, N-1], \tag{2}$$

initialized as $W_0(x) = \mathbb{1}_{\mathcal{B}}(x), \forall x \in \mathscr{S}$, and where $\mathbb{1}_{\mathcal{C}}$ denotes the indicator function of set $\mathcal{C} \subseteq \mathscr{S}$. The Belman recursion in (2) indicates that the value functions W_k are always equal to one within the target set $\mathcal{B}$, while their supports are contained in the set $\mathcal{A}$ (namely, they are equal to zero over the complement of $\mathcal{A}$). We are thus only interested in computing the value functions over the set $\mathcal{A}\setminus\mathcal{B}$, which allows simplifying the recursion in (2) as follows, for $k \in [0, N-1]$:

$$W_{k+1}(x) = T(\mathcal{B}|x) + \int_{\mathcal{A}\setminus\mathcal{B}} W_k(y) T(dy|x), \quad W_0(x) = 0, \quad \forall x \in \mathcal{A}\setminus\mathcal{B}. \tag{3}$$

Let us denote with $\mathbb{B}(\mathcal{A}\backslash\mathcal{B})$ the space of bounded and measurable functions $f : \mathcal{A}\backslash\mathcal{B} \to \mathbb{R}$, and let us assign to this space the infinity norm $\|f\|_\infty = \sup\{|f(x)|, x \in \mathcal{A}\backslash\mathcal{B}\}$, $\forall f \in \mathbb{B}(\mathcal{A}\backslash\mathcal{B})$. The affine operator $\mathcal{R}_{\mathcal{A},\mathcal{B}}$, defined over $\mathbb{B}(\mathcal{A}\backslash\mathcal{B})$ by

$$\mathcal{R}_{\mathcal{A},\mathcal{B}} f(x) = T(\mathcal{B}|x) + \int_{\mathcal{A}\backslash\mathcal{B}} f(y) T(dy|x), \quad \forall f \in \mathbb{B}(\mathcal{A}\backslash\mathcal{B}), \quad \forall x \in \mathcal{A}\backslash\mathcal{B}, \quad (4)$$

characterizes the solution of the recursion in (3) as $W_k(x) = \mathcal{R}^k_{\mathcal{A},\mathcal{B}}(W_0)(x)$, for any $k = 1, 2, ..., N$.

3 Approximation Schemes and Error Quantification

The solution of the recursion in (3) cannot be characterized analytically in general. The goal of this section is to propose numerical schemes for approximating the value functions $W_k, k = 0, 1, \ldots, N$, with an explicit quantification of the approximation error. While previous work proposed approximations of the value functions W_k by piece-wise constant functions [1,2,8,9], in this contribution we are interested in considering approximations via higher-order interpolations.

3.1 Quantification of the Error of a Projection over a Function Space

Consider a function space $\Phi = span\{\phi_1(x), \phi_2(x), \cdots, \phi_n(x)\}$ as a subset of $\mathbb{B}(\mathcal{A}\backslash\mathcal{B})$, and a projection operator $\Pi_{\mathcal{A}\backslash\mathcal{B}} : \mathbb{B}(\mathcal{A}\backslash\mathcal{B}) \to \Phi$ that satisfies the inequality

$$\|\Pi_{\mathcal{A}\backslash\mathcal{B}}(f) - f\|_\infty \leq \mathcal{E}(f) \quad (5)$$

under some regularity conditions on f (beyond $f \in \mathbb{B}(\mathcal{A}\backslash\mathcal{B})$, see assumptions in Theorem 1), and where the bound $\mathcal{E}$ depends on the properties of the function f. With focus on a linear projection operator, the next result provides a useful tool for approximating the solution of the reach-avoid problem.

Theorem 1. *Assume that a linear operator $\Pi_{\mathcal{A}\backslash\mathcal{B}}$ satisfies the inequality*

$$\left\|\Pi_{\mathcal{A}\backslash\mathcal{B}}(t(y|\cdot)) - t(y|\cdot)\right\|_\infty \leq \epsilon, \quad \forall y \in \mathcal{A}, \quad (6)$$

and that there exists a finite constant $\mathcal{M}$, such that

$$\int_{\mathcal{A}\backslash\mathcal{B}} \left|\Pi_{\mathcal{A}\backslash\mathcal{B}}(t(y|x))\right| dy \leq \mathcal{M}, \quad \forall x \in \mathcal{A}\backslash\mathcal{B}. \quad (7)$$

Define the value functions $\bar{W}_k$ as approximations of the value functions W_k (cfr. (4)), by

$$\bar{W}_k = (\Pi_{\mathcal{A}\backslash\mathcal{B}} \mathcal{R}_{\mathcal{A},\mathcal{B}})^k (W_0), \quad k = 0, 1, \ldots, N. \quad (8)$$

Then it holds that

$$\|W_k - \bar{W}_k\|_\infty \leq E_k, \quad k = 1, 2, ..., N, \quad (9)$$

where the error E_k satisfies the difference equation

$$E_{k+1} = \mathcal{M}E_k + \mathcal{L}(\mathcal{A})\epsilon,$$

initialized by $E_0 = 0$, and where $\mathcal{L}(\mathcal{A})$ denotes the Lebesgue measure of the set $\mathcal{A}$.

Corollary 1. *Under the assumptions raised in* (6)-(7)*, the error E_k can be alternatively expressed explicitly as*

$$E_k = \epsilon\mathcal{L}(\mathcal{A})\frac{1-\mathcal{M}^k}{1-\mathcal{M}}, \text{ for } \mathcal{M} \neq 1, \quad \text{and} \quad E_k = \epsilon\mathcal{L}(\mathcal{A})k, \text{ for } \mathcal{M} = 1.$$

One possible general choice for the constant $\mathcal{M}$ is $\mathcal{M} = 1 + \epsilon\mathcal{L}(\mathcal{A}\backslash\mathcal{B})$.

Notice that the above error converges if $\mathcal{M} < 1$ as k goes to infinity, which makes the result applicable to the approximate computation of the infinite-horizon reach-avoid property (unbounded-until operator) with a finite approximation error.

3.2 Construction of the Projection Operator

In the ensuing sections we focus, for the sake of simplicity, on a state space that is Euclidean, namely $\mathscr{S} = \mathbb{R}^d$, where d is its finite dimension. In Section 5 we extend the upcoming results to be valid over general models known as Stochastic Hybrid Systems.

We discuss a general form for the interpolation operator. Let $\phi_j : \mathcal{D} \subset \mathbb{R}^d \to \mathbb{R}, j = 1, \cdots, n$, be independent functions defined over a generic set $\mathcal{D}$. The interpolation operator $\Pi_{\mathcal{D}}$ is defined as a projection map into the function space $\Phi = span\{\phi_1(x), \phi_2(x), \cdots, \phi_n(x)\}$, which projects any function $f : \mathcal{D} \to \mathbb{R}$ to a unique function $\Pi_{\mathcal{D}}(f) = \sum_{j=1}^{n} \alpha_j\phi_j$, using a finite set of data $\{(x_j, f(x_j))|x_j \in \mathcal{D}, j = 1, \cdots, n\}$ and such that $\Pi_{\mathcal{D}}(f)(x_j) = f(x_j)$. The operator $\Pi_{\mathcal{D}}$ is guaranteed to verify the inequality in (5), namely $\|\Pi_{\mathcal{D}}(f) - f\|_\infty \leq \mathcal{E}_{\mathcal{D}}(f)$, under some regularity assumptions on its argument function f (cfr. Corollary 2).

With focus on the problem described in Section 2, let us select a partition $\{\mathcal{D}_i\}_{i=1}^m$ for the set $\mathcal{A}\backslash\mathcal{B}$, with finite cardinality m. Using a basis $\{\phi_{ij}\}_{j=1}^n$, let us introduce the interpolation operators $\Pi_{\mathcal{D}_i}$ for the projection over each partition set $\mathcal{D}_i$, which is done as described above by replacing the domain $\mathcal{D}$ with $\mathcal{D}_i$. Finally, let us introduce the (global) linear operator $\Pi_{\mathcal{A}\backslash\mathcal{B}}$ on a function $f : \mathcal{A}\backslash\mathcal{B} \to \mathbb{R}$ by

$$\Pi_{\mathcal{A}\backslash\mathcal{B}}(f) = \sum_{i=1}^{m} \mathbb{1}_{\mathcal{D}_i}\Pi_{\mathcal{D}_i}(f|_{\mathcal{D}_i}), \tag{10}$$

where $f|_{\mathcal{D}_i}$ represents the restriction of the function f over the partition set $\mathcal{D}_i$. The following result holds:

Theorem 2. *The operator in* (10) *satisfies the inequality in* (5) *with constant $\mathcal{E}(f) = \max_{i=1,\ldots,m} \mathcal{E}_{\mathcal{D}_i}(f|_{\mathcal{D}_i})$, and where $\|\Pi_{\mathcal{D}_i}(f|_{\mathcal{D}_i}) - f|_{\mathcal{D}_i}\|_\infty \leq \mathcal{E}_{\mathcal{D}_i}(f|_{\mathcal{D}_i})$.*

Corollary 2. *The result in Theorem 1 can be tailored to the operator in* (10) *and applied to the density* $t = f$*, under the assumptions* (6)-(7) *on* t *and using the following two quantities:*

$$\epsilon = \max_i \epsilon_i, \text{ where } \|\Pi_{\mathcal{D}_i}(t(y|\cdot)|_{\mathcal{D}_i}) - t(y|\cdot)|_{\mathcal{D}_i}\|_\infty \leq \epsilon_i, \text{ for all } y \in \mathcal{A};$$

$$\mathcal{M} = \max_i \mathcal{M}_i, \text{ where } \int_{\mathcal{A}\setminus\mathcal{B}} |\Pi_{\mathcal{D}_i}(t(y|x))|\, dy \leq \mathcal{M}_i, \text{ for all } x \in \mathcal{D}_i.$$

Here ϵ_i *represents the interpolation error on the density function over the partition set* $\mathcal{D}_i$*.*

3.3 Approximation Algorithm

An advantage of the interpolation operator in (10) is that $\Pi_{\mathcal{A}\setminus\mathcal{B}}(f)$ is fully characterized by the interpolation coefficients α_{ij}, such that

$$\Pi_{\mathcal{A}\setminus\mathcal{B}}(f) = \sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_{ij}\phi_{ij}\mathbb{1}_{\mathcal{D}_i}.$$

The set of interpolation coefficients α_{ij} are computable by matrix multiplication based on the data $\{f(x_{ij})\}_{i,j=1}^{m,n}$, where the matrix depends on the interpolation points x_{ij} and on the basis functions ϕ_{ij} and can be computed off-line (see step 5 in Algorithm 1).

Let us now focus on the recursion in (8), $\bar{W}_{k+1} = \Pi_{\mathcal{A}\setminus\mathcal{B}}\mathcal{R}_{\mathcal{A},\mathcal{B}}(\bar{W}_k)$, given the initialization $\bar{W}_0 = 0$, for the approximate computation of the value functions. This recursion indicates that the approximate value functions $\bar{W}_k, k = 1, \ldots, N$, belong to the image of the operator $\Pi_{\mathcal{A}\setminus\mathcal{B}}$. Let us express these value functions by

$$\bar{W}_k = \sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_{ij}^k \phi_{ij}\mathbb{1}_{\mathcal{D}_i},$$

where α_{ij}^k denote the interpolation coefficients referring to $\bar{W}_k$ (at step k). This suggests that we need to store and update the coefficients α_{ij}^k for each iteration in (8). Writing the recursion in the form $\bar{W}_{k+1} = \Pi_{\mathcal{A}\setminus\mathcal{B}}\left(\mathcal{R}_{\mathcal{A},\mathcal{B}}(\bar{W}_k)\right)$ indicates that it is sufficient to evaluate the function $\mathcal{R}_{\mathcal{A},\mathcal{B}}(\bar{W}_k)$ over the interpolation points in order to compute the coefficients α_{ij}^{k+1}. In the following, the pair i, s indicate the indices of the related partition sets, namely $\mathcal{D}_i, \mathcal{D}_s$, whereas the pair of indices j, t show the ordering positions within partition sets. For an arbitrary interpolation point x_{st} we have:

$$\begin{aligned}\mathcal{R}_{\mathcal{A},\mathcal{B}}(\bar{W}_k)(x_{st}) &= T(\mathcal{B}|x_{st}) + \int_{\mathcal{A}\setminus\mathcal{B}} \bar{W}_k(y)t(y|x_{st})dy \\ &= T(\mathcal{B}|x_{st}) + \sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_{ij}^k \int_{\mathcal{D}_i} \phi_{ij}(y)t(y|x_{st})dy.\end{aligned}$$

Introducing the following quantities

$$Q(s,t) = \int_{\mathcal{B}} t(y|x_{st})dy, \quad P_{ij}(s,t) = \int_{\mathcal{D}_i} \phi_{ij}(y)t(y|x_{st})dy,$$

we have that

$$\bar{W}_{k+1}(s,t) = \mathcal{R}_{\mathcal{A},\mathcal{B}}(\bar{W}_k)(x_{st}) = Q(s,t) + \sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_{ij}^k P_{ij}(s,t).$$

Algorithm 1 provides a general procedure for the discrete computation of the interpolation coefficients and of the approximate value functions.

Algorithm 1. Approximate computation of the value functions $\bar{W}_k$

Require: Density function $t(y|x)$, safe set $\mathcal{A}\backslash\mathcal{B}$
1: Select a finite m-dimensional partition of the set $\mathcal{A}\backslash\mathcal{B} = \cup_{i=1}^{m}\mathcal{D}_i$ ($\mathcal{D}_i$ are non-overlapping)
2: For each $\mathcal{D}_i$, select interpolation basis functions ϕ_{ij} and points $x_{ij} \in \mathcal{D}_i$, where $j = 1, \ldots, n$
3: Compute $P_{ij}(s,t) = \int_{\mathcal{D}_i} \phi_{ij}(y)t(y|x_{st})dy$, where $1 \le i, s \le m$ and $1 \le j, t \le n$
4: Compute matrix Q with entries $Q(s,t) = \int_{\mathcal{B}} t(y|x_{st})dy$
5: Compute matrix representation of operators $\Pi_{\mathcal{D}_i}$
6: Set $k = 0$ and $\bar{W}_0(i,j) = 0$ for all i, j
7: **if** $k < N$ **then**
8: Compute interpolation coefficients α_{ij}^k given $\bar{W}_k(i,j)$, using matrices in step 5
9: Compute values $\bar{W}_{k+1}(s,t)$ based on $\bar{W}_{k+1}(s,t) = Q(s,t) + \sum_i \sum_j \alpha_{ij}^k P_{ij}(s,t)$
10: $k = k + 1$
11: **end if**
Ensure: Approximate value functions $\bar{W}_k, k = 0, 1, \ldots, N$

Next, we provide a condition on the selection of the basis functions and of the interpolation points, leading to a simplification of Algorithm 1.

Theorem 3 ([13]). *Assume that there exists a choice of interpolation points x_{ij} and of basis functions ϕ_{ij} such that*

$$\det \begin{bmatrix} \phi_{i1}(x_{i1}) & \cdots & \phi_{in}(x_{i1}) \\ \vdots & \ddots & \vdots \\ \phi_{i1}(x_{in}) & \cdots & \phi_{in}(x_{in}) \end{bmatrix} \neq 0, \quad \forall i \in \{1, 2, \cdots, m\}.$$

Then, there additionally exists an equivalent basis made up of functions ψ_{ij} such that

$$span\{\psi_{i1}, \psi_{i2}, \cdots, \psi_{in}\} = span\{\phi_{i1}, \phi_{i2}, \cdots, \phi_{in}\}$$

for all i, and which is related to the interpolation coefficients $\alpha_{ij}^k = \bar{W}_k(i,j)$.

Theorem 3 ensures that by utilizing the basis functions ψ_{ij} step 5 in Algorithm 1 can be skipped, and that the main update (steps 8 and 9) can be simplified as follows:

$$\bar{W}_{k+1}(s,t) = Q(s,t) + \sum_{i=1}^{m}\sum_{j=1}^{n} \bar{W}_k(i,j)P_{ij}(s,t), \quad \bar{W}_0(i,j) = 0.$$

A sufficient condition for the satisfaction of the assumption in Theorem 3 is the selection of a basis $\{\phi_{i1}, \cdots, \phi_{in}\}$ as a Chebyshev (or Haar) system [13], for all i. In this case, the choice of the distinct interpolation points x_{ij} can be made freely, for each partition set $\mathcal{D}_i$ (instances of this selection will be given below).

In Algorithm 1, the interpolation points x_{ij} are in general pair-wise distinct. Extending the domain of interpolation $\mathcal{D}_i$ to its closure $\bar{\mathcal{D}}_i$, it is legitimate to use boundary points as interpolation points, which can lead to a reduction of the number of integrations required in Algorithm 1. However, special care should be taken, since the interpolation operator should produce a continuous output over the boundaries of the neighboring partition sets. In the ensuing sections, we will exploit this feature upon selecting equally spaced points.

4 Special Forms of the Projection Operator

In this section we leverage known interpolation theorems for the construction of the projection operator $\mathit{\Pi}_{\mathcal{A}\backslash\mathcal{B}}$. These theorems are presented over a general domain $\mathcal{D}$ and are then used to derive specific error bounds for the problem of interest presented in Section 2.[1]

4.1 Piece-Wise Constant Approximations

We focus on the approximation of a function by a piece-wise constant one, which has inspired the previous work in [1,2,8,9]. The procedure is detailed in Algorithm 2, while the associated error is quantified in Theorem 4.

Consider a continuous, partially differentiable scalar field $f : \mathcal{D} \subset \mathbb{R}^d \to \mathbb{R}$ such that $\|\frac{\partial f}{\partial x}\| \leq M_0, \forall x \in \mathcal{D}$. Then $|f(x) - f(x')| \leq M_0\|x - x'\|, \forall x, x' \in \mathcal{D}$.

Theorem 4. *Suppose the density function $t(\cdot|x)$ is Lipschitz continuous with constant $\mathcal{M}_0$:*

$$|t(y|x) - t(y|x')| \leq \mathcal{M}_0\|x - x'\|, \quad \forall x, x' \in \mathcal{A}\backslash\mathcal{B}.$$

Then the approximation error of Algorithm 2 is upper bounded by the quantity $N\mathcal{L}(\mathcal{A})\mathcal{M}_0\delta$, where $\delta = \max_i \delta_i$ is the partition size of $\cup_{i=1}^{m}\mathcal{D}_i = A\backslash\mathcal{B}$, with $\delta_i = \sup\{\|x - x'\| : x, x' \in \mathcal{D}_i\}$.

[1] In the rest of the article, we employ normal typeset for bounds derived from general interpolation theorems, whereas calligraphic letters are used for theorems developed specifically for this article.

Algorithm 2. Piece-wise constant computation of the value functions $\bar{W}_k$

Require: Density function $t(y|x)$, safe set $\mathcal{A}\backslash\mathcal{B}$
1: Select a finite m-dimensional partition of the set $\mathcal{A}\backslash\mathcal{B} = \cup_{i=1}^{m}\mathcal{D}_i$ ($\mathcal{D}_i$ are non-overlapping)
2: For each $\mathcal{D}_i$, select one representative point $x_i \in \mathcal{D}_i$
3: Compute matrix P with entries $P(i,j) = \int_{\mathcal{D}_i} t(y|x_j)dy$, where $1 \leq i,j \leq m$
4: Compute vector Q with entries $Q(j) = \int_{\mathcal{B}} t(y|x_j)dy$
5: Set $k = 0$ and $\bar{W}_0(i) = 0$ for all i
6: **if** $k < N$ **then**
7: Compute the vector $\bar{W}_{k+1}$ based on $\bar{W}_{k+1} = Q + \bar{W}_k P$
8: $k = k + 1$
9: **end if**
Ensure: Approximate value functions $\bar{W}_k, k = 0, 1, \ldots, N$

Notice that in some cases [17] it is possible to find a constant $\mathcal{M} = \max_{x\in\mathcal{A}\backslash\mathcal{B}} \int_{\mathcal{A}\backslash\mathcal{B}} t(y|x)dy$ that is less than one, which leads to an error (cfr. Corollary 1) that converges as time horizon N grows.

Let us compare Algorithms 1 and 2 in terms of their computational complexity. Algorithm 1 requires $mn(mn+1)$ integrations in the marginalization steps (3 and 4), whereas $m(m+1)$ integrations are required in Algorithm 2. Furthermore, steps 5 and 8 in Algorithm 1 can be skipped only if a Chebyshev (Haar) system can be selected, whereas these steps are not needed at all in Algorithm 2. As a bottom line, higher interpolation orders increase the computational complexity of the approximation procedure, however this can as well lead to a lower global approximation error. Since the global approximation error depends on the local partitioning sets (their diameter, size, and the local continuity of the density function), for a given error higher interpolation procedures may require partitions with lower cardinality.

4.2 Higher-Order Approximations for One-Dimensional Systems

In this section we study higher-order interpolations over the real axis, where the partition sets $\mathcal{D}_i$ are real intervals. We use this simple setting to quantify the error related to the approximate solution of the reach-avoid problem. In order to assess the effect of the choice of the interpolation points on the approximation error and on the computational complexity of the method, we compare two different sets of interpolation points: equally spaced points and Chebyshev nodes.

Theorem 5 ([13]). *Let f be a real $(n+1)$-times continuously differentiable function on the bounded (one-dimensional) interval $\mathcal{D} = [\alpha, \beta]$. For the interpolation polynomial $\Pi_{\mathcal{D}}(f) \in span\{1, x, x^2, ..., x^n\}$, with $(n+1)$ pair-wise distinct points $\{x_0, x_1, ..., x_n\} \subset \mathcal{D}$, and condition $\Pi_{\mathcal{D}}(f)(x_j) = f(x_j), j = 0, \ldots, n$, there exist a $\xi \in \mathcal{D}$ such that*

$$f(x) - \Pi_{\mathcal{D}}(f)(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{j=0}^{n}(x - x_j), \quad \forall x \in \mathcal{D}.$$

Equally spaced interpolation points. The following result can be adapted from [13].

Theorem 6. *Consider equally spaced interpolation points* $x_0, x_1, ..., x_n$*:*

$$x_j = \alpha + j\frac{\beta - \alpha}{n}, \quad j = 0, 1, 2, ..., n.$$

The interpolation error is upper bounded, $\forall x \in \mathcal{D}$*, by*

$$|f(x) - \Pi_{\mathcal{D}}(f)(x)| \leq \frac{M_n}{4(n+1)} \left(\frac{\beta - \alpha}{n}\right)^{n+1},$$

where $M_n = \max_{x \in \mathcal{D}} |f^{n+1}(x)|$.

Application to the reach-avoid problem. Consider a one dimensional reach-avoid problem with a partitioning of $\mathcal{A} \backslash \mathcal{B} = \cup_{i=1}^{m} \mathcal{D}_i$ which is such that $\mathcal{D}_i = [\alpha_i, \beta_i]$. Define the interpolation operator $\Pi_{\mathcal{D}_i}(t|_{\mathcal{D}_i})$ over the basis $\Phi = span\{1, x, x^2, ..., x^n\}$ using equally spaced interpolation points $x_{ij} \in \mathcal{D}_i, j = 0, \ldots, n$. Then we can easily derive the following constants:

$$\mathcal{M}_n = \max_{x,y \in \mathcal{A} \backslash \mathcal{B}} \left| \frac{\partial^{n+1} t(y|x)}{\partial x^{n+1}} \right|, \qquad \epsilon = \frac{\mathcal{M}_n}{4(n+1)} \left(\frac{\delta}{n}\right)^{n+1},$$

and $\delta_i = \beta_i - \alpha_i, \delta = \max_i \delta_i, i = 1, 2, ..., m$. Changing the basis of interpolation gives us the opportunity to obtain another value for $\mathcal{M}$ to be used in the error computation. Let us select the interpolation basis functions to be Lagrange polynomials:

$$L_{ij}(x) = \prod_{s=1, s \neq j}^{n+1} \frac{x - x_{is}}{x_{ij} - x_{is}}.$$

This leads to a projection with a special form, namely $\Pi_{\mathcal{D}_i}(t(y|x)|_{\mathcal{D}_i}) = \sum_{j=1}^{n+1} \alpha_{ij} x^{j-1} = \sum_{j=1}^{n+1} t(y|x_{ij}) L_{ij}(x)$. Computing the constants $\kappa_i = \max_{x \in \mathcal{D}_i} \sum_{j=1}^{n+1} |L_{ij}(x)|$ yields the following choice of $\mathcal{M}$:

$$\int_{\mathcal{A} \backslash \mathcal{B}} |\Pi_{\mathcal{D}_i}(t(y|x)|_{\mathcal{D}_i})| \, dy \leq \kappa_i \int_{\mathcal{A} \backslash \mathcal{B}} t(y|x_{ij}) dy \leq \kappa_i, \text{ and } \mathcal{M} = \max_i \kappa_i.$$

Having the values of ϵ and $\mathcal{M}$ we are ready to implement Algorithm 1 for equally spaced points and polynomial basis functions of degree at most n, with the pre-specified error of Theorem 1.

Chebyshev nodes. The following statement can be adapted from [13].

Theorem 7. *Let f be a real $(n+1)$-times continuously differentiable function on the bounded interval $\mathcal{D} = [\alpha, \beta]$. For the interpolation polynomial $\Pi_{\mathcal{D}}(f) \in span\{1, x, x^2, ..., x^n\}$ with Chebyshev nodes*

$$x_j = \frac{\alpha+\beta}{2} + \frac{\beta-\alpha}{2}\cos\left(\frac{2j+1}{2(n+1)\pi}\right), \quad j = 0, 1, 2, ..., n,$$

and values $\Pi_{\mathcal{D}}(f)(x_j) = f(x_j)$, we have

$$|f(x) - \Pi_{\mathcal{D}}(f)(x)| \leq \frac{M_n}{2^n(n+1)!}\left(\frac{\beta-\alpha}{2}\right)^{n+1}, \quad \forall x \in \mathcal{D},$$

where $M_n = \max_{x\in\mathcal{D}} |f^{n+1}(x)|$.

Application to the reach-avoid problem. We can implement Algorithm 1 for Chebyshev nodes and Chebyshev polynomials of degree n, given a pre-specified error in Theorem 1, and with the following value of ϵ:

$$\epsilon = \frac{\mathcal{M}_n}{2^n(n+1)!}\left(\frac{\delta}{2}\right)^{n+1},$$

where the quantity $\mathcal{M}_n$ is that defined for equally spaced points. The only difference between the selection of equally spaced points and of Chebyshev nodes is the value of ϵ. The ratio of ϵ for these two cases (denoted respectively ϵ_1 and ϵ_2) is presented in Table 1 as a function of n (interpolation order). The advantage gained by using Chebyshev nodes is distinctive over larger values of the interpolation order.

Table 1. Ratio between equally spaced pints (ϵ_1) vs. Chebyschev nodes (ϵ_2), expressed with double digit precision, for different orders of interpolation order (n).

n	1	2	3	4	5	6	7	8	9	10	11	12
$\frac{\epsilon_2}{\epsilon_1}$	0.50	0.50	0.42	0.33	0.25	0.19	0.14	0.10	0.07	0.05	0.04	0.03

It is worth mentioning that, unlike the piece-wise constant case [1,2,8,9], with higher-order approximation approaches the global error is a nonlinear function of the partition size δ, namely it depends on a power of the partition size contingent on the order of the selected interpolation operator.

4.3 Bilinear Interpolation for Two-Dimensional Systems

We directly tailor the results above to a general two-dimensional system.

Theorem 8. *Consider a partially differentiable function $f(x_1, x_2)$, defined (for simplicity) over the unit square $\mathcal{D} = [0, 1]^2$. For the interpolation operator*

$$\begin{aligned}\Pi_{\mathcal{D}}(f)(x_1, x_2) =& a_1 + a_2x_1 + a_3x_2 + a_4x_1x_2 \\ =& x_1(1-x_2)f(1,0) + x_1x_2f(1,1) + (1-x_1)(1-x_2)f(0,0) + (1-x_1)x_2f(0,1),\end{aligned}$$

the error is upper bounded by

$$\|f - \Pi_{\mathcal{D}}(f)\|_\infty \leq \frac{1}{8}\left[M_{x_1^2} + M_{x_2^2} + 2M_{x_1^2 x_2} + 2M_{x_2^2 x_1}\right],$$

where $\left|\frac{\partial^2 f}{\partial x_i^2}\right| \leq M_{x_i^2}, \left|\frac{\partial^3 f}{\partial x_i^2 x_{3-i}}\right| \leq M_{x_i^2 x_{3-i}}, i = 1, 2, \quad \forall (x_1, x_2) \in \mathcal{D}.$

Application to the reach-avoid problem. With focus on a two-dimensional reach-avoid problem, consider a uniform partition (using squared partition sets) of size δ for the set $\mathcal{A}\backslash\mathcal{B}$. We employ a bilinear interpolation within each partition set $\mathcal{D}_i = [\alpha_{i1}, \alpha_{i2}] \times [\beta_{i1}, \beta_{i2}]$ with basis $\{\phi_1(x) = 1, \phi_2(x) = x_1, \phi_3(x) = x_2, \phi_4(x) = x_1 x_2\}$, or with Lagrange polynomials

$$\psi_{i1}(x) = \frac{(\alpha_{i2} - x_1)(\beta_{i2} - x_2)}{(\alpha_{i2} - \alpha_{i1})(\beta_{i2} - \beta_{i1})}, \qquad \psi_{i2}(x) = \frac{(\alpha_{i2} - x_1)(x_2 - \beta_{i1})}{(\alpha_{i2} - \alpha_{i1})(\beta_{i2} - \beta_{i1})},$$
$$\psi_{i3}(x) = \frac{(x_1 - \alpha_{i1})(\beta_{i2} - x_2)}{(\alpha_{i2} - \alpha_{i1})(\beta_{i2} - \beta_{i1})}, \qquad \psi_{i4}(x) = \frac{(x_1 - \alpha_{i1})(x_2 - \beta_{i1})}{(\alpha_{i2} - \alpha_{i1})(\beta_{i2} - \beta_{i1})},$$

and compute the associated error, given the following value for ϵ:

$$\epsilon = \frac{\delta^2}{16}\left[\mathcal{M}_{x_1^2} + \mathcal{M}_{x_2^2} + \delta\sqrt{2}\mathcal{M}_{x_1^2 x_2} + \delta\sqrt{2}\mathcal{M}_{x_2^2 x_1}\right],$$

where $\left|\frac{\partial^2 t}{\partial x_i^2}(y|x)\right| \leq \mathcal{M}_{x_i^2}, \left|\frac{\partial^3 t}{\partial x_i^2 x_{3-i}}(y|x)\right| \leq \mathcal{M}_{x_i^2 x_{3-i}}, i = 1, 2, \forall x, y \in A\backslash\mathcal{B}$. Note that the basis function ψ_{ij} is non-negative on the partition set $\mathcal{D}_i$ and that $\sum_{j=1}^4 \psi_{ij}(x) = 1$, which leads to a constant $\mathcal{M} = \max_{x \in A\backslash\mathcal{B}} \int_{A\backslash\mathcal{B}} t(y|x)dy \leq 1$.

4.4 Trilinear Interpolation for Three-Dimensional Systems

We now apply the results above to a general three-dimensional system.

Theorem 9. *Consider a partially differentiable function $f(x_1, x_2, x_3)$, defined (for simplicity) over the unit cube $\mathcal{D} = [0, 1]^3$. For the interpolation operator*

$$\begin{aligned}\Pi_{\mathcal{D}}(f)(x_1, x_2, x_3) =& a_1 + a_2 x_1 + a_3 x_2 + a_4 x_3 + a_5 x_1 x_2 + a_6 x_1 x_3 + a_7 x_2 x_3 + a_8 x_1 x_2 x_3 \\ =& (1 - x_1)(1 - x_2)(1 - x_3) f(0, 0, 0) + x_1 x_2 x_3 f(1, 1, 1) \\ &+ x_1(1 - x_2)(1 - x_3) f(1, 0, 0) + (1 - x_1) x_2 x_3 f(0, 1, 1) \\ &+ (1 - x_1) x_2 (1 - x_3) f(0, 1, 0) + x_1 (1 - x_2) x_3 f(1, 0, 1) \\ &+ (1 - x_1)(1 - x_2) x_3 f(0, 0, 1) + x_1 x_2 (1 - x_3) f(1, 1, 0),\end{aligned}$$

the error is upper bounded by the expression

$$\begin{aligned}\|f - \Pi_{\mathcal{D}}(f)\|_\infty \leq \frac{1}{8}[&M_{x_1^2} + M_{x_2^2} + M_{x_3^2} + 2M_{x_1^2 x_2} + 2M_{x_2^2 x_1} + 2M_{x_1^2 x_3} \\ &+ 2M_{x_3^2 x_1} + 2M_{x_2^2 x_3} + 2M_{x_3^2 x_2} + 6M_{x_1 x_2 x_3}],\end{aligned}$$

where $\left|\frac{\partial^2 f}{\partial x_i^2}\right| \leq M_{x_i^2}, \left|\frac{\partial^3 f}{\partial x_i^2 x_j}\right| \leq M_{x_i^2 x_j}, \left|\frac{\partial^3 f}{\partial x_1^2 x_2 x_3}\right| \leq M_{x_1 x_2 x_3}, \forall x = (x_1, x_2, x_3) \in \mathcal{D}$.

Application to the reach-avoid problem. With focus on a three-dimensional reach-avoid problem, consider a uniform partition (using cubic sets) of size δ for the set $\mathcal{A}\backslash\mathcal{B}$. We employ a trilinear interpolation within each partition set and compute the associated error, given the following value for ϵ:

$$\epsilon = \frac{\delta^2}{24}\left[\mathcal{M}_{x_1^2} + \mathcal{M}_{x_2^2} + \mathcal{M}_{x_3^2}\right] + \frac{\delta^3}{12\sqrt{3}}\left[\mathcal{M}_{x_1^2x_2} + \mathcal{M}_{x_2^2x_1} + \mathcal{M}_{x_2^2x_3} + \mathcal{M}_{x_3^2x_2} + \mathcal{M}_{x_1^2x_3} + \mathcal{M}_{x_3^2x_1} + 3\mathcal{M}_{x_1x_2x_3}\right],$$

where, $\forall x = (x_1, x_2, x_3), y = (y_1, y_2, y_3) \in D$, $\left|\frac{\partial^2 t}{\partial x_i^2}(y|x)\right| \leq M_{x_i^2}$, $\left|\frac{\partial^3 t}{\partial x_i^2 x_j}(y|x)\right| \leq M_{x_i^2x_j}$, and $\left|\frac{\partial^3 t}{\partial x_1^2 x_2 x_3}(y|x)\right| \leq M_{x_1x_2x_3}$. Similar to the bilinear interpolation case, the function ψ_{ij} is non-negative on the partition set $\mathcal{D}_i$ and $\sum_{j=1}^{8}\psi_{ij}(x) = 1$, which leads to a constant $\mathcal{M} = \max_{x\in\mathcal{A}\backslash\mathcal{B}}\int_{\mathcal{A}\backslash\mathcal{B}} t(y|x)dy \leq 1$.

5 Extensions to Stochastic Models with Hybrid State Spaces

Stochastic Hybrid Systems are Markov processes defined over a hybrid state space $\mathscr{S}$ made up of a finite, disjoint union of continuous domains, namely $\mathscr{S} = \cup_{q\in\mathcal{Q}}\{q\}\times\mathbb{R}^{n(q)}$, where $\mathcal{Q} = \{q_1, q_2, \cdots, q_{\mathfrak{m}}\}$, and the function $n : \mathcal{Q} \to \mathbb{N}$ assigns to each discrete location $q \in \mathcal{Q}$ a (finite) dimension for the associated continuous domain $\mathbb{R}^{n(q)}$. The conditional stochastic kernel $T : \mathscr{B}(\mathscr{S}) \times \mathscr{S} \to [0, 1]$ on $\mathscr{S}$ is fully characterized by three kernels T_q, T_x, T_r, dealing respectively with the discrete evolution over locations, the continuous evolution in the domain of a given location, and the continuous reset between domains of different locations:

$$T(\{q'\}\times A_{q'}|(q,x)) = T_q(q'|(q,x)) \times \begin{cases} T_x(A_{q'}|(q,x)), & q' = q, \\ T_r(A_{q'}|(q,x), q'), & q' \neq q. \end{cases}$$

Consider a safe set $\mathcal{A} = \cup_{q\in\mathcal{Q}}\{q\}\times\mathcal{A}_q$ and a target set $\mathcal{B} = \cup_{q\in\mathcal{Q}}\{q\}\times\mathcal{B}_q$, where $\mathcal{B}_q \subset \mathcal{A}_q$. Since the conditional kernels T_x, T_r admit density functions t_x, t_r, we can define the operator $\mathcal{R}_{\mathcal{A},\mathcal{B}}$ acting on $f \in \mathbb{B}(\mathcal{A}\backslash\mathcal{B})$ as

$$\mathcal{R}_{\mathcal{A},\mathcal{B}}f(q,x) = T(\mathcal{B}|(q,x)) + T_q(q|(q,x))\int_{\mathcal{A}_q\backslash\mathcal{B}_q} f(q,y)t_x(y|(q,x))dy + \sum_{\bar{q}\neq q} T_q(\bar{q}|(q,x))\int_{\mathcal{A}_{\bar{q}}\backslash\mathcal{B}_{\bar{q}}} f(\bar{q},y)t_r(y|(q,x),\bar{q})dy, \quad \forall q\in\mathcal{Q}, \forall x\in\mathcal{A}_q\backslash\mathcal{B}_q.$$

Given a partition $\mathcal{A}_q\backslash\mathcal{B}_q = \cup_i\mathcal{D}_{q,i}$ and a basis of interpolation functions $\{\psi_{q,ij}(x)\}$, we can construct the projection operator $\mathit{\Pi}_{\mathcal{A}\backslash\mathcal{B}}$ on $\mathbb{B}(\mathcal{A}\backslash\mathcal{B})$ by separately interpolating over the continuous domains associated to each discrete location. The following holds:

Theorem 10. *Suppose the conditional kernels of the SHS model satisfy the following inequalities*

$$\|\Pi_{\mathcal{A}\setminus\mathcal{B}}(T_q(q|(q,\cdot))t_x(y|(q,\cdot))) - T_q(q|(q,\cdot))t_x(y|(q,\cdot))\|_\infty \leq \mathcal{E}_x, \quad \forall q \in \mathcal{Q}, \forall y \in \mathcal{A}_q,$$
$$\|\Pi_{\mathcal{A}\setminus\mathcal{B}}(T_q(\bar{q}|(q,\cdot))t_r(y|(q,\cdot),\bar{q})) - T_q(\bar{q}|(q,\cdot))t_r(y|(q,\cdot),\bar{q})\|_\infty \leq \mathcal{E}_r, \quad \forall q,\bar{q} \in \mathcal{Q}, \bar{q} \neq q, \forall y \in \mathcal{A}_{\bar{q}},$$

then the following error bound can be established:

$$\|\mathcal{R}^k_{\mathcal{A},\mathcal{B}}(W_0) - (\Pi_{\mathcal{A}\setminus\mathcal{B}}\mathcal{R}_{\mathcal{A},\mathcal{B}})^k(W_0)\|_\infty \leq E_k, \quad W_0 = 0,$$
$$E_{k+1} = \lambda(\mathcal{E}_x + (\mathfrak{m}-1)\mathcal{E}_r) + \kappa E_k, \quad E_0 = 0,$$

where $\lambda = \max_q \mathcal{L}(A_q)$, $\kappa = \max\left\{\sum_j |\psi_{q,ij}(x)| \middle| x \in A_{q,i}, \forall i, q\right\}$, *and* $\mathfrak{m}$ *is the cardinality of the set of discrete locations.*

6 Case Studies

The probabilistic safety (or invariance) problem over a finite time horizon can be defined as follows:

$$P_x(\mathcal{A}) \doteq P\{\forall k \in [0,N], X_k \in \mathcal{A} | X_0 = x\}. \tag{11}$$

Safety is the dual of reachability, which in turn is a special case of the reach-avoid problem. In order to compute the solution of the safety problem over the safe set $\mathcal{A}$, we can compute that of the reach-avoid problem with a safe set $\mathscr{S}$ and a target set $\mathcal{A}^c = \mathscr{S}\setminus\mathcal{A}$. In this instance, the operator $\mathcal{R}_{\mathscr{S},\mathcal{A}^c}$ is used to compute the associated value functions W_k, which leads to the solution of the safety problem as $1 - W_N$. The errors associated to this procedure can be computed exactly as done for the reach-avoid problem. We develop a few case studies to investigate the probabilistic safety problem.

6.1 A One-Dimensional Case Study

Consider a probabilistic safety problem over the safe set $\mathcal{A} = [0,2]$ and the time horizon $N = 10$, over a model characterized by the kernel $T(dy|x) = g(x+c-y)dy$, where $c = 1.3035$, and the function g is defined as:

$$g(t) = \begin{cases} 3.57485\dfrac{1}{t^2}\exp\left(-t - \dfrac{1}{t}\right), & t > 0, \\ 0, & t \leq 0. \end{cases}$$

Selecting an approximation error $E_N = 0.01$, we compute the required number of partition sets to abide by such figure. Using piece-wise constant approximations based on a global Lipschitz constant (cfr. Sec. 4.1) yields a value $\mathcal{M}_0 = 6.90$ and the error function $E_N = N\mathcal{L}(\mathcal{A})\mathcal{M}_0\delta$. This leads to a required number of partition

sets $m = 27616$ and a total number of integrations $m(m+1) = 7.6 \times 10^8$ (the number of integrations is here conceived as a proxy for computational complexity).

Now consider algorithms and error bounds developed for higher-order approximations. The constants $\mathcal{M}_n$ are: $\mathcal{M}_1 = 88.93, \mathcal{M}_2 = 2063.65, \mathcal{M}_3 = 79064.41, \mathcal{M}_4 = 5428040$, whereas $\mathcal{M}$ is computed based on the following optimization problem:

$$\mathcal{M} = \max_{x \in \mathcal{A}} \int_{\mathcal{A}} t(y|x)dy = \max_{x \in \mathcal{A}} \int_0^2 g(x+c-y)dy = \max_{x \in \mathcal{A}} \int_{x+c-2}^{x+c} g(u)du,$$

which leads to $x_{opt} = 0.82$ and $\mathcal{M} = 0.96$.

Table 2 compares the number of partition sets and the number of integrations required to reach an approximation error $E_N = 0.01$, using equally spaced points and Chebyshev nodes. Notice that the two methods coincide for $n = 0$. The formulas for the number of integrations are an adaptation of the corresponding ones developed to assess Algorithm 1 (this case deals with invariance, rather than the more general reach-avoid for Algorithm 1). Similar outcomes, performed for an experiment with error $E_N = 0.001$, are also reported. These results show that Chebyshev nodes require in general a lower number of partition sets and therefore fewer integrations. The values are comparable since the ratio ϵ_2/ϵ_1 is smaller for larger values of n, as per Table 1. Notice further that equally spaced points give the opportunity to select common boundary points over adjacent partition sets as interpolation points, which can lead to a reduction on the associated number of integrations. However, interestingly the complexity is in general not monotonically decreasing with the order.

Table 2. Number of partition sets and integrations for equally spaced points (indexed by 1) and for Chebyshev nodes (indexed by 2), given two error bounds $E_N = 0.01, 0.001$.

uniform partitioning	total # of partitions		# of integrations	
$E_N = 0.01$	m_1	m_2	$m_1(n+1)(m_1 n+1)$	$m_2^2(n+1)^2$
piecewise constant, $n=0$	23357	23357	$5.5 \cdot 10^8$	$5.5 \cdot 10^8$
piecewise linear, $n=1$	275	194	$1.5 \cdot 10^5$	94864
piecewise quadratic, $n=2$	67	53	27135	25281
third-order, $n=3$	36	29	15696	13456
fourth-order, $n=4$	28	22	15820	12100
uniform partitioning	total # of partitions		# of integrations	
$E_N = 0.001$	m_1	m_2	$m_1(n+1)(m_1 n+1)$	$m_2^2(n+1)^2$
piecewise constant, $n=0$	233563	233563	$5.5 \cdot 10^{10}$	$5.5 \cdot 10^{10}$
piecewise linear, $n=1$	868	614	1508584	1507984
piecewise quadratic, $n=2$	143	114	123123	116964
third-order, $n=3$	64	52	49408	43264
fourth-order, $n=4$	43	35	37195	30625

6.2 A Two-Dimensional Case Study

Consider a d-dimensional linear, stochastic difference equation over $\mathbb{R}^d$

$$x(k+1) = Ax(k) + w(k), \quad k \in \mathbb{N},$$

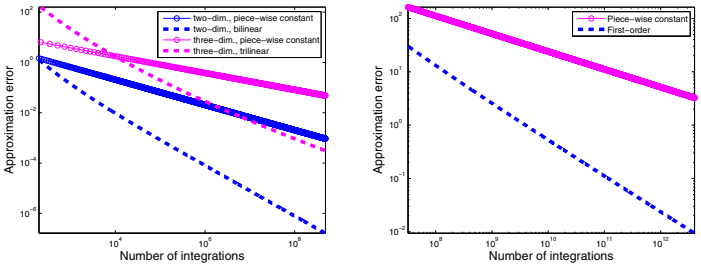
where $w(k), k \geq 0$, is the process noise, taken to be Normal i.i.d. random variables with zero mean and covariance matrix Σ: $w(k) \sim \mathcal{N}(0, \Sigma)$. Given any point $x \in \mathbb{R}^d$ at any time, the distribution at the next time can be characterized by a transition probability kernel $T(\cdot|x) \sim \mathcal{N}(\cdot; Ax, \Sigma)$. For a detailed description of the model and of its parameters the reader may refer to [8]. Let us consider the probabilistic invariance problem over a safe set $\mathcal{A} = [-1, 1]^d$, namely a hypercube pointed at the origin, and a time horizon $[0, N]$. Select a two dimensional state space $d = 2$ and a covariance matrix $\Sigma = 0.5\mathbb{I}_2$. The following constants are needed to compute the error: $\mathcal{M} = 0.71$, $\mathcal{M}_{x_1^2} = 2.23$, $\mathcal{M}_{x_2^2} = 0.72$, $\mathcal{M}_{x_1^2 x_2} = 3.80$, $\mathcal{M}_{x_1 x_2^2} = 2.17$. Table 3 compares the complexity of piece-wise constant and bilinear approximations, for different values of the global error E_N. Similarly, Figure 1a (on the left) compares the two approximations over the probabilistic safety problem (blue lines). The vertical axis represents the global approximation error, whereas the horizontal axis indicates the corresponding number of integrations, pointing to the computational complexity of each method. For a given computational complexity, bilinear interpolations approximate the solution with less error and their performance is dimensionally better in compared to the piece-wise constant approximations. Similarly, for a given error threshold, less computations are required when using bilinear interpolations.

Table 3. Piece-wise constant versus bilinear approximations

	piece-wise constant		bilinear	
error	# of partitions per dimension	# of integrations	# of partitions per dimension	# of integrations
E_N	m_1	m_1^2	m_2	$4(m_2+1)^2$
0.1	206	$4.2 \cdot 10^4$	18	1444
0.01	2053	$4.2 \cdot 10^6$	49	10^4
0.001	20525	$4.2 \cdot 10^8$	145	$8.5 \cdot 10^4$
0.0001	205241	$4.2 \cdot 10^{10}$	448	$8.1 \cdot 10^5$

6.3 A Three-Dimensional Case Study

Consider the above system with three dimensional state space $d = 3$ and covariance matrix $\Sigma = 0.5\mathbb{I}_3$. The following constants are needed to compute the error: $\mathcal{M} = 0.60, \mathcal{M}_{x_1^2} = 2.66, \mathcal{M}_{x_2^2} = 0.33, \mathcal{M}_{x_3^2} = 1.50, \mathcal{M}_{x_1^2 x_2} = 3.47, \mathcal{M}_{x_2^2 x_1} = 1.28, \mathcal{M}_{x_2^2 x_3} = 0.95, \mathcal{M}_{x_3^2 x_2} = 1.92, \mathcal{M}_{x_1^2 x_3} = 8.37, \mathcal{M}_{x_3^2 x_1} = 6.27, \mathcal{M}_{x_1 x_2 x_3} = 2.56$. Table 4 compares piece-wise constant and trilinear approximations, for different values of the global error E_N. Similarly, Figure 1a (on the left) compares the two approximations over the solution of the safety problem (magenta lines). Recall that there is a tradeoff between local computations and global error for higher-order interpolations. Thus, if we consider a large global error, piece-wise approximations may be computationally favorable (left of the crossing in the magenta curves). However, for small error bounds the performance of trilinear interpolations is much better in comparison with that of piece-wise constant approximations.



(a) 2- and 3-dimensional models, Secs. 6.2, 6.3 **(b)** Hybrid model, Sec. 6.4

Fig. 1. Error comparison between piece-wise constant versus higher-order approximations, as a function of their computational complexity, for three case studies.

Table 4. Piece-wise constant versus trilinear approximations

	piece-wise constant		trilinear	
error	# of partitions per dimension	# of integrations	# of partitions per dimension	# of integrations
E_N	m_1	m_1^3	m_2	$8(m_2+1)^3$
0.1	383	$5.6 \cdot 10^7$	30	$2.4 \cdot 10^5$
0.01	3825	$5.6 \cdot 10^{10}$	78	$3.9 \cdot 10^6$
0.001	38250	$5.6 \cdot 10^{13}$	220	$8.6 \cdot 10^7$
0.0001	382498	$5.6 \cdot 10^{16}$	681	$2.5 \cdot 10^9$

6.4 Case Study for a Hybrid Model

Consider the hybrid model of a chemical reaction network, with continuous dynamics described by stochastic difference equations, where time is discrete with sampling interval Δ (see [9] for a complete derivation of the model and for its parameters):

$$\begin{cases} x_1(k+1) = k_r \Delta q(k) + (1-\gamma_r \Delta) x_1(k) + \sqrt{k_r \Delta q(k) + \gamma_r \Delta x_2(k)}\, w_1(k) \\ x_2(k+1) = k_p \Delta x_1(k) + (1-\gamma_p \Delta) x_2(k) + \sqrt{k_p \Delta x_1(k) + \gamma_p \Delta x_2(k)}\, w_2(k). \end{cases}$$

The model has two locations $\mathcal{Q} = \{q_1, q_2\}$ indicating a gene in active or inactive mode. The variables x_1, x_2 are concentrations of m-RNA and of a protein, respectively. The signals $w_i(k), i = 1, 2, k \in \mathbb{N} \cup \{0\}$, are independent standard Normal random variables. The transition kernels can be directly derived from the above dynamics [9]. The safe set $\mathcal{A}$ is selected to cover an interval of 10% variation around the steady state of the model. We study the probabilistic safety of $\mathcal{A}$ over a 10-step interval.

Figure 1b compares the approximation errors of piece-wise constant and first-order approximations. The total number of integrations differ roughly only by a factor of two. Furthermore, considering for instance 1000 bins per dimension,

the piece-wise constant (zeroth-order) approximation has a global error equal to 32.64, whereas the first-order approximation leads to an error equal to 0.62, with only twice as many integrations involved in the procedure.

7 Conclusions

This contribution has put forward new algorithms, based on higher-order function approximation, for the efficient computation of approximate solutions of probabilistic specifications expressed as PCTL formulae over Markov processes on general state spaces (and in particular over Stochastic Hybrid Systems).

The authors plan to extend the technique to nested PCTL formulae, to further investigate its convergence properties, and to integrate the presented procedures within the algorithms worked out in [8,9], with the goal of developing a flexible software tool for abstraction and verification of Stochastic Hybrid Systems.

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