PAC Model Checking of Black-Box Continuous-Time Dynamical Systems

Bai Xue, Member, IEEE, Miaomiao Zhang, Arvind Easwaran and Qin Li

Abstract—In this paper we present a novel model checking approach to finite-time safety verification of black-box continuoustime dynamical systems within the framework of probably approximately correct (PAC) learning. The black-box dynamical systems are the ones, for which no model is given but whose states changing continuously through time within a finite time interval can be observed at some discrete time instants for a given input. The new model checking approach is termed as PAC model checking due to incorporation of learned models with correctness guarantees expressed using the terms error probability and confidence. Based on the error probability and confidence level, our approach provides statistically formal guarantees that the time-evolving trajectories of the black-box dynamical system over finite time horizons fall within the range of the learned model plus a bounded interval, contributing to insights on the reachability of the black-box system and thus on the satisfiability of its safety requirements. The learned model together with the bounded interval is obtained by scenario optimization, which boils down to a linear programming problem. Three examples demonstrate the performance of our approach.

Index Terms—Black-box Dynamical Systems; PAC Model Checking; Linear Programming.

I. INTRODUCTION

The complexity of today's technological applications induces a quest for automation, leading to many black-box intelligent cyber-physical systems and thus being difficult to reason about [25]. Many of these systems operate in safetycritical context and hence safety-critical systems themselves [32]. Therefore, reasonable performance guarantees should be obtained before the systems are deployed.

Black-box checking, introduced by Peled at al. [31], is often used for verifying non-stochastic black-box systems, based on experiments that interface with them. It performs checks on the system itself. The black-box checking is a combination of model checking and testing: model checking [12] checks properties of a model of the system, but not the system itself. In contrary, testing is usually applied to the actual system and checks whether the system conforms with the model, further serving to improve the model. They are two complementary approaches for enhancing the reliability of black-box systems. In the black-box checking, whenever a model is created, model checking may reveal a fault in the system or show that the model was not good enough and needs to be learned further if the fault is spurious. If model checking does not reveal a fault, equivalence between the model and the black-box system is checked via testing. In case, non-equivalence is detected, then the model needs to be further learned. The checking-testing-learning repeated process is costly generally. Recently, a method combining optimization-based falsification and black-box checking was proposed to falsify specifications for black-box cyber-physical systems in [40].

Another technique to verification of black-box systems is statistical model checking (SMC) [35], [45]. SMC is pioneered by Younes and Simmons in the discrete case in [47], which is based on Sequential Probability Ratio Test [41]. It is a compromise between verification and testing, which is based on sampling executions of the system and then deciding whether the samples provide a statistical evidence for the satisfaction or violation of the specification based on hypothesis testing [34]. SMC is now widely accepted in various research areas such as software engineering, in particular for industrial applications [13], or even for solving problems originating from systems biology [11]. There are several reasons for this success. First, SMC is very simple to understand, implement and use. Second, it does not require extra modelling or specification effort, but simply an executable system that can be simulated and checked against state-based properties. Third, it avoids the state space explosion in verification and thus can be applied to analyze systems with large state spaces. Consequently, there are variety of SMC tools such as PLASMA-Lab [3], Ymer [46], VeStA [36], MRMC [24], MC2 [20], UPPAAL-SMC [14] and so on. In order to further improve the efficiency of SMC, Bayesian SMC was proposed in [23], [48], which is a SMC based on Bayesian statistics. The aforementioned SMC approaches for black-box systems are free of mathematical models and perform checks on the system itself by sampling executions of the system. However, the usefulness of mathematical models is well documented. The mathematical models not only help us to understand the system, but also are instrumental to yield insight into the complex processes involved in the system by extracting the essential meaning of some hypotheses. Also, they allow

Corresponding Authors: Bai Xue and Miaomiao Zhang

B. Xue is with State Key Lab. of Computer Science, Institute of Software, CAS, and University of Chinese Academy of Sciences, Beijing, China email: xuebai@ios.ac.cn

Miaomiao Zhang is with School of Software Engineering, Tongji University, China email: miaomiao@tongji.edu.cn

A. Easwaran is with School of Computer Science and Engineering, Nanyang Technological University (NTU), Singapore email: arvinde@ntu.edu.sg.

Q. Li is with Shanghai Key Laboratory of Trustworthy Computing East China Normal University, Shanghai, China email: qli@sei.ecnu.edu.cn.

Manuscript received April 17, 2020; revised June 17, 2020; accepted July 6, 2020. This article was presented in the International Conference on Embedded Software 2020 and appears as part of the ESWEEK-TCAD special issue.

This work has been supported through grants by NSFC under grant No. 61872341, 61836005, 61972284, the CAS Pioneer Hundred Talents Program under grant No. Y8YC235015, the MoE, Singapore, Tier-2 grant #MOE2019-T2-2-040, and the foundation of Shenzhen Institute of Artificial Intelligence and Robotics for Society and the foundation of National Trusted Embedded Software Engineering Technology Research Center.

to study the effects of changes in their components and/or environmental conditions on the system's trajectories, i.e., they allow the control and optimization of the system. Thus, the introduction of mathematical models with appropriate degree of complexity into SMC would contribute a lot to the analysis of the black-box system, not only in the verification of its specifications but also in understanding the complex mechanisms underlying and thus further optimizing the system. Consequently, model learning based SMC approaches are also proposed. For example, [1], [26]-[28] considered black-box systems modelled by Markov decision processes and inferred probabilistic models with the purpose of model checking. The work in [29] combined stochastic learning and abstraction with respect to some property for analyzing black-box systems modelled by Markov decision processes. The work in [4] presented an approach for black-box systems modelled by Markov decision processes to unbounded reachability analysis via SMC. The technique is based on delayed Q-learning, a form of reinforcement learning. Generally, the exact learning algorithms require checking equivalence between the model and the system, which is difficult and undecidable. Regression models were used in [17] for finding the regions in the parameter space that lead to satisfaction or violation of given specification with probabilistic coverage guarantees based on conformal regression. Recently, learning procedure within the PAC learning framework is proposed, e.g., [2], [10], [19], [30].

In this paper we propose a novel SMC approach for finite-time safety verification of black-box continuous-time dynamical systems within the framework of PAC learning [18]. The black-box continuous-time dynamical systems are the ones, for which no model is given but whose states changing continuously through time over finite time horizons can be observed at some discrete time instants for a given input. The proposed new model checking, also termed as PAC model checking, is built upon learned models within the framework of PAC learning. In the PAC model checking, correctness guarantees of the learned models are expressed using the terms error probability and confidence level. We show that the time-evolving trajectories of the black-box system over a specified finite time horizon fall within the range of the learned model plus a bounded interval with statistical guarantees, which is further used to characterize the satisfiability of safety requirements. Given an error probability and a confidence level, which are two fundamental parameters in PAC learning, the model together with the bounded interval is computed via scenario optimization, which is widely used for computing solutions to robust optimization problems based on finite randomization of infinite constraints [5]. The scenario optimization, which finally boils down to a linear program in our approach, is constructed from a family of independent and identically distributed datum collected by executing the system. Three examples demonstrate the performance of our approach. Our contributions are summarized as follows.

1). We propose a novel PAC model checking approach for finite-time safety verification of black-box continuous-time dynamical systems. In this approach the trajectories of the black-box system over finite time horizons are shown to fall within the range of a model plus a bounded interval with error probabilities and confidence levels. This reachability analysis is instrumental in characterizing the satisfiability of safety requirements of the black-box system.

2). A linear programming based approach is proposed to synthesize the model and the bounded interval. The size of the linear programming problem could be independent of the one of the black-box system, thus rendering our approach suitable for large-scale systems.

Related Work

As mentioned above, there are many works on verifying black-box systems. In this subsection we just discuss the closely related works to the present one.

The works [2], [19] considered (unbounded) reachability for Markov decision processes (and stochastic games in [2]) and inferred the transition probabilities with PAC guarantees. The work [30] proposed an algorithm for constructing PAC confidence sets for deep neural networks. The work in [43] computed safe inputs for a black-box system such that the system's final outputs fall within a safe range with PAC guarantees. In contrast, our approach focuses on analysis of continuous-time systems, and infers that the time-evolving trajectories of the black-box system over finite time horizons fall within the range of a model plus a bounded interval with PAC guarantees. The closest work in spirit to the present one is [10], which considered verification of sequential programs by learning models of the set of feasible paths of programs within the framework of PAC learning. The model learning algorithm in [10] is based on counterexample guided abstraction refinement. However, our approach considers continuoustime systems and infers an approximation to the trajectories of the system over the specified finite time horizon within the framework of PAC learning, in which linear programs are used for learning models.

In the framework of simulation-driven reachability analysis [15], a PAC based method was proposed for learning discrepancy functions in [16] for safety verification of hybrid systems with black-box modules. The problem of learning discrepancy functions is reduced to a problem of learning linear separators. Although a PAC discrepancy function is computed in [16], a characterization on how well the trajectories satisfy the learned discrepancy function is not given and thus a formal quantitative assessment on the satisfiability of safety properties is not presented if a valid discrepancy function is not obtained. Generally, valid discrepancy functions rather than PAC ones for black-box systems are challenging to obtain. In contrast, a formal characterization of the satisfiability of safety properties is given based on the computation of PAC models in our PAC model checking method.

When the continuous-time systems of interest are modeled by ordinary differential equations or delay differential equations, and the equations are explicitly given, there are many well-developed model-based reachability analysis techniques over finite time horizons, e.g., Taylor-model method [9], simulation-driven reachability method [15] and set-boundary reachability method [44], for safety verification of these systems. However, our method focuses on black-box continuoustime dynamical systems, whose mathematical abstractions are



Fig. 1. An illustration of the system (1).

not acquired and which are only represented by a family of datum. Such systems can not be handled by existing model-based reachability analysis techniques.

The remainder of this paper is structured as follows. In Section II we formalize the concept of black-box continuoustime dynamical systems and the problem of interest in this paper. Section III elucidates our PAC model checking approach. After demonstrating the performance of our approach on three examples in Section IV, we conclude this paper in Section V.

II. PRELIMINARIES

In this section we present the concept of black-box continuous-time dynamical systems and the related problems, as well as a brief introduction on scenario optimization. The notations are used throughout this paper: $\mathbb{R}_{\geq 0}$ denotes the set of nonnegative real values. $\mathbb{R}_{>0}$ denotes the set of positive real values. Vectors are denoted by boldface letters. *Besides, the ground truth trajectories in all examples are obtained based on the combination of Runge-Kutta simulation methods and linear interpolation methods.*

A. Problem Formulation

In this paper we consider a black-box continuous-time dynamical system, whose dynamics are governed by a formula of the following form:

$$y(t) = b(\boldsymbol{x}_0, t), \tag{1}$$

where $\boldsymbol{x}_0 = (x_{0,1}, \ldots, x_{0,n})^\top \in \mathcal{X}_0$ is the input of the system, the set $\mathcal{X}_0 \subseteq \mathbb{R}^n$ is compact, $t \in [0, T]$ with $T \in \mathbb{R}_{>0}$ is the time variable, y(t) is the state of the system at time t, and $b(\cdot, \cdot) : \mathcal{X}_0 \times [0, T] \to \mathbb{R}$ is the system mapping which is unknown. Besides, we have the following assumptions.

Assumption 1. 1). The system (1) runs well, including the onboard sensors, and thus it can provide us any family of finite datum we need. Also, the provided datum are free of noise.

2). Suppose that the time horizon [0,T] is endowed with a σ -algebra \mathcal{D}_t and a probability P_t over \mathcal{D}_t is assigned. Also, we assume that the set \mathcal{X}_0 of inputs is endowed with a σ -algebra $\mathcal{D}_{\mathbf{x}_0}$ and that a probability $P_{\mathbf{x}_0}$ over $\mathcal{D}_{\mathbf{x}_0}$ is assigned. Throughout this paper, we use the uniform distribution P_t on [0,T] and $P_{\mathbf{x}_0}$ on \mathcal{X}_0 to illustrate our method, although our method is not confined to this particular distribution.

The system (1) is illustrated in Fig. 1. Given an input $x_0 \in \mathcal{X}_0$, the trajectory of the system (1) with the input x_0 is denoted by $y_{x_0}(\cdot) : [0,T] \to \mathbb{R}$.

Systems of the form (1) are all around us, especially nowadays. For example, many AI systems such as robotics and self-driving cars are leaving academic laboratories and entering real-world applications. Unfortunately, many of these systems can not explain their results even to their makers, let alone to end-users [7]. They operate like black boxes, which can be viewed in terms of a family of observed datum, without any knowledge of their internal workings.

In this paper we propose a PAC model checking approach for finite-time safety verification of the system (1). The safety verification problem is widely studied in computer science, e.g., [22]. In our approach, the key is to obtain a model with appropriate degree of complexity, which is learned based on a family of collected datum within the framework of PAC learning and can characterize the system (1) with correctness guarantees expressed with error probabilities and confidence levels. For computing such models, we should address the problems summarized below:

Problem 1. 1.1 What datum should we use?

- 1.2 How can we learn a mathematical model efficiently based on the collected datum?
- 1.3 What is the discrepancy between the trajectories of the learned mathematical model and the system (1)?

After computing the model, we will address the safety verification problem below.

Problem 2. Given a set $Uns \subseteq \mathbb{R}$ of unsafe states, when the trajectories of the computed model are shown to avoid the set Uns, how can we formally characterize the satisfiability of the safety property of avoiding the unsafe set Uns for the black-box system (1) over the time horizon [0, T]?

We in the sequel solve Problems 1 and 2 based on scenario optimization.

Remark 1. Our method can be straightforwardly extended to vector valued mappings of the form $\mathbf{b}(\cdot, \cdot) : \mathcal{X}_0 \times [0, T] \to \mathbb{R}^q$ with q > 1, but the scalar valued mappings $b(\cdot, \cdot) : \mathcal{X}_0 \times [0, T] \to \mathbb{R}$ are considered for ease of exposition.

B. Scenario Optimization

This subsection gives a brief introduction on scenario optimization. It provides statistical solutions to robust optimization problems based on solving finite randomization of infinite convex constraints.

A robust optimization problem of interest is as follows:

$$\min_{\boldsymbol{\gamma}\in\Gamma\subseteq\mathbb{R}^m} \boldsymbol{c}^{\top}\boldsymbol{\gamma}
s. t. \boldsymbol{f}_{\boldsymbol{\delta}}(\boldsymbol{\gamma}) \leq 0, \forall \boldsymbol{\delta} \in \Delta,$$
(2)

where $f_{\delta}(\gamma)$ are continuous and convex functions over the m-dimensional optimization variable γ for every $\delta \in \Delta$. Also, the sets Γ and Δ are convex and closed.

Generally, it is challenging to solve (2). The work in [5] proposed a scenario optimization approach for solving (2) with statistically formal guarantees.

Definition 1. Suppose that Δ is endowed with a σ -algebra D and that a probability P over D is assigned. The scenario optimization of (2) is to obtain an approximate solution to (2) via solving the convex program (3), which is constructed by

$$\min_{\boldsymbol{\gamma} \in \Gamma \subseteq \mathbb{R}^m} \boldsymbol{c}^\top \boldsymbol{\gamma}$$

s. t. $\wedge_{i=1}^K \boldsymbol{f}_{\boldsymbol{\delta}_i}(\boldsymbol{\gamma}) \leq 0.$ (3)

(3) relaxes (2) in that it only considers a finite subset of the infinitely many constraints of (2). A mathematically rigorous relation, which holds irrespective of the underlying probability P, between the solutions of the two systems can be drawn [6].

Theorem 1. If (3) is feasible and attains a unique optimal solution γ_K^* , and

$$\epsilon \ge \frac{2}{K} (\ln \frac{1}{\beta} + m), \tag{4}$$

where $\epsilon \in (0, 1)$ and $\beta \in (0, 1)$ are respectively a user-chosen error level and confidence level, then with at least $1 - \beta$ confidence, γ_K^* satisfies all constraints in Δ but at most a fraction of probability measure ϵ , i.e., $P(\{\delta \in \Delta \mid f_{\delta}(\gamma_K^*) \leq 0\}) \leq \epsilon$, where the confidence β is the K-fold probability P^K in $\Delta^K = \Delta \times \ldots \times \Delta$, which is the set to which the extracted sample $(\delta_1, \ldots, \delta_K)$ belongs.

The above conclusion still holds if the uniqueness of optimal solutions to (3) is removed [5], since a unique optimal solution can always be obtained according to Tie-break rule if multiple optimal solutions occur. Moreover, since β appears under the sign of logarithm in (4), it can be made small, like 10^{-10} or 10^{-20} , without increasing K significantly. Recently, scenario optimization was used to compute probably approximately safe inputs for a black-box system such that the system's final outputs fall within a safe range in [43], and perform safety verification of hybrid systems in [42].

III. PAC MODEL CHECKING

In this paper we present our PAC model checking approach for safety verification of the black-box system (1) by solving Problems 1 and 2.

A. Datum Extraction

In this subsection we introduce what datum to use in learning a model of the system (1) in our approach and how to obtain them, i.e., solve Problem 1.1.

We first extract a family of independent and identically distributed time instances $(t_j)_{j=1}^M$ from the time interval [0, T]according to the probability distribution P_t . Moreover, a family of independent and identically distributed inputs $(\boldsymbol{x}_{0,i})_{i=1}^N$ is also extracted from the set \mathcal{X}_0 according to the probability distribution $P_{\boldsymbol{x}_0}$. The process of obtaining $(t_j)_{j=1}^M$ and $(\boldsymbol{x}_{0,i})_{i=1}^N$ does not need to run or /simulate the system (1). The numbers M and N rely on how accurate one wants the learned model to achieve. The relationship is elucidated in Subsection III-B.

Next we need to run the system (1) to obtain its internal datum. For each extracted input $x_{0,i}$, i = 1, ..., N, we feed it to the system (1) and then run it until the time T. In this process, the on-board sensors will help observe and record the states of the system (1) at the time instance t_j ,

j = 1, ..., M. This is realistic for some systems nowadays, since smart sensors are taking over almost every sphere of human life. For example, RADAR, LIDAR, GPS and computer vision are widely used to work coherently for identifying the position, velocity and other states of the vehicle. We denote the family of observed states by $(y_{i,j})_{i=1,...,N,j=1,...,M}$, where $y_{i,j}$ denotes the state of the system (1) at time t_j with the input $\boldsymbol{x}_{0,i}, i = 1, ..., N, j = 1, ..., M$.

So far, we obtain a family of datum $((x_{0,i}, t_j, y_{i,j}))_{j=1,...,N}^{i=1,...,N}$. Each data is a triple $(x_0, t, y(t))$, where x_0 is the input of the system (1), $t \in [0,T]$ is the time instance and y(t) is the state of the system (1) with the input x_0 at time t. The process of running the system (1) can be regarded as a testing process. However, our method goes further than testing techniques. We meanwhile collect a family of datum and then use these datum to compute models for characterizing the system (1) formally.

In our experiment, we assume that the input $x_{0,i}$ is noisefree and the on-board sensors work perfectly such that the observed datum are free of noise as well, i.e., $y_{i,j}$ is the exact state of the system (1) with the input $x_{0,i}$ at time $t = t_j$, i = 1, ..., N, j = 1, ..., M. This assumption may be too ideal in practice since input and sensor noise often exists. We would relax it in our future work.

B. Safety Verification

In this section we elucidate our approach for solving Problems 1.2, 1.3 and 2 based on the family of datum obtained from the process in Subsection III-A. We first consider the system (1) with one trajectory, and then multiple trajectories and finally all trajectories from the input set \mathcal{X}_0 .

1) One Trajectory Verification: In this subsection, we solve Problems 1.2, 1.3 and 2 for the system (1) with a single input. Concretely, given a discrete-time trajectory of the system (1) with the input $\boldsymbol{x}_{0,i}$, which is represented by a family of datum $\left((\boldsymbol{x}_{0,i}, t_j, y_{i,j})\right)_{j=1}^M$ with $(t_j)_{j=1}^M$ and $(y_{i,j})_{j=1}^M$ obtained in Subsection III-A, we would compute a model $z(t) = w(\boldsymbol{x}_{0,i}, t)$ with $w(\boldsymbol{x}_{0,i}, \cdot) : [0, T] \to \mathbb{R}$ to characterize $y_{\boldsymbol{x}_{0,i}}(\cdot) : [0, T] \to \mathbb{R}$.

PAC Models: In computing a model, we consider a linearlyparameterized model template $w(c_1, \ldots, c_k, \boldsymbol{x}_{0,i}, t), k \geq 1$ such that $w(c_1,\ldots,c_k,\boldsymbol{x}_{0,i},t)$ is for $t \in [0,T]$ a linear function in c_1, \ldots, c_k , which are unknown parameters. This model can be a polynomial function over t, or a more general nonlinear function over t. For instance, consider a twodimensional system with input state variable $\boldsymbol{x} = (x_1, x_2)^{\top}$, $w(c_1, c_2, \boldsymbol{x}, t) = c_1 x_1 t + c_2 x_2 t^2$ is a linear function in c_1 and c_2 , and $w(c_1, c_2, \boldsymbol{x}, t) = c_1 e^{x_1 x_2} t + c_2 \ln(x_2 t^2)$ is also a linear function over c_1 and c_2 . Such models can be the ones parameterized with orthonormal basis functions, which are able to represent a set of physical systems [21]. For ease of exposition, we use c to denote $(c_l)_{l=1,\ldots,k}$ in the reminder of this paper. Generally, a model template of appropriate degree of complexity should be chosen in order to avoid the overfitting issue and facilitate the reachability analysis. In practice, engineering insight and physical knowledge would facilitate the selection of model templates.

Then we construct the following linear program over c for computing a mathematical model based on the family of given datum $((\mathbf{x}_{0,i}, t_i, y_{i,j}))^M$:

$$\min_{c,\xi} \xi
s. t. \text{ for each } j = 1, ..., M :
w(c, x_{0,i}, t_j) - b(x_{0,i}, t_j) \le \xi,
b(x_{0,i}, t_j) - w(c, x_{0,i}, t_j) \le \xi,
- U_c \le c_l \le U_c, l = 1, ..., k,
0 \le \xi \le U_{\xi},$$
(5)

which is equivalent to

$$\min_{\boldsymbol{c},\boldsymbol{\xi}} \xi$$
s. t. for each $j = 1, \dots, M$:

$$w(\boldsymbol{c}, \boldsymbol{x}_{0,i}, t_j) - y_{i,j} \leq \boldsymbol{\xi}, \qquad (6)$$

$$y_{i,j} - w(\boldsymbol{c}, \boldsymbol{x}_{0,i}, t_j) \leq \boldsymbol{\xi}, \qquad -U_c \leq c_l \leq U_c, l = 1, \dots, k, \qquad 0 \leq \boldsymbol{\xi} \leq U_{\boldsymbol{\xi}},$$

where $U_c \in \mathbb{R}_{\geq 0}$ is a pre-specified upper bound for c_l , $l = 1, \ldots, k$, and $U_{\xi} \in \mathbb{R}_{\geq 0}$ is a pre-specified upper bound for ξ .

Denote the optimal solution to (6) by (c^*, ξ^*) . Thus, we obtain a model $z(t) = w(c^*, x_{0,i}, t)$, whose discrepancy with the system (1) is characterized by two approximation parameters: error probability $\epsilon \in (0, 1)$ and confidence level $\beta \in (0, 1)$. This is formally stated in Theorem 2.

Theorem 2. Let (c^*, ξ^*) be an optimal solution to (6), $\epsilon \in (0, 1)$, $\beta \in (0, 1)$ and

$$\epsilon \ge \frac{2}{M} \left(\ln \frac{1}{\beta} + k + 1 \right). \tag{7}$$

Then we have that with at least $1 - \beta$ confidence,

$$P_t\left(\left\{t\in[0,T]\middle|\begin{array}{c} |w(\boldsymbol{c}^*,\boldsymbol{x}_{0,i},t)-b(\boldsymbol{x}_{0,i},t)|\\ &\leq\xi^*\end{array}\right\}\right)\geq 1-\epsilon.$$
(8)

Proof. The conclusion is easily obtained by Theorem 1. \Box

Actually, the computed mathematical model $z(t) = w(c^*, x_{0,i}, t)$ is a PAC model [37], [38] with accuracy level ϵ and confidence level β . The accuracy parameter ϵ in Theorem 2 determines how far the learned model can be from the real one. This corresponds to the "approximately correct". A confidence parameter β indicates how likely the learned model is to meet that accuracy requirement. This corresponds to the "probably" part. Under the data access model that we are investigating, these approximations are inevitable. Since the training set $((x_{0,i}, t_j, y_{i,j}))_{j=1}^{M}$ is randomly generated, there may always be a small chance that it will happen to be noninformative (for example, there is always some chance that the training set will contain only one domain point, sampled over and over again). Furthermore, even when we are lucky



Fig. 2. An illustration of the discrepancy between the mathematical model $z(t) = w(\mathbf{c}^*, \mathbf{x}_{0,i}, t)$ and the system $y(t) = b(\mathbf{x}_{0,i}, t)$ for $t \in [0, T]$.

enough to get a training sample that does faithfully represent [0, T], because it is just a finite sample, there may always be some finite details of [0, T] that it fails to reflect. The accuracy parameter ϵ allows forgiving the learned model for making minor errors.

One Trajectory Verification: Based on Theorem 2, we in this subsection solve Problem 2 for the system (1) with one trajectory $y_{\boldsymbol{x}_0,i}(\cdot) : [0,T] \to \mathbb{R}$ using the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^*, \boldsymbol{x}_{0,i}, t)$ within the framework of PAC learning.

We first characterize the reachability of the trajectory $y_{\boldsymbol{x}_0,i}(\cdot) : [0,T] \to \mathbb{R}$ using the mathematical model $z(t) = w(\boldsymbol{c}^*, \boldsymbol{x}_{0,i}, t)$ plus the computed ξ^* . We denote the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^*, \boldsymbol{x}_{0,i}, t)$ by $z_{\boldsymbol{x}_{0,i}}(\cdot) : [0,T] \to \mathbb{R}$. From Theorem 2, we have that with confidence of at least $1 - \beta$,

$$y_{\boldsymbol{x}_{0,i}}(t) \in [z_{\boldsymbol{x}_{0,i}}(t) - \xi^*, z_{\boldsymbol{x}_{0,i}}(t) + \xi^*]$$
(9)

for all t in [0, T] but at most a fraction of probability measure ϵ , i.e., with confidence of at least $1 - \beta$, the amount of time for the trajectory $y_{\boldsymbol{x}_{0,i}}(\cdot) : [0,T] \to \mathbb{R}$ staying within the ξ^* neighborhood of the trajectory $z_{\boldsymbol{x}_{0,i}}(\cdot) : [0,T] \to \mathbb{R}$ exceeds $T(1-\epsilon)$. A graph explanation is further presented in Fig. 2 to enhance the understanding of (9). In Fig. 2, $y_{\boldsymbol{x}_{0,i}}(t) \notin [z_{\boldsymbol{x}_{0,i}}(t) - \xi^*, z_{\boldsymbol{x}_{0,i}}(t) + \xi^*]$ for $t \in [t_1, t_2] \cup [t_3, t_4] \cup [t_5, t_6]$. According to Theorem 2, $t_6 - t_5 + t_4 - t_3 + t_2 - t_1 \leq \epsilon T$ with confidence of at least $1 - \beta$.

Then we solve Problem 2 based on the formal reachability characterization given above. That is,

if $[z_{\boldsymbol{x}_{0,i}}(t) - \xi^*, z_{\boldsymbol{x}_{0,i}}(t) + \xi^*]$ does not intersect the unsafe set Uns for $t \in [0, T]$, i. e., $[z_{\boldsymbol{x}_{0,i}}(t) - \xi^*, z_{\boldsymbol{x}_{0,i}}(t) + \xi^*] \cap \text{Uns} = \emptyset$ for $t \in [0, T]$, we have that the amount of time the system (1) with the input $\boldsymbol{x}_{0,i}$ spends inside the unsafe set Uns does not exceed ϵT , with confidence of at least $1 - \beta$.

If β in Theorem 2 is extremely small (smaller than 10^{-20}), then we have a priori practical certainty that the total amount of unsafe time does not exceed ϵT . As explained in Subsection II-B, the confidence level $1 - \beta$ can be made large without increasing the size M of samples significantly. This framework is useful in those situations where the system (1) is able to tolerate the exposure to a deteriorating agent for a limited amount of time. For example, let us consider a solarpowered autonomous vehicle. Regions without solar exposure are considered to be unsafe, since the vehicle's battery could be drained after a period of time. However, it would be inefficient to plan a path for the vehicle completely avoiding all these shaded regions. Instead, a more reasonable requirement would be that the amount of time the vehicle spends in the shaded regions is small.

Remark 2. Our approach can also be used to characterize the case that there exists $t \in [0,T]$ such that $[z_{\mathbf{x}_{0,i}}(t) - \xi^*, z_{\mathbf{x}_{0,i}}(t) + \xi^*] \cap \text{Uns} \neq \emptyset$. For this case, we need to compute a value $\tau \ge 0$, which is larger than or equal to the amount of time such that $[z_{\mathbf{x}_{0,i}}(t) - \xi^*, z_{\mathbf{x}_{0,i}}(t) + \xi^*] \cap \text{Uns} \neq \emptyset$. Further, we have that the amount of time the system (1) with the input $\mathbf{x}_{0,i}$ spends inside the unsafe set Uns does not exceed $\epsilon T + \tau$, with confidence of at least $1 - \beta$.

In the following we use an example from a Van-der-Pol oscillator to enhance the understanding of our approach.

Example 1. Consider a system with T = 10, $\mathbf{x}_{0,i} = (1.4, 2.3)^{\top}$ and $\text{Uns} = \{y \in \mathbb{R} \mid y \geq 3\}$, whose internal dynamics are described by an ordinary differential equation which generally describes a Van-der-Pol oscillator [39]:

$$\begin{cases} \frac{dx_1}{dt} = x_2\\ \frac{dx_2}{dt} = (1 - x_1^2)x_2 - x_1 \end{cases}$$
 (10)

We assume that the trajectory of the system (1) in this example describes the time evolution of the state x_1 in (10), i.e., $y(t) = b(\mathbf{x}_{0,i}, t) = x_1(t)$ for $t \in [0, 10]$. The ground truth trajectory $y_{\mathbf{x}_{0,i}}(\cdot) : [0,T] \to \mathbb{R}$, is illustrated in Fig. 3. It is used to extract datum $((\mathbf{x}_{0,i}, t_j, y_{i,j}))_{j=1}^M$ and perform comparisons. The method of constructing the ground truth trajectory is introduced in the beginning of Section II.

Let $\beta = 10^{-20}$ and $\epsilon = 0.01$. In this example we use M = 10811 and a polynomial $w(\mathbf{c}, \mathbf{x}_{0,i}, t)$ of degree 6 over t as a mathematical model to perform computations. Since $\mathbf{x}_{0,i}$ is known, $w(\mathbf{c}, \mathbf{x}_{0,i}, t)$ is of the form $\sum_{i=0}^{6} c_i t^i$. Note that the number k+1 of decision variables in (6) is 8 and consequently $M \geq 10811$ according to Theorem 2.

We obtain $\xi^* = 0.33$ via solving the linear program (6) with $U_c = U_{\xi} = 100$. Therefore, we have that with confidence of at least $1 - 10^{-20}$,

$$y_{\boldsymbol{x}_{0,i}}(t) \in [z_{\boldsymbol{x}_{0,i}}(t) - 0.33, z_{\boldsymbol{x}_{0,i}}(t) + 0.33]$$
(11)

for all t in [0,10] except at most a fraction of probability measure 0.01, where $z_{\boldsymbol{x}_{0,i}}(\cdot) : [0,T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^*, \boldsymbol{x}_{0,i}, t)$. We also take the time step $\Delta t = 10^{-5}$ and the corresponding states $(y_{\boldsymbol{x}_{0,i}}(j\Delta t))_{j=0}^{10^6}$ on the ground truth trajectory to verify the satisfiability of (11), i.e., whether $y_{\boldsymbol{x}_{i,0}}(j\Delta t) \in [\boldsymbol{z}_{\boldsymbol{x}_{0,i}}(j\Delta t) - 0.33, \boldsymbol{z}_{\boldsymbol{x}_{0,i}}(j\Delta t) + 0.33]$ holds for $j \in \{0, 1, \dots, 10^6\}$. The satisfiability ratio is 100%.

Since $[z_{\boldsymbol{x}_{0,i}}(t) - 0.33, z_{\boldsymbol{x}_{0,i}}(t) + 0.33] \cap \text{Uns} = \emptyset$ for $t \in [0, 10]$, we have that the amount of time the system (1) with the input $(1.4, 2.3)^{\top}$ spends inside the unsafe set Uns does not exceed 0.1, with confidence of at least $1 - 10^{-20}$.

2) Multiple Trajectories Verification: In Subsection 3.2.1 we considered one trajectory characterization of the system (1). In this subsection we extend the method in Subsection 3.2.1 to multiple trajectories characterization. These trajectories are the ones of the system (1) with inputs $x_{0,1}, \ldots, x_{0,N}$.



Fig. 3. An illustration of the trajectory reachability for Example 1. The green curve denotes the ground truth trajectory. The red curve denotes $z_{\boldsymbol{x}_{0,i}}(\cdot) + \xi^* : [0, 10] \to \mathbb{R}$ and $z_{\boldsymbol{x}_{0,i}}(\cdot) - \xi^* : [0, 10] \to \mathbb{R}$ respectively.

This extension is straightforward. We just need to enrich the constraints in (6) by incorporating these discrete-time trajectories $((\boldsymbol{x}_{0,1}, t_j, \boldsymbol{y}_{1,j}))_{j=1}^M, \ldots, ((\boldsymbol{x}_{0,N}, t_j, \boldsymbol{y}_{N,j}))_{j=1}^M$, consequently resulting in the following linear program:

$$\min_{\boldsymbol{c},\boldsymbol{\xi}} \xi$$
s. t. for each $j = 1, \dots, M$ and $i = 1, \dots, N$:

$$w(\boldsymbol{c}, \boldsymbol{x}_{0,i}, t_j) - y_{i,j} \leq \xi, \qquad (12)$$

$$y_{i,j} - w(\boldsymbol{c}, \boldsymbol{x}_{0,i}, t_j) \leq \xi, \qquad -U_c \leq c_l \leq U_c, l = 1, \dots, k, \qquad 0 \leq \xi \leq U_{\xi},$$

where $U_c \in \mathbb{R}_{\geq 0}$ is a given upper bound for c_l , l = 1, ..., k, and $U_{\xi} \in \mathbb{R}_{\geq 0}$ is a given upper bound for ξ . Denote the optimal solution to (12) by (c^{**}, ξ^{**}) .

We denote the trajectory of the mathematical model $z(t) = w(\mathbf{c}^*, \mathbf{x}_0, t)$ with the input \mathbf{x}_0 by $z_{\mathbf{x}_0}(\cdot) : [0, T] \to \mathbb{R}$. Similarly, we have the following theorem for the solution obtained via solving the linear program (12).

Theorem 3. Let (c^{**}, ξ^{**}) be an optimal solution to (12), $\epsilon \in (0, 1), \beta \in (0, 1)$ and

$$\epsilon \ge \frac{2}{M} \left(\ln \frac{1}{\beta} + k + 1 \right). \tag{13}$$

Then for each input $\mathbf{x}_{0,i}$, i = 1, ..., N, we have that with at least $1 - \beta$ confidence,

$$P_t(\{t \in [0,T] \mid |w(\boldsymbol{c}^{**}, \boldsymbol{x}_{0,i}, t) - b(\boldsymbol{x}_{0,i}, t)| \le \xi^{**}\}) \ge 1 - \epsilon.$$

Proof. According to the scenario optimization in Subsection II-B, we have that with at least $1 - \beta$ confidence,

$$P_t(\{t \in [0,T] \mid \wedge_{i=1}^N | w(\boldsymbol{c}^{**}, \boldsymbol{x}_{0,i}, t) - b(\boldsymbol{x}_{0,i}, t) | \le \xi^{**} \}) \ge 1 - \epsilon.$$

Since

$$P_t(\{t \in [0,T] \mid |w(\boldsymbol{c}^{**}, \boldsymbol{x}_{0,i}, t) - b(\boldsymbol{x}_{0,i}, t)| \le \xi^{**}\}) \ge P_t(\{t \in [0,T] \mid \wedge_{i=1}^M |w(\boldsymbol{c}^{**}, \boldsymbol{x}_{0,i}, t) - b(\boldsymbol{x}_{0,i}, t)| \le \xi^{**}\})$$

for $i \in \{1, \dots, M\}$, the conclusion follows directly. \Box

From Theorem 3, we have that for each trajectory $y_{\boldsymbol{x}_{0,i}}(\cdot)$: $[0,T] \to \mathbb{R}$ of the system (1) with the input $\boldsymbol{x}_{0,i}$, $i = 1, \ldots, N$, with confidence of at least $1 - \beta$,

$$y_{\boldsymbol{x}_{0,i}}(t) \in [z_{\boldsymbol{x}_{0,i}}(t) - \xi^{**}, z_{\boldsymbol{x}_{0,i}}(t) + \xi^{**}]$$

for all t in [0, T] but at most a fraction of probability measure ϵ , i.e., with confidence of at least $1 - \beta$, each of the N trajectories of the system (1) deviates from the corresponding one of the mathematical model $\boldsymbol{z}(t) = w(\boldsymbol{c}^{**}, \boldsymbol{x}_0, t)$ by at most ξ^{**} for all $t \in [0, T]$ but at most a fraction ϵ .

Consequently, the solution to Problem 2 for the system (1) with multiple trajectories is presented below:

If $[z_{\mathbf{x}_{0,i}}(t) - \xi^{**}, z_{\mathbf{x}_{0,i}}(t) + \xi^{**}]$ does not intersect the unsafe set Uns for $t \in [0, T]$, $i \in \{1, \ldots, N\}$, we have that the amount of time the system (1) with the input $\mathbf{x}_{0,i}$ spends inside the unsafe set Uns does not exceed ϵT , with confidence of at least $1 - \beta$.

It is worth remarking that the family of inputs $(x_{0,i})_{i=1}^N$ here does not require to be extracted independently according to the probability distribution P_{x_0} . They can be arbitrary N inputs of interest in the set \mathcal{X}_0 .

Example 2. Let's take the system in Example 1 as an instance to illustrate the case of two trajectories verification. These two trajectories, which are presented in Fig. 4, respectively describe the time evolution of the state x_1 in (10) with two different inputs $\mathbf{x}_{0,1} = (1.25, 2.28)^{\top}$ and $\mathbf{x}_{0,2} = (1.55, 2.32)^{\top}$.

Let $\beta = 10^{-20}$ and $\epsilon = 0.01$. In this example we use M = 26211 and a polynomial $w(\mathbf{c}, \mathbf{x}_0, t)$ of degree 6 as a mathematical model, which is input-dependent and is linear in \mathbf{c} , to perform computations. The number k + 1 of decision variables in (6) is 85 and thus $M \ge 26211$ from Theorem 2.

We obtain $\xi^{**} = 0.34$ via solving the linear program (12) with $U_c = U_{\xi} = 100$. Thus, for each i = 1, 2, we have that with confidence of at least $1 - 10^{-20}$, $y_{\mathbf{x}_{0,i}}(t) \in [z_{\mathbf{x}_{0,i}}(t) - 0.34, z_{\mathbf{x}_{0,i}}(t) + 0.34]$ for all $t \in [0, 10]$ except a small fraction 0.01, where $z_{\mathbf{x}_{0,i}}(\cdot) : [0, T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w(\mathbf{c}^{**}, \mathbf{x}_{0,i}, t)$. Like Example I, within the Monte-Carlo testing framework, we take the time step $\Delta t = 10^{-5}$ and the corresponding states $(y_{\mathbf{x}_{0,i}}(j\Delta t))_{j=0}^{10^6}$ on the ground truth trajectory with the input $\mathbf{x}_{0,i}$ to verify whether $y_{\mathbf{x}_{0,i}}(j\Delta t) \in [z_{\mathbf{x}_{0,i}}(j\Delta t) - 0.34, z_{\mathbf{x}_{0,i}}(j\Delta t) + 0.34]$ for $j \in \{0, 1, \ldots, 10^6\}$, where i = 1, 2. The satisfiability ratio is 100% for both of these two trajectories.

Since $[z_{\boldsymbol{x}_{0,i}}(t) - 0.34, z_{\boldsymbol{x}_{0,i}}(t) + 0.34] \cap \text{Uns} = \emptyset$ for $t \in [0, 10]$ and i = 1, 2, we have that the amount of time the system (1) with each of the two inputs $\boldsymbol{x}_{0,1} = (1.25, 2.28)^{\top}$ and $\boldsymbol{x}_{0,2} = (1.55, 2.32)^{\top}$ spends inside the unsafe set Uns does not exceed 0.1, with confidence of at least $1 - 10^{-20}$.

3) All Trajectories Verification: In this subsection we further extend the method in Subsection 3.2.2 for multiple trajectories verification to all trajectories verification of the system (1) with the input set \mathcal{X}_0 . Unlike in Subsection 3.2.2, the family of inputs $(\boldsymbol{x}_i)_{i=1}^N$ in this situation should be extracted independently according to the probability distribution $P_{\boldsymbol{x}_0}$.

Theorem 4. Let (c^{**}, ξ^{**}) be an optimal solution to (12), $\epsilon_1 \in (0, 1), \ \beta_1 \in (0, 1), \ \epsilon_2 \in (0, 1), \ \beta_2 \in (0, 1), \ and$

$$\epsilon_1 \ge \frac{2}{M} (\ln \frac{1}{\beta_1} + k + 1), \tag{14}$$

$$\epsilon_2 \ge \frac{2}{N} (\ln \frac{1}{\beta_2} + k + 1).$$
 (15)



Fig. 4. An illustration of two trajectories reachability for Example 2 with inputs $\boldsymbol{x}_{0,1} = (1.25, 2.28)^{\top}$ and $\boldsymbol{x}_{0,2} = (1.55, 2.32)^{\top}$. The green curves denote the two ground truth trajectories. From middle to right (i = 1, 2): the green curve denotes $\boldsymbol{y}_{\boldsymbol{x}_{0,i}}(\cdot) : [0, T] \to \mathbb{R}$, and the red curves correspond to $\boldsymbol{z}_{\boldsymbol{x}_{0,i}}(\cdot) + \boldsymbol{\xi}^{**} : [0, T] \to \mathbb{R}$ and $\boldsymbol{z}_{\boldsymbol{x}_{0,i}}(\cdot) - \boldsymbol{\xi}^{**} : [0, T] \to \mathbb{R}$ respectively.

Then we have that with at least $1-\beta_2$ confidence, $P_{\boldsymbol{x}_0}(\{\boldsymbol{x}_0 \mid \boldsymbol{x}_0 \in \mathcal{X}\}) \geq 1-\epsilon_2$, where $\mathcal{X} =$

$$\left\{ \boldsymbol{x}_0 \in \mathcal{X}_0 \middle| \begin{array}{c} P_t \left(\left\{ t \in [0,T] \middle| \begin{array}{c} |w(\boldsymbol{c}^{**}, \boldsymbol{x}_0, t) - b(\boldsymbol{x}_0, t)| \\ \leq \xi^{**} \end{array} \right\} \right) \\ \geq 1 - \epsilon_1, \text{ with confidence of at least } 1 - \beta_1. \end{array} \right\}.$$

Proof. Let us fix the time instances t_1, \dots, t_M firstly, we have that with confidence of at least $1 - \beta_2$,

$$P_{\boldsymbol{x}_0}\left(\left\{\boldsymbol{x}_0 \in \mathcal{X}_0 \middle| \bigwedge_{j=1}^M |w(\boldsymbol{c}^{**}, \boldsymbol{x}_0, t_j) - b(\boldsymbol{x}_0, t_j)| \le \xi^{**}\right\}\right)$$

$$\ge 1 - \epsilon_2$$

Let $\tilde{\mathcal{X}}_0 = \{ \boldsymbol{x}_0 \in \mathcal{X}_0 \mid \bigwedge_{j=1}^M | w(\boldsymbol{c}^{**}, \boldsymbol{x}_0, t_j) - b(\boldsymbol{x}_0, t_j) | \leq \xi^{**} \}$. Obviously, $\boldsymbol{x}_{0,i} \in \tilde{\mathcal{X}}_0$, $i = 1, \ldots, N$. For $\boldsymbol{x}_0 \in \tilde{\mathcal{X}}_0$, we can add the constraints involving \boldsymbol{x}_0 to the linear program (12) and obtain the following linear program:

$$\min_{c,\xi} \xi$$
s. t. for each $j = 1, ..., M$ and $i = 1, ..., N$:
 $w(c, x_{0,i}, t_j) - y_{i,j} \le \xi,$
 $y_{i,j} - w(c, x_{0,i}, t_j) \le \xi,$
 $w(c, x_0, t_j) - b(x_0, t_j) \le \xi,$
 $b(x_0, t_j) - w(c, x_0, t_j) \le \xi,$
 $-U_c \le c_l \le U_c, l = 1, ..., k,$
 $0 \le \xi \le U_{\xi}.$
(16)

Obviously, (c^{**}, ξ^{**}) is also an optimal solution to (16). Since the time instances t_1, \dots, t_M are also extracted independently according to the distribution P_t , Theorem 3 indicates that with confidence of at least $1 - \beta_1$,

$$P_t(\{t \in [0,T] \mid |w(\boldsymbol{c}^{**}, \boldsymbol{x}_0, t) - b(\boldsymbol{x}_0, t)| \le \xi^{**}\}) \ge 1 - \epsilon_1$$

for $x_0 \in \tilde{\mathcal{X}}_0$. Thus, we have $\tilde{\mathcal{X}}_0 \subseteq \mathcal{X}$ and consequently the conclusion follows.

From Theorem 4, we have that with confidence of at least $1 - \beta_2$, the probability measure of the set \mathcal{X} is larger than $1 - \epsilon_2$. The set \mathcal{X} is a set of inputs such that the trajectory of the system (1) with each of them does not deviate from the corresponding one of the model $z(t) = w(\mathbf{c}^{**}, \cdot, \cdot) : \mathbb{R}^n \times [0, T] \to \mathbb{R}$ by ξ^{**} for all $t \in [0, T]$ but at most a fraction ϵ_1 . Thus, the solution to Problem 2 for the system (1) with all

trajectories originating from the set \mathcal{X}_0 is presented below:

If $[z_{\boldsymbol{x}_0}(t) - \xi^{**}, z_{\boldsymbol{x}_0}(\cdot) + \xi^{**}] \cap \text{Uns} = \emptyset$ for $\boldsymbol{x}_0 \in \mathcal{X}_0$ and $t \in [0, T]$, we have that with confidence of at least $1 - \beta_2$, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside Uns does not exceed $\epsilon_1 T$ with confidence of at least $1 - \beta_1$, is larger than $1 - \epsilon_2$.

Although the size of the linear program (12) for computing PAC models does not depend on the dimension of the system (1), it heavily depends on $\epsilon_1, \beta_1, \epsilon_2, \beta_2$ and the number of unknown parameters in a pre-specified PAC model template according to inequalities (14) and (15) in Theorem 4.

Example 3. Let's take the system in Example 1 again as an instance to illustrate the case of all trajectories characterization. The input set is assumed to be $\mathcal{X}_0 = [1.25, 1.55] \times [2.28, 2.32]$.

The input set is assumed to be $\mathcal{X}_0 = [1.25, 1.55] \times [2.28, 2.32]$. Let $\beta_1 = 10^{-10}$, $\epsilon_1 = 0.3$, $\beta_2 = 10^{-10}$ and $\epsilon_2 = 0.5$. In this example we use M = 207, N = 125 and a polynomial $w(\mathbf{c}, t)$ of degree 6 as a mathematical model, which is input-independent and is linear in \mathbf{c} , to perform computations. The number k + 1 of decision variables in (12) is 8 and consequently $M \ge 207$ and $N \ge 125$ according to Theorem 4. The computation time for solving the resulting linear program is 150.32 seconds. The reason that an inputindependent model is used is to reduce the number of decision variables in (12), which further results in reduction of the size of extracted samples according to inequalities (14) and (15) and thus reduction of the size of the linear program (12). These computations were performed on an i7-7500U 2.70GHz CPU with 32G RAM running Windows 10.

We obtain $\xi^{**} = 0.38$ via solving the linear program (12) with $U_c = U_{\xi} = 100$. Therefore, with confidence of at least $1 - 10^{-10}$, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1 - 10^{-10}$,

$$y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 0.38, z_{\boldsymbol{x}_0}(t) + 0.38]$$
(17)

for all $t \in [0, 10]$ but at most a fraction 0.3, is larger than 0.5, where $z_{\boldsymbol{x}_0}(\cdot) : [0,T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^{**}, t)$. Within the Monte-Carlo testing framework, we extract 10^4 inputs $(\boldsymbol{x}'_{i,0})_{i=1}^{10^4}$ from \mathcal{X}_0 independently according to the probability distribution $P_{\boldsymbol{x}_0}$ and then obtain their corresponding ground truth trajectories for validating the above conclusion. Like Example 1, we take the time step $\Delta t = 10^{-5}$ and the states $(y_{\boldsymbol{x}'_{0,i}}(j\Delta t))_{j=0}^{10^6}$ on



Fig. 5. An illustration of all trajectories reachability for Example 3 with $\mathcal{X}_0 = [1.25, 1.55] \times [2.28, 2.32]$. The green curves denote the trajectories generated by the extracted N inputs. The red curves denote $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ respectively.



Fig. 6. An illustration of Monte Carlo validation for Example 3. The green curves denote the extracted 10⁴ trajectories, and the red curves denote $w(\boldsymbol{c}^{**},\cdot)+\boldsymbol{\xi}^{**}:[0,T] \rightarrow \mathbb{R}$ and $w(\boldsymbol{c}^{**},\cdot)-\boldsymbol{\xi}^{**}:[0,T] \rightarrow \mathbb{R}$ respectively.

the ground truth trajectory with the input $\mathbf{x}'_{0,i}$ to verify the satisfiability of (17), where $i = 1, \ldots, 10^4$. The satisfiability ratio of 10^4 inputs such that

$$y_{\boldsymbol{x}'_{0,i}}(j\Delta t) \in [z_{\boldsymbol{x}'_{0,i}}(j\Delta t) - 0.38, z_{\boldsymbol{x}'_{0,i}}(j\Delta t) + 0.38]$$

for all $j \in \{0, \dots, 10^6\}$ but at most a fraction 0.05, is 100%.

Since $[z_{x_0}(t) - \xi^{**}, z_{x_0}(\cdot) + \xi^{**}] \cap \text{Uns} = \emptyset$ for $x_0 \in \mathcal{X}_0$ and $t \in [0, 10]$, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside Uns does not exceed 3 with at least $1 - 10^{-10}$ confidence, is larger than 0.5.

IV. EXPERIMENTS

In this section we demonstrate the performance of our approach on three examples. All computations were performed on an i7-7500U 2.70GHz CPU with 32G RAM running Windows 10.

Example 4. In this example we consider a black-box system of the form (1) with T = 10, $\mathcal{X}_0 = [1.0, 1.1]^9$ and $\text{Uns} = \{y \in \mathbb{R} \mid y \leq -3\}$, which describes the time evolution of the state x_1 in the following 9-dimensional biological model [8]:

$$\begin{cases} \dot{x}_1(t) = 3x_3(t) - x_1(t)x_6(t), \dot{x}_2(t) = x_4(t) - x_2(t)x_6(t), \\ \dot{x}_3(t) = x_1(t)x_6(t) - 3x_3(t), \dot{x}_4(t) = x_2(t)x_6(t) - x_4(t), \\ \dot{x}_5(t) = 3x_3(t) + 5x_1(t) - x_5(t), \\ \dot{x}_6(t) = 5x_5(t) + 3x_3(t) + x_4(t) \\ - x_6(t)(x_1(t) + x_2(t) + 2x_8(t) + 1), \\ \dot{x}_7(t) = 5x_4(t) + x_2(t) - 0.5x_7(t), \\ \dot{x}_8(t) = 5x_7(t) - 2x_6(t)x_8(t) + x_9(t) - 0.2x_8(t), \\ \dot{x}_9(t) = 2x_6(t)x_8(t) - x_9(t). \end{cases}$$



Fig. 7. An illustration of trajectories reachability for Example 4 with the polynomial PAC model of degree 2. The green curves denote the extracted 181 trajectories. The red curves denote $w(c^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w(c^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ respectively.

Let $\epsilon_1 = 0.2$, $\beta_1 = 10^{-10}$, $\epsilon_2 = 0.3$ and $\beta_2 = 10^{-10}$. In this example we compute two polynomial models of degree 2 and 5 to illustrate our method.

1). We use M = 271, N = 181 and a polynomial $w(\mathbf{c}, t)$ of degree 2 as a mathematical model, which is inputindependent and is linear in \mathbf{c} , to perform computations. Note that the number k + 1 of decision variables in (12) is 4 and consequently $M \ge 271$ and $N \ge 181$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$ we obtain $\xi^{**} = 0.17$. The computation time is 167.43 seconds. Therefore, according to Theorem 4, we conclude that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1 - 10^{-10}$,

$$y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 0.17, z_{\boldsymbol{x}_0}(t) + 0.17]$$

for all $t \in [0, 10]$ but at most a fraction 0.2, is larger than 0.7, where $z_{\mathbf{x}_0}(\cdot) : [0, T] \to \mathbb{R}$ is the trajectory of the model $z(t) = w(\mathbf{c}^{**}, t)$. The reachability analysis is illustrated in Fig. 7. Like Example 3, within the Monte-Carlo framework, we also extract 10^4 inputs $(\mathbf{x}'_{i,0})_{i=1}^{10^4}$ to verify the conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\mathbf{x}'_{i,0}}(j\Delta t) \in [z_{\mathbf{x}'_{i,0}}(j\Delta t) - 0.17, z_{\mathbf{x}'_{i,0}}(j\Delta t) + 0.17]$ for all $j \in \{0, \dots, 10^6\}$ but at most a fraction 0.05, is larger than 97.87\%, where $\Delta t = 10^{-5}$.

Since $[z_{\mathbf{x}_0}(t) - 0.17, z_{\mathbf{x}_0}(t) + 0.17] \cap \text{Uns} = \emptyset$ for $t \in [0, 10]$ and $\mathbf{x}_0 \in \mathcal{X}_0$, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside Uns does not exceed 2 with confidence of at least $1 - 10^{-10}$, is larger than 0.7.

2). We use M = 301, N = 201 and a polynomial $w(\mathbf{c}, t)$ of degree 5 as a mathematical model, which is inputindependent and is linear in \mathbf{c} , to perform computations. Note that the number k + 1 of decision variables in (12) is 7 and consequently $M \ge 301$ and $N \ge 201$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$ we obtain $\xi^{**} = 0.12$. The computation time is 223.83 seconds. Therefore, according to Theorem 4, we conclude that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1 - 10^{-10}$,

$$y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 0.12, z_{\boldsymbol{x}_0}(t) + 0.12]$$

for all $t \in [0, 10]$ but at most a fraction 0.2, is larger than 0.7, where $z_{\boldsymbol{x}_0}(\cdot) : [0, T] \to \mathbb{R}$ is the trajectory of the model



Fig. 8. An illustration of trajectories reachability for Example 4 with the polynomial model of degree 5. The green curves denote the extracted 201 trajectories. The red curves denote $w(c^{**}, \cdot) - \xi^{**}$: $[0, T] \rightarrow \mathbb{R}$ and $w(c^{**}, \cdot) + \xi^{**} : [0, T] \rightarrow \mathbb{R}$ respectively.



Fig. 9. An illustration of Monte Carlo validation for Example 4. The green curves denote the extracted 10⁴ trajectories. The red curves denote $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ respectively, where $w(\mathbf{c}^{**}, \cdot)$ is the model of degree 5. The blue curves denote $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ respectively, where $w(\mathbf{c}^{**}, \cdot)$ is the model of degree 2.

 $z(t) = w(\mathbf{c}^{**}, t)$. The reachability analysis is illustrated in Fig. 8. Within the Monte-Carlo framework we use the 10^4 inputs $(\mathbf{x}'_{i,0})_{i=1}^{10^4}$ in the first case to verify the conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\mathbf{x}'_{i,0}}(j\Delta t) \in [z_{\mathbf{x}'_{i,0}}(j\Delta t) - 0.12, z_{\mathbf{x}'_{i,0}}(j\Delta t) + 0.12]$ for all $j \in \{0, \ldots, 10^6\}$ but at most a fraction 0.05, is larger than 98.56%, where $\Delta t = 10^{-5}$.

Similarly, due to the fact that $[z_{x_0}(t) - 0.12, z_{x_0}(t) + 0.12] \cap$ Uns = \emptyset for $t \in [0, 10]$ and $x_0 \in \mathcal{X}_0$, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside the unsafe set Uns does not exceed 2 with confidence of at least $1 - 10^{-10}$, is larger than 0.7.

From the comparison results illustrated in Fig. 9 for the above two cases with the same PAC guarantees, i.e., ϵ_1 , ϵ_2 , β_1 and β_2 are the same, we observe that polynomial models of higher degree could describe the internal dynamics of the system (1) more exactly, but with more computation time.

Example 5. To demonstrate the applicability of our approach to higher dimensional systems, we consider a scalable system of the form (1) with T = 2, $\mathcal{X}_0 = [0.5, 0.6]^{101}$ and $\text{Uns} = \{y \in \mathbb{R} \mid y \geq 3.0\}$, describing the time evolution of the state x_1 in an ordinary differential equation [33]:

$$\begin{cases} \dot{x}_1(t) = 1 + \frac{1}{l} \left(\sum_{i=1}^{l} x_{i+1}(t) + x_{i+2}(t) \right), \\ \dot{x}_2(t) = x_3(t), \dot{x}_3(t) = -10 \sin x_2(t) - x_2(t) \\ \dots \\ \dot{x}_{2l}(t) = x_{2l+1}(t), \dot{x}_{2l+1}(t) = -10 \sin x_{2l}(t) - x_2(t) \end{cases}$$

where l = 50.



Fig. 10. An illustration of all trajectories reachability for Example 5 with a polynomial model of degree 2. The green curves denote the extracted 271 trajectories. The red curves denote $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ respectively.

Let $\epsilon_1 = 0.2$, $\beta_1 = 10^{-10}$, $\epsilon_2 = 0.2$ and $\beta_2 = 10^{-10}$. In this example we compute two polynomial models of degree 2 and 4 to illustrate our method.

1). We use M = 271, N = 271 and a polynomial w(c, t) of degree 2 as a mathematical model, which is input-independent, to perform computations. Note that the number k + 1 of decision variables in (12) is 4 and consequently $M \ge 271$ and $N \ge 271$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$, we obtain that $\xi^{**} = 0.36$. The computation time is 398.23 seconds. According to Theorem 4, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1 - 10^{-10}$,

$$y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 0.36, z_{\boldsymbol{x}_0}(t) + 0.36]$$

for all $t \in [0,2]$ but at most a fraction 0.2, is larger than 0.8, where $z_{\boldsymbol{x}_0}(\cdot) : [0,T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^{**}, t)$. The reachability analysis is illustrated in Fig. 10. Like Example 4, within the Monte-Carlo testing framework, we also extract 10^4 inputs $(\boldsymbol{x}'_{i,0})_{i=1}^{10^4}$ to verify the above conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\boldsymbol{x}'_{i,0}}(j\Delta t) \in [z_{\boldsymbol{x}'_{i,0}}(j\Delta t) - 0.36, z_{\boldsymbol{x}'_0}(j\Delta t) + 0.36]$ for all $j \in \{0, \ldots, 10^5\}$ is equal to 98.07%, where $\Delta t = \frac{2}{10^5}$ and $i = 1, \ldots, 10^4$.

Since $[z_{\boldsymbol{x}_0}(t) - 0.36, z_{\boldsymbol{x}_0}(t) + 0.36] \cap \text{Uns} = \emptyset$ for $t \in [0, 2]$ and $\boldsymbol{x}_0 \in \mathcal{X}_0$, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside Uns does not exceed 0.4 with at least $1 - 10^{-10}$ confidence, is larger than 0.8.

2). We use M = 291, N = 291 and a polynomial $w(\mathbf{c}, t)$ of degree 4 as a mathematical model, which is input-independent, to perform computations. Note that the number k + 1 of decision variables in (12) is 6 and consequently $M \ge 291$ and $N \ge 291$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$, we obtain that $\xi^{**} = 0.12$. The computation time is 398.23 seconds. According to Theorem 4, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1 - 10^{-10}$,

$$y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 0.12, z_{\boldsymbol{x}_0}(t) + 0.12]$$

for all $t \in [0, 2]$ but at most a fraction 0.2, is larger than 0.8, where $z_{\boldsymbol{x}_0}(\cdot) : [0, T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w(\boldsymbol{c}^{**}, t)$. The reachability analysis is illustrated in Fig. 11. Also, within the Monte-Carlo testing framework



Fig. 11. An illustration of trajectories reachability for Example 5 with a polynomial model of degree 4. The green curves denote the extracted 291 trajectories. The red curves denote $w(c^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w(c^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ respectively.



Fig. 12. An illustration of Monte Carlo validation for Example 5. The green curves denote the 10^4 trajectories. The red curves denote $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ respectively, where $w(\mathbf{c}^{**}, \cdot)$ is the PAC model of degree 4. The blue curves denote $w(\mathbf{c}^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ and $w(\mathbf{c}^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ respectively, where $w(\mathbf{c}^{**}, \cdot)$ is the PAC model of degree 2.

we use the 10^4 inputs $(\mathbf{x}'_{i,0})_{i=1}^{10^4}$ in the first case to verify the above conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\mathbf{x}'_{i,0}}(j\Delta t) \in [z_{\mathbf{x}'_{i,0}}(j\Delta t) - 0.12, z_{\mathbf{x}'_0}(j\Delta t) + 0.12]$ for all $j \in \{0, \ldots, 10^5\}$ is equal to 1, where $\Delta t = \frac{2}{10^5}$ and $i = 1, \ldots, 10^4$.

Similar to the first case, we have that with at least $1-10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside the unsafe set Uns does not exceed 0.4 with confidence of at least $1-10^{-10}$, is larger than 0.8.

Like Example 4, by comparing the results in Fig. 12 for the above two cases with the same PAC guarantees, i.e., ϵ_1 , ϵ_2 , β_1 and β_2 are the same, we also obtain that polynomial models of higher degree could capture the internal dynamics of the system (1) more exactly, but with more computation time.

Example 6. In this example we show a strategy to overcome the issue of solving large-scale linear programs based on a black-box system of the form (1) which describes the time evolution of the state x_1 in the two-dimensional delay differential equation

$$\begin{cases} \dot{x}_1(t) = ax_1(t)(1 - \frac{x_1(t)}{m}) + bx_1(t)x_2(t) \\ \dot{x}_2(t) = cx_2(t) + dx_1(t - \tau)x_2(t - \tau) \end{cases}$$

where $\tau = 0.1$, a = 0.25, m = 200, b = -0.01, c = -1.00and d = 0.01. The delay differential equation was a model for predator-prey populations.

Assume that T = 10, the initial condition $\mathbf{x}(t)$ over $t \in [-0.1, 0]$ is a constant vector falling within $\mathcal{X}_0 = \{(x_1, x_2) \mid (x_1 + 5)^2 + (x_2 + 5)^2 \leq 1\}$ and $\text{Uns} = \{y \mid y \geq 40\}.$

Let $\epsilon_1 = 0.1$, $\beta_1 = 10^{-10}$, $\epsilon_2 = 0.1$ and $\beta_2 = 10^{-10}$. In this example we first use input-dependent polynomial models of degree 4 to illustrate this strategy, and then use inputindependent polynomial models of degree 4 to illustrate it.

1). Input-dependent Models: If a generic polynomial inputdependent model template of degree 4, which is formed by choosing all monomials of degree up to 4 as the basis polynomials, is employed, the number k + 1 of decision variables in (12) is 36 and consequently $M \ge 1181$ and $N \ge 1181$ according to Theorem 4. This leads to a large-scale linear program, producing heavy computational burden. As a result, we did not obtain results within two hours via solving this large-scale linear program.

Our strategy for avoiding large-scale linear programs is as follows: a small family of datum is first employed to compute an initial estimate of the coefficients c, and then determine the values of some coefficients based on the computed c and leave the remaining ones unknown, reducing the number of decision variables in (12) and thus the size of the resulting linear program.

In the experiment we first solve the linear program (12) with M = 50 and N = 50 to obtain a model $w'(\mathbf{c}^{**}, \mathbf{x}, t)$ with the computation time of 1.82 seconds, and then use the computed $w'(\boldsymbol{c}^{**}, \boldsymbol{x}, t)$ to perform computations on the linear program (12) with M = N = 481 and $U_c = U_{\xi} = 100$. Note that the number k + 1 of decision variables in (12) becomes 1 in this setting and consequently $M \ge 481$ and $N \ge 481$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$, we obtain that $\xi^{**} = 1.49$ with the computation time of 268.67 seconds. The reachability analysis is illustrated in Fig. 13. Therefore, according to Theorem 4, we conclude that with at least 1 - 10^{-10} confidence, the probability measure of inputs in \mathcal{X}_0 such that with confidence of at least $1-10^{-10}$, $y_{\boldsymbol{x}_0}(t) \in [z_{\boldsymbol{x}_0}(t) - 10^{-10}]$ $1.49, z_{x_0}(t)+1.49$ for all $t \in [0, 10]$ but at most a fraction 0.1, is larger than 0.9, where $z_{\boldsymbol{x}_0}(\cdot):[0,T] \to \mathbb{R}$ is the trajectory of the mathematical model $z(t) = w'(c^{**}, x, t)$. Also, within the Monte-Carlo framework, we extract 10⁴ inputs $(\mathbf{x}'_{i,0})_{i=1}^{10^4}$ to verify the above conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\boldsymbol{x}'_{i,0}}(j\Delta t) \in [z_{\boldsymbol{x}'_{i,0}}(j\Delta t) - 1.49, z_{\boldsymbol{x}'_{i,0}}(j\Delta t) + 1.49, z_{\boldsymbol{x}''_{i,0}}(j\Delta t) + 1.49, z_{\boldsymbol{x}''_{i,0}}$ 1.49] for all $j \in \{0, ..., 10^6\}$ is 100%, where $\Delta t = 10^{-5}$.

Since $[z_{x_0}(t) - 1.49, z_{x_0}(t) + 1.49] \cap \text{Uns} = \emptyset$ for $t \in [0, 10]$ and $x_0 \in \mathcal{X}_0$, we have that with at least $1 - 10^{-10}$ confidence, the probability measure of inputs in \mathcal{X}_0 such that the amount of time the system (1) with each of them spends inside Uns does not exceed 1 with confidence of at least $1 - 10^{-10}$, is larger than 0.9.

2). Input-independent Models: If an input-independent polynomial template of degree 4 is used to perform computations, the number k + 1 of decision variables in (12) is 6 and consequently $M \ge 581$ and $N \ge 581$ according to Theorem 4. Via solving the linear program (12) with M = N = 581 and $U_c = U_{\xi} = 100$, we obtain $\xi^{**} = 24.84$ with the computation time of 6634.51 seconds. The reachability analysis is illustrated in Fig. 14.

We also adopt the strategy presented in the above case for reducing the computation cost. We first solve the linear program (12) with M = N = 50 and $U_c = U_{\xi} = 100$ to obtain a $w'(\mathbf{c}^{**}, t)$ with the computation time of 1.65



Fig. 13. An illustration of trajectories reachability for Example 6 with the input-dependent model $w'(\boldsymbol{c}^*, \boldsymbol{x}, t)$. The green curves denote some extracted trajectories. The red curves denote the corresponding $w'(\boldsymbol{c}^{**}, \boldsymbol{x}, \cdot) - \xi^{**}$: $[0, T] \rightarrow \mathbb{R}$ and $w'(\boldsymbol{c}^{**}, \boldsymbol{x}, \cdot) + \xi^{**}$: $[0, T] \rightarrow \mathbb{R}$ respectively.



Fig. 14. An illustration of trajectories reachability for Example 6 with the input-independent model $w(c^*, t)$. The green curves denote some extracted trajectories. The red curves denote the corresponding $w(c^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w(c^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ with $\xi^{**} = 24.84$ respectively. The blue curves denote the corresponding $w'(c^{**}, \cdot) - \xi^{**} : [0, T] \to \mathbb{R}$ and $w'(c^{**}, \cdot) + \xi^{**} : [0, T] \to \mathbb{R}$ with $\xi^{**} = 25.96$ respectively.

seconds, and then use the computed $w'(\mathbf{c}^{**}, t)$ to perform computations on the linear program (12) with M = N = 481and $U_c = U_{\xi} = 100$. Note that the number k + 1 of decision variables in (12) becomes 1 in this setting and consequently $M \ge 481$ and $N \ge 481$ according to Theorem 4. Via solving (12) with $U_c = U_{\xi} = 100$, we obtain that $\xi^{**} = 25.96$ with the computation time of 71.09 seconds. The reachability analysis is illustrated in Fig. 14 as well. The safety guarantee is the same with the case of using input-dependent models. Similarly, within the Monte-Carlo framework, we use the 10^4 inputs $(\mathbf{x}'_{i,0})_{i=1}^{10^4}$ in the first case to verify the above conclusion, and obtain that the ratio of 10^4 inputs such that $y_{\mathbf{x}'_{i,0}}(j\Delta t) \in [z_{\mathbf{x}'_{i,0}}(j\Delta t) - 25.96, z_{\mathbf{x}'_{i,0}}(j\Delta t) + 25.96]$ for all $j \in \{0, \ldots, 10^6\}$ is equal to 100%, where $\Delta t = 10^{-5}$.

Via comparing the results in Fig. 13 and 14 for the above two cases with the same PAC guarantees, i.e., ϵ_1 , ϵ_2 , β_1 and β_2 are the same, we conclude that input-dependent polynomial models could capture the internal dynamics of the system (1) more exactly than input-independent ones, but also with more computation cost.

V. CONCLUSION

In this paper we proposed a novel PAC model checking approach for finite-time safety verification of black-box continuous-time dynamical systems, which are represented by observed datum, within the framework of PAC learning. In this approach, a PAC model of the system was computed such that the time-evolving trajectories of the black-box dynamical system over finite-time horizons fall within the range of the PAC model plus a bounded interval with error probabilities and confidence levels, thus facilitating the formal characterization of the satisfiability of safety requirements. Both the PAC model and the bounded interval were obtained via scenario optimization, which finally boil down to a linear program. Three examples demonstrated the performance of our approach.

In the future we would extend our method to safety verification of black-box systems, whose internal mechanisms are described by hybrid dynamical systems that exhibit both continuous and discrete dynamic behavior. Also, we would like to extend our method for safety verification of black-box systems with noise measurements and inputs.

REFERENCES

- B. K. Aichernig and M. Tappler. Probabilistic black-box reachability checking (extended version). *Formal methods in system design*, 54(3):416–448, 2019.
- [2] P. Ashok, J. Křetínský, and M. Weininger. Pac statistical model checking for markov decision processes and stochastic games. In *CAV'19*, pages 497–519. Springer, 2019.
- [3] B. Boyer, K. Corre, A. Legay, and S. Sedwards. Plasma-lab: A flexible, distributable statistical model checking library. In *QEST'13*, pages 160– 164. Springer, 2013.
- [4] T. Brázdil, K. Chatterjee, M. Chmelik, V. Forejt, J. Křetínský, M. Kwiatkowska, D. Parker, and M. Ujma. Verification of markov decision processes using learning algorithms. In *ATVA'14*, pages 98– 114. Springer, 2014.
- [5] G. C. Calafiore and M. C. Campi. The scenario approach to robust control design. *IEEE Transactions on Automatic Control*, 51(5):742– 753, 2006.
- [6] M. C. Campi, S. Garatti, and M. Prandini. The scenario approach for systems and control design. *Annual Reviews in Control*, 33(2):149–157, 2009.
- [7] D. Castelvecchi. Can we open the black box of ai? *Nature News*, 538(7623):20, 2016.
- [8] X. Chen. Reachability Analysis of Non-Linear Hybrid Systems Using Taylor Models. PhD thesis, Fachgruppe Informatik, RWTH Aachen University, 2015.
- [9] X. Chen, E. Ábrahám, and S. Sankaranarayanan. Flow*: An analyzer for non-linear hybrid systems. In CAV'13, pages 258–263. Springer, 2013.
- [10] Y.-F. Chen, C. Hsieh, O. Lengál, T.-J. Lii, M.-H. Tsai, B.-Y. Wang, and F. Wang. Pac learning-based verification and model synthesis. In *ICSE'16*, pages 714–724. IEEE, 2016.
- [11] E. M. Clarke, J. R. Faeder, C. J. Langmead, L. A. Harris, S. K. Jha, and A. Legay. Statistical model checking in biolab: Applications to the automated analysis of t-cell receptor signaling pathway. In *CMSB'08*, pages 231–250. Springer, 2008.
- [12] E. M. Clarke, O. Grumberg, and D. E. Long. Model checking and abstraction. ACM transactions on Programming Languages and Systems (TOPLAS), 16(5):1512–1542, 1994.
- [13] E. M. Clarke and P. Zuliani. Statistical model checking for cyberphysical systems. In ATVA'11, pages 1–12. Springer, 2011.
- [14] A. David, K. G. Larsen, A. Legay, M. Mikučionis, and D. B. Poulsen. Uppaal smc tutorial. *International Journal on Software Tools for Technology Transfer*, 17(4):397–415, 2015.
- [15] P. S. Duggirala, S. Mitra, M. Viswanathan, and M. Potok. C2E2: A verification tool for stateflow models. In *TACAS'15*, pages 68–82. Springer, 2015.
- [16] C. Fan, B. Qi, S. Mitra, and M. Viswanathan. Dryvr: Data-driven verification and compositional reasoning for automotive systems. In *CAV'17*, pages 441–461. Springer, 2017.
- [17] C. Fan, X. Qin, and J. Deshmukh. Parameter searching and partition with probabilistic coverage guarantees. arXiv preprint arXiv:2004.00279, 2020.
- [18] M. Fränzle, S. Gerwinn, P. Kröger, A. Abate, and J.-P. Katoen. Multiobjective parameter synthesis in probabilistic hybrid systems. In *FOR-MATS'15*, pages 93–107. Springer, 2015.
- [19] J. Fu and U. Topcu. Probably approximately correct mdp learning and control with temporal logic constraints. arXiv preprint arXiv:1404.7073, 2014.
- [20] R. Grosu and S. A. Smolka. Monte carlo model checking. In TACAS'05, pages 271–286. Springer, 2005.
- [21] R. Horst and H. Tuy. Global optimization: Deterministic approaches. Springer Science & Business Media, 2013.

- [22] F. Immler. Verified reachability analysis of continuous systems. In TACAS'15, pages 37–51. Springer, 2015.
- [23] S. K. Jha, E. M. Clarke, C. J. Langmead, A. Legay, A. Platzer, and P. Zuliani. A bayesian approach to model checking biological systems. In *CMSB'09*, pages 218–234. Springer, 2009.
- [24] J.-P. Katoen, I. S. Zapreev, E. M. Hahn, H. Hermanns, and D. N. Jansen. The ins and outs of the probabilistic model checker mrmc. *Performance evaluation*, 68(2):90–104, 2011.
- [25] E. A. Lee. Cyber physical systems: Design challenges. In ISORC'08, pages 363–369. IEEE, 2008.
- [26] H. Mao, Y. Chen, M. Jaeger, T. D. Nielsen, K. G. Larsen, and B. Nielsen. Learning probabilistic automata for model checking. In *QEST'11*, pages 111–120. IEEE, 2011.
- [27] H. Mao, Y. Chen, M. Jaeger, T. D. Nielsen, K. G. Larsen, and B. Nielsen. Learning markov decision processes for model checking. arXiv preprint arXiv:1212.3873, 2012.
- [28] H. Mao, Y. Chen, M. Jaeger, T. D. Nielsen, K. G. Larsen, and B. Nielsen. Learning deterministic probabilistic automata from a model checking perspective. *Machine Learning*, 105(2):255–299, 2016.
- [29] A. Nouri, B. Raman, M. Bozga, A. Legay, and S. Bensalem. Faster statistical model checking by means of abstraction and learning. In *RV'14*, pages 340–355. Springer, 2014.
- [30] S. Park, O. Bastani, N. Matni, and I. Lee. Pac confidence sets for deep neural networks via calibrated prediction. arXiv preprint arXiv:2001.00106, 2019.
- [31] D. Peled, M. Y. Vardi, and M. Yannakakis. Black box checking. In Formal Methods for Protocol Engineering and Distributed Systems, pages 225–240. Springer, 1999.
- [32] R. Rajkumar, I. Lee, L. Sha, and J. Stankovic. Cyber-physical systems: the next computing revolution. In *Design Automation Conference*, pages 731–736. IEEE, 2010.
- [33] S. Ratschan. Simulation based computation of certificates for safety of dynamical systems. In FORMATS'17, pages 303–317. Springer, 2017.
- [34] D. Reijsbergen, P. de Boer, W. R. W. Scheinhardt, and B. R. Haverkort. On hypothesis testing for statistical model checking. *Int. J. Softw. Tools Technol. Transf.*, 17(4):377–395, 2015.
- [35] K. Sen, M. Viswanathan, and G. Agha. Statistical model checking of black-box probabilistic systems. In CAV'04, pages 202–215. Springer, 2004.
- [36] K. Sen, M. Viswanathan, and G. A. Agha. VESTA: A statistical modelchecker and analyzer for probabilistic systems. In *QEST'05*, pages 251– 252. IEEE Computer Society, 2005.
- [37] S. Shalev-Shwartz and S. Ben-David. Understanding machine learning: From theory to algorithms. Cambridge university press, 2014.
- [38] L. Valiant. Probably Approximately Correct: NatureÕs Algorithms for Learning and Prospering in a Complex World. Basic Books (AZ), 2013.
- [39] B. Van der Pol. Lxxxviii. on "relaxation-oscillations". *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 2(11):978–992, 1926.
- [40] M. Waga. Falsification of cyber-physical systems with robustness-guided black-box checking. In HSCC'20, pages 1–13, 2020.
- [41] A. Wald. Sequential tests of statistical hypotheses. The Annals of Mathematical Statistics, 16(2):117–186, 1945.
- [42] B. Xue, M. Fränzle, H. Zhao, N. Zhan, and A. Easwaran. Probably approximate safety verification of hybrid dynamical systems. In *ICFEM'19*, pages 236–252. Springer, 2019.
- [43] B. Xue, Y. Liu, L. Ma, X. Zhang, M. Sun, and X. Xie. Safe inputs approximation for black-box systems. In *ICECCS'19*, pages 180–189. IEEE, 2019.
- [44] B. Xue, Q. Wang, S. Feng, and N. Zhan. Over- and under-approximating reach sets for perturbed delay differential equations. *IEEE Transactions* on Automatic Control, pages 1–1, 2020.
- [45] H. L. Younes. Probabilistic verification for "black-box" systems. In CAV'05, pages 253–265. Springer, 2005.
- [46] H. L. Younes. Ymer: A statistical model checker. In CAV'05, pages 429–433. Springer, 2005.
- [47] H. L. Younes and R. G. Simmons. Probabilistic verification of discrete event systems using acceptance sampling. In CAV'02, pages 223–235. Springer, 2002.
- [48] P. Zuliani, A. Platzer, and E. M. Clarke. Bayesian statistical model checking with application to stateflow/simulink verification. *Formal Methods in System Design*, 43(2):338–367, 2013.