

Data-driven verification and synthesis of stochastic systems through barrier certificates

Ali Salamati, Abolfazl Lavaei, Sadegh Soudjani, and Majid Zamani

Abstract In this work, we study verification and synthesis problems for safety specifications over unknown discrete-time stochastic systems. When a model of the system is available, barrier certificates have been successfully applied for ensuring the satisfaction of safety specifications. In this work, we formulate the computation of barrier certificates as a robust convex program (RCP). Solving the acquired RCP is hard in general because the model of the system that appears in one of the constraints of the RCP is unknown. We propose a data-driven approach that replaces the uncountable number of constraints in the RCP with a finite number of constraints by taking finitely many random samples from the trajectories of the system. We thus replace the original RCP with a scenario convex program (SCP) and show how to relate their optimizers. We guarantee that the solution of the SCP is a solution of the RCP with a priori guaranteed confidence when the number of samples is larger than a pre-computed value. This provides a lower bound on the safety probability of the original unknown system together with a controller in the case of synthesis. We also discuss an extension of our verification approach to a case where the associated robust program is non-convex and show how a similar methodology can be applied. Finally, the applicability of our proposed approach is illustrated through three case studies.

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1 introduction

Ensuring safety and temporal requirements on cyber-physical systems is becoming more important in many applications including self-driving cars, power grids, traffic networks, and integrated medical devices. Complex requirements for such real-life practical systems can be expressed as linear temporal logic formulae [1]. Model-based approaches for satisfying such requirements have been studied extensively in the literature [2, 3, 4, 5]. In the setting of formal approaches for stochastic systems, a number of abstraction-based methods has been developed for the verification and synthesis of dynamical systems in order to either verify the desired specifications or synthesize controllers enforcing these systems to satisfy such specifications [6, 7, 8, 9, 10]. In order to improve scalability of abstraction-based methods, some other techniques such as sequential gridding [11, 12], discretization-free abstraction [13], and compositional abstraction-based techniques [14] have been introduced in the literature in order to efficiently deal with the verification and synthesis problems.

An approach for formal verification and synthesis with respect to safety specifications in dynamical systems is to use a notion of barrier certificates [15]. Barrier certificates have been the focus of the recent literature as an abstraction-free technique that is scalable with the dimension of the system, i.e., they do not require construction of an abstraction of the system and can provide directly the controller together with the guarantee on the satisfaction of the safety specification [16], [17], [18]. A barrier-based methodology is introduced in [15] in order to verify safety in deterministic hybrid systems. In [19], a framework is proposed for safety verification of stochastic systems using barrier certificates which is extended to stochastic hybrid systems. The authors in [20] present barrier certificates that ensure collision-free behaviors in multi-robot systems by minimizing the difference between the actual and the nominal controllers subject to safety constraints. In [21], a compositional analysis is proposed for verifying the safety of an interconnection of subsystems using barrier certificates. The results in [22] uses barrier certificates for the synthesis of controllers against complex requirements expressed as co-safe linear temporal logic formulas.

The common requirement of the approaches mentioned above is the fact that they need a mathematical model of the system. However, a precise model of dynamical systems is either not available in many application scenarios or too complex to be of any use. Therefore, there is a need to develop approaches which are capable of verifying or synthesizing controllers against safety specifications only based on collected data from the system.

Related Literature. Data-driven methods have gained significant attentions recently for formally verifying some desired specifications. A data-enabled predictive

control is introduced in [23] that utilizes noisy data of the system and produces optimal control inputs ensuring the satisfaction of desired chance constraints with high probability. A data-driven model predictive control scheme is proposed in [24] which only requires initially measured input-output trajectories together with an upper bound on the dimension of the unknown system. In [25], a methodology is developed in order to make a single-input single-output system stable only based on data. The stability problem of black-box linear switching systems with desired confidences is investigated in [26] based on collected data. This approach is extended in [27] by providing a methodology for computing the invariant sets of discrete-time black-box systems. A novel Bayes-adaptive planning algorithm for data-efficient verification of uncertain Markov decision processes is introduced in [28]. A framework is proposed in [29] to provide a formal guarantee on data-driven model identification and controller synthesis. In [30], a methodology is developed for providing a probabilistic confidence over the verification of signal temporal logic properties for partially unknown stochastic systems based on collected data.

An optimization-based approach is proposed in [31] to learn a control barrier certificate through safe trajectories under suitable Lipschitz smoothness assumption on the dynamical system. A sub-linear algorithm is developed in [32] for the barrier-based data-driven model validation of dynamical systems which computes the barrier function using a large dataset of trajectories. In [33], a two-step procedure is proposed to synthesize a controller for an unknown nonlinear system, where the first step is to learn a Gaussian process as a replacement of the unknown dynamics, and the second step is to construct the control barrier function for the learned dynamics.

A data-driven optimization called *scenario convex program* (SCP) is introduced in [34] to solve robust convex optimizations. This approach replaces the infinite number of constraints in the robust optimization with a finite number of constrained by sampling the uncertain variables from their distributions. The approach relates the feasibility of the SCP to that of the robust optimization while providing bounds on the probability of violating the constraints. The results in [35] studies the same approach and relates worst-case violation of the constraints to the probability of their violation. While [34, 35] focus on feasibility, the authors in [36] establish a quantitative relation between the optimal value of the robust optimization and its associated SCP.

Contributions. Here, we propose formal verification and synthesis procedures for unknown stochastic systems with respect to safety specifications based on collected data. We first cast a barrier-based safety problem as a robust convex program (RCP). Solving the obtained RCP is hard in general because the unknown model of the system appears in the constraints. To tackle this issue, we resort to a scenario-driven approach by collecting samples from the system. Using the results in [36], we connect the optimal solution of the acquired scenario convex program (SCP) with that of the original RCP. We provide a lower bound on the safety probability of the unknown stochastic unknown system using a certain number of data which is computed according to the desired confidence. We extend this result to provide a new confidence bound for a class of non-convex barrier-based safety problems.

We conclude the paper by three case studies to illustrate the applicability of our approach.

A limited subset of the results proposed here was presented in [37]. This paper extends [37] in three main directions. First and foremost, we extend the results from verification to the synthesis of safety controllers based on sampled data. Second, we develop verification results for a class of non-convex safety problems which makes the approach suitable to larger classes of systems. Finally, we improved the case studies by dealing with higher dimensional systems to show the usability of our approach to a wider range of applications.

Outline. The structure of this paper is as follows. Section 2 gives the system definition and the problem statement, and presents the safety verification of stochastic systems using barrier certificates. In Section 3, we introduce the scenario convex program for the barrier-based safety problem and we connect its optimizer to that of the original optimization. Our approach for the safety verification of the unknown stochastic system is presented in Section 4. In Section 5, we explain our data-driven synthesis approach which enforces the safety specification with a certain confidence. An extension of the verification problem for a class of non-convex safety problems is discussed in Section 6. To illustrate the effectiveness of our approach, three case studies are presented in Section 7. Finally, Section 8 concludes the paper.

2 Preliminaries and Problem Statement

2.1 Notations and Preliminaries

The set of positive integers, non-negative integers, real numbers, non-negative real numbers, and positive real numbers are denoted by $\mathbb{N} := \{1, 2, 3, \dots\}$, $\mathbb{N}_0 := \{0, 1, 2, \dots\}$, \mathbb{R} , \mathbb{R}_0^+ , and \mathbb{R}^+ , respectively. We denote the indicator function by $\mathbb{1}_{\mathcal{A}}(X) : X \rightarrow \{0, 1\}$, where $\mathbb{1}_{\mathcal{A}}(x)$ is 1 if and only if $x \in \mathcal{A}$, and 0 otherwise. Notation $\mathbf{1}_m$ is used to indicate a column vector of ones in $\mathbb{R}^{m \times 1}$. We denote by $\|x\|$ the Euclidean norm of any $x \in \mathbb{R}^n$. We also denote the induced norm of any matrix $A \in \mathbb{R}^{m \times n}$ by $\|A\| = \sup_{x \neq 0} \|Ax\|/\|x\|$. Given N vectors $x_i \in \mathbb{R}^{n_i}$, $n_i \in \mathbb{N}$, and $i \in \{1, \dots, N\}$, we use $[x_1; \dots; x_N]$ and $[x_1, \dots, x_N]$ to denote the corresponding column and row vectors, respectively, with dimension $\sum_i n_i$. The absolute value of a real number x is denoted by $|x|$. If a system, denoted by \mathcal{S} , satisfies a property Ψ during a time horizon \mathcal{H} , it is denoted by $\mathcal{S} \models_{\mathcal{H}} \Psi$. We also use \models in this paper to show the feasibility of a solution for an optimization problem.

The sample space of random variables is denoted by Ω . The Borel σ -algebra on a set X is denoted by $\mathfrak{B}(X)$. The measurable space on X is denoted by $(X, \mathfrak{B}(X))$. We have two probability spaces in this work. The first one is represented by $(X, \mathfrak{B}(X), \mathbb{P})$ which is the probability space defined over the state space X with \mathbb{P} as a probability measure. The second one, $(V_w, \mathfrak{B}(V_w), \mathbb{P}_w)$, defines the probability space over V_w for the random variable w affecting the stochastic system with \mathbb{P}_w as its probability measure. With a slight abuse of the notation, we use the same \mathbb{P} and \mathbb{P}_w when the

product measures are needed in the formulations. Considering a random variable z , $\text{Var}(z) := \mathbb{E}(z^2) - (\mathbb{E}(z))^2$ denotes its variance with \mathbb{E} being the expectation operator.

2.2 System Definition

In this work, we first deal with (potentially) unknown discrete-time continuous-space stochastic dynamical systems as formalized next.

Definition 1 A discrete-time stochastic system (dt-SS) is a tuple $\mathcal{S} = (X, V_w, w, f)$, where the Borel set $X \subset \mathbb{R}^n$ is the state space of the system, the Borel set V_w is the uncertainty space, $w := \{w(t) : \Omega \rightarrow V_w, t \in \mathbb{N}_0\}$ is a sequence of independent and identically distributed (i.i.d.) random variables on the Borel space V_w with some distribution \mathbb{P}_w , and the map $f : X \times V_w \rightarrow X$ is a measurable function that characterizes the state evolution of the system. The state trajectory of the system is constructed according to

$$\mathcal{S} : x(t+1) = f(x(t), w(t)), \quad t \in \mathbb{N}_0. \quad (1)$$

We denote a finite trajectory of the system by $\xi(t) := x(0)x(1) \dots x(t)$, $t \in \mathbb{N}_0$.

In this work, we assume that the map f and the distribution of the uncertainty \mathbb{P}_w are unknown. Instead, we assume we can collect *independent* and *identically distributed* state pairs (x_i, x_i^+) by initializing the system at x_i and observing its next state x_i^+ . The collected dataset is denoted by

$$\mathcal{D} := \left\{ (x_i, f(x_i, w_j)) \right\}_{i,j} \subset X^2. \quad (2)$$

2.3 Problem Statement

Definition 2 Given a set of initial states $X_{in} \subset X$, a set of unsafe states $X_u \subset X$, and a finite time horizon $\mathcal{H} \in \mathbb{N}_0$, the system \mathcal{S} is called safe if all trajectories of \mathcal{S} that start from X_{in} never reach X_u within horizon \mathcal{H} . We denote this safety property by Ψ and its satisfaction by \mathcal{S} is written as $\mathcal{S} \models_{\mathcal{H}} \Psi$.

The safety property in the sense of Definition 2 is schematically depicted in Fig. 1.

Since the system is stochastic and we do not know the distribution of w and the map f , we are interested in establishing a lower bound on the probability that the safety property Ψ is satisfied by the trajectories of \mathcal{S} while using only a dataset of the form (2). Now, we state the main problem we are interested to solve here.

Problem 1 Consider an unknown dt-SS \mathcal{S} as in Definition 1. Provide a lower bound $(1 - \rho) \in [0, 1]$ on the probability of satisfying Ψ , *i.e.*,

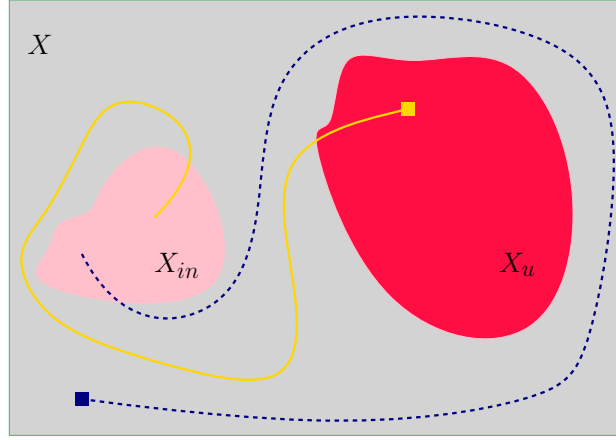


Fig. 1 A set X containing initial and unsafe sets X_{in} and X_u . The (blue) dashed line illustrates a safe trajectory of the system, whereas the yellow one demonstrates an unsafe trajectory.

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho,$$

together with a confidence $(1 - \beta) \in [0, 1]$ using only a dataset \mathcal{D} of the form (2). Moreover, establish a connection between the required size of dataset \mathcal{D} and the desired confidence $1 - \beta$.

Note that $\rho = 1$ gives a trivial lower bound on the probability. Therefore, we are interested in finding a potentially tight lower bound.

Fig. 2 shows an overview of our approach for solving Problem 1 by connecting the related optimizations and results in the paper. Our first step is to cast the formulation of safety problem as an optimization that depends on the model of the system using the concept of barrier certificate.

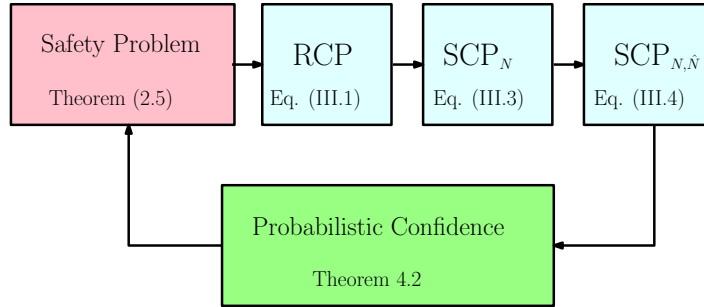


Fig. 2 A schematic overview of the proposed scenario-driven approach towards verification of the safety specification.

2.4 Safety Verification via Barrier Certificates

Definition 3 Given a dt-SS $\mathcal{S} = (X, V_w, w, f)$, a nonnegative function $B : X \rightarrow \mathbb{R}_0^+$ is called a barrier certificate (BC) for \mathcal{S} if there exist constants $\lambda > 1$ and $c \in \mathbb{R}_0^+$ such that

$$B(x) \leq 1, \quad \forall x \in X_{in}, \quad (3)$$

$$B(x) \geq \lambda, \quad \forall x \in X_u, \quad (4)$$

$$\mathbb{E} \left[B(f(x, w)) \mid x \right] \leq B(x) + c, \quad \forall x \in X, \quad (5)$$

where $X_{in} \subset X$ and $X_u \subset X$ are initial and unsafe sets corresponding to a given safety specification Ψ , respectively.

Next theorem, borrowed from [22], provides a lower bound on the probability of satisfaction of the safety specification for a dt-SS.

Theorem 1 Consider a dt-SS \mathcal{S} and a safety specification Ψ . Assume there exists a non-negative barrier certificate $B(x)$ which satisfies conditions (3)-(5) with constants λ and c . Then

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \frac{1 + c \mathcal{H}}{\lambda}, \quad (6)$$

with $\mathcal{H} \in \mathbb{N}_0$ being the finite time horizon associated with Ψ .

In this work, we consider polynomial-type barrier certificates denoted by $B(b, x)$, where b is the vector containing the coefficients of the polynomial. Such a polynomial with degree $k \in \mathbb{N}_0$ has the form

$$B(b, x) = \sum_{\iota_1=0}^k \dots \sum_{\iota_n=0}^k b_{\iota_1, \dots, \iota_n} (x_1^{\iota_1} \dots x_n^{\iota_n}), \quad (7)$$

with $b_{\iota_1, \dots, \iota_n} = 0$ for $\iota_1 + \dots + \iota_n > k$. Hence, finding a polynomial barrier certificate reduces to determining the coefficients of the polynomial, namely $b_{\iota_1, \dots, \iota_n}$. In the next section, we provide our data-driven approach for the construction of polynomial-type barrier certificates.

3 Data-driven Safety Verification

We first cast the barrier-based safety problem in Theorem 1 as a robust convex programming (RCP). We then provide a scenario-based approach in order to solve the obtained RCP using data collected from the system.

Satisfying the conditions of Theorem 1 is equivalent to having a non-positive value for the optimal solution of the following RCP (i.e., $\mathcal{K} \leq 0$):

$$\text{RCP} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z (g_z(x, d)) \leq 0, z \in \{1, \dots, 5\}, \forall x \in X, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_n}], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \end{cases} \quad (8)$$

in which,

$$\begin{aligned} g_1(x, d) &= -\text{B}(b, x) - \mathcal{K}, \\ g_2(x, d) &= \text{B}(b, x) \mathbb{1}_{X_{in}}(x) - 1 - \mathcal{K}, \\ g_3(x, d) &= -\text{B}(b, x) \mathbb{1}_{X_u}(x) + \lambda - \mathcal{K}, \\ g_4(x, d) &= \frac{1 + c \mathcal{H}}{\rho} - \lambda - \mathcal{K}, \\ g_5(x, d) &= \mathbb{E}[\text{B}(b, f(x, w)) \mid x] - \text{B}(b, x) - c - \mathcal{K}, \end{aligned} \quad (9)$$

where $(1 - \rho)$ is a given lower bound for the safety probability.

Remark 1 The RCP (8) is in fact a robust convex optimization. It is a convex optimization since the constraints are convex with respect to decision variables in d and objective function. It is a robust optimization since the constraints have to hold for all $x \in X$.

Remark 2 The RCP (8) always has a feasible solution. For instance, by choosing coefficients of $\text{B}(b, x)$ equal to zero, $\lambda = 2$, $c = 0$, and $\mathcal{K} \geq \frac{1}{\rho} - 2$, we get a feasible solution for the RCP. Moreover, the barrier certificate obtained from this RCP satisfies conditions (3)-(5) as long as $\mathcal{K} \leq 0$.

Finding an optimal solution for the RCP in (8) is hard in general because the map f is unknown, the probability measure \mathbb{P}_w is also unknown (thus the expectation in g_5 cannot be computed analytically), and there are infinitely many constraints in the robust optimization since $x \in X$, where X is a continuous set. To tackle this, we first assign a probability distribution to the state set, take N i.i.d. samples $\{x_1, x_2, \dots, x_N\}$ from this distribution, and replace the robust quantifier $\forall x \in X$ with $\forall x_i \in X, i \in \{1, 2, \dots, N\}$. This results in the following scenario convex program denoted by SCP_N :

$$\text{SCP}_N : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z g_z(x_i, d) \leq 0, \forall i \in \{1, \dots, N\}, \\ & z \in \{1, \dots, 5\}, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_n}], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0. \end{cases} \quad (10)$$

Remark 3 Note that our results presented in this paper are valid for any choice of the probability distribution \mathbb{P} over the state set. From the algorithmic perspective, this distribution affects the collected data points x_i and the optimal solution of the SCP_N .

The confidence formulated in our paper is also with respect to this distribution. We choose \mathbb{P} to be a uniform distribution in the case study section.

To tackle the issue of unknown \mathbb{P}_w , we replace the expectation in g_5 with its empirical approximation by sampling \hat{N} i.i.d. values w_j , $j \in \{1, \dots, \hat{N}\}$, from \mathbb{P}_w for each x_i , which gives the following scenario convex program denoted by $\text{SCP}_{N, \hat{N}}$:

$$\text{SCP}_{N, \hat{N}} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z \bar{g}_z(x_i, d) \leq 0, \forall i \in \{1, \dots, N\}, \\ & z \in \{1, \dots, 5\}, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_n}], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \end{cases} \quad (11)$$

where $\bar{g}_z := g_z$ for all $z \in \{1, 2, 3, 4\}$ and

$$\bar{g}_5(x_i, d) := \frac{1}{\hat{N}} \sum_{j=1}^{\hat{N}} \text{B}(b, f(x_i, w_j)) - \text{B}(b, x_i) - c + \delta - \mathcal{K}. \quad (12)$$

In $\text{SCP}_{N, \hat{N}}$, $f(x_i, w_j)$ is the next state of the system from the current state x_i with the noise realization w_j . Therefore, the solution of the $\text{SCP}_{N, \hat{N}}$ can be obtained using only the dataset \mathcal{D} without the knowledge of f and \mathbb{P}_w . The optimal value for the objective function of $\text{SCP}_{N, \hat{N}}$ is denoted by $\mathcal{K}^*(\mathcal{D})$. We also denote by $\hat{\text{B}}(b, x | \mathcal{D})$ the barrier function constructed based on the solution of $\text{SCP}_{N, \hat{N}}$ in (11).

Note that $\bar{g}_5(x_i, d)$ in (12) has an additional parameter $\delta > 0$ compared to g_5 . This parameter is added to make the last inequality more conservative in order to capture the error coming from replacing the expectation with the empirical mean. We use Chebyshev's inequality [38] to quantify such an error with the associated confidence. Let us define the variance of the empirical approximation as

$$\sigma^2 := \text{Var}\left(\frac{1}{\hat{N}} \sum_{j=1}^{\hat{N}} \text{B}(b, f(x, w_j))\right), \quad (13)$$

where the variance is taken with respect to w_j . We assume that there is a bound \hat{M} such that

$$\text{Var}(\text{B}(b, f(x, w))) \leq \hat{M}, \quad \forall x \in X. \quad (14)$$

This assumption gives us a bound for σ^2 in (13) as $\sigma^2 \leq \frac{\hat{M}}{\hat{N}}$ due to w_j being independent. The idea of replacing the expectation by the empirical mean in an optimization problem and relating the associated solutions based on Chebyshev's inequality is also used in [39]. Next theorem shows that the barrier certificate computed using the optimal solution of the $\text{SCP}_{N, \hat{N}}$ is a feasible barrier certificate for SCP_N in (10) with a certain confidence.

Theorem 2 *Let $\hat{\text{B}}(b, x | \mathcal{D})$ be a feasible solution of the $\text{SCP}_{N, \hat{N}}$ for some $\delta > 0$, and assume the inequality (14) holds with a given \hat{M} . Then for any $\beta_s \in (0, 1]$, we get*

$$\mathbb{P}_w\left(\hat{\mathbf{B}}(b, x | \mathcal{D}) \models \text{SCP}_n\right) \geq 1 - \beta_s, \quad (15)$$

provided that the number of samples in the empirical mean satisfies $\hat{N} \geq \frac{\hat{M}}{\delta^2 \beta_s}$.

Proof By the statement of the theorem, we have $\hat{\mathbf{B}}(b, x | \mathcal{D}) \models \text{SCP}_{n, \hat{N}}$. The difference between the empirical mean in (12) and the expected value in (10) can be quantified by invoking the Chebyshev's inequality as:

$$\mathbb{P}_w\left(\left|\mathbb{E}[\mathbf{B}(b, f(x, w)) | x] - \frac{1}{\hat{N}} \sum_{j=1}^{\hat{N}} \mathbf{B}(b, f(x, w_j))\right| \leq \delta\right) \geq 1 - \frac{\sigma^2}{\delta^2}, \quad (16)$$

where $\delta \in \mathbb{R}^+$, and σ^2 is defined in (13) [38]. Since all the first four feasibility conditions are the same as in (10) and (11), $\hat{\mathbf{B}}(b, x | \mathcal{D})$ is a feasible solution for those conditions of SCP_n with probability one. The only remaining concern is the last feasibility condition. According to (16), one can deduce that $\hat{\mathbf{B}}(b, x | \mathcal{D})$ is a feasible solution for SCP_n with a confidence of at least $1 - \frac{\sigma^2}{\delta^2}$. Furthermore, we have $\sigma^2 \leq \frac{\hat{M}}{\hat{N}}$ by having $\text{Var}(\mathbf{B}(b, f(x, w))) \leq \hat{M}$, and hence

$$\mathbb{P}_w(\hat{\mathbf{B}}(b, x | \mathcal{D}) \models \text{SCP}_n) \geq 1 - \frac{\hat{M}}{\delta^2 \hat{N}}.$$

By the above inequality, we get $\beta_s \geq \frac{\hat{M}}{\delta^2 \hat{N}}$ and consequently $\hat{N} \geq \frac{\hat{M}}{\delta^2 \beta_s}$. This completes the proof. \square

Remark 4 When the system has additive noise, *i.e.*,

$$x(t+1) = f_a(x(t)) + w(t),$$

the condition (14) can be established by having a bound on $f_a(\cdot)$ and bounds on moments of the noise w . For instance, in the case of one-dimensional systems (*i.e.*, $n = 1$), we have $\mathbf{B}(b, x) = \sum_{t=0}^k b_t x^t$ and the variance of $\mathbf{B}(\cdot)$ can be expanded as follows:

$$\begin{aligned}
\text{Var}(\mathbf{B}(b, f(x, w))) &= \text{Var}\left(\sum_{\iota=0}^k b_{\iota} f(x, w)^{\iota}\right) \\
&= \text{Var}\left(\sum_{\iota=0}^k b_{\iota} (f_a(x) + w)^{\iota}\right) = \text{Var}\left(\sum_{\iota} \sum_{j=0}^{\iota} b_{\iota} \binom{\iota}{j} f_a(x)^{\iota-j} w^j\right) \\
&= \text{Var}\left(\sum_{j=1}^k g_j(x) w^j\right) \text{ with } g_j(x) := \sum_{\iota=j}^k b_{\iota} \binom{\iota}{j} f_a(x)^{\iota-j} \\
&= \sum_{j=1}^k \sum_{z=1}^k g_j(x) g_z(x) (\mathbb{E}[w^{j+z}] - \mathbb{E}[w^j] \mathbb{E}[w^z]).
\end{aligned}$$

This means the variance can be bounded using upper bounds of $f_a(\cdot)$ and moments of w .

As it can be seen from Theorem 2, higher number of samples \hat{N} is needed in order to have a smaller empirical approximation error δ , and to provide a better confidence bound. In fact, \hat{N} and δ are required to solve the $\text{SCP}_{N, \hat{N}}$ in (11). Later in the next section, we show how the value of β_s affects the total confidence concerning the safety of the stochastic system.

4 Safety Guarantee over Unknown Stochastic Systems

In the previous section, we established the connection between the two optimizations SCP_N and $\text{SCP}_{N, \hat{N}}$, and showed that the solution of $\text{SCP}_{N, \hat{N}}$ is a feasible solution for SCP_N with a certain confidence if the number of samples \hat{N} is chosen appropriately (cf. Theorem 2). In this section, we focus on the relation between the original RCP and the SCP_N utilizing the fundamental result of [36] and provide an end-to-end safety guarantee over the unknown stochastic system with a priori guaranteed confidence. To do so, we need to raise the following assumption.

Assumption Functions g_1, g_2, g_3 , and g_5 are all Lipschitz continuous with respect to x with Lipschitz constants $L_{x_1}, L_{x_2}, L_{x_3}$, and L_{x_5} , respectively. Denote the maximum Lipschitz constant by $L_x := \max\{L_{x_1}, L_{x_2}, L_{x_3}, L_{x_5}\}$.

Theorem 4 Consider an unknown dt-SS as in (1) and safety specification Ψ . Let Assumption 3 hold with constant L_x . Assume \hat{N} is selected for the $\text{SCP}_{N, \hat{N}}$ as in Theorem 2 in order to provide confidence $1 - \beta_s$. Define the number of samples $N \geq N(\bar{\epsilon}, \beta)$, with

$$N(\bar{\epsilon}, \beta) := \min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^{Q+2} \binom{N}{i} \bar{\epsilon}^i (1 - \bar{\epsilon})^{N-i} \leq \beta \right\}, \quad (17)$$

where $\epsilon, \beta \in [0, 1]$ with $\epsilon \leq L_x$, $\bar{\epsilon} := (\frac{\epsilon}{L_x})^n$, and Q is the number of coefficients of barrier certificate. Suppose $\mathcal{K}^*(\mathcal{D})$ is the optimal value of the optimization problem in (11) using \hat{N} and N and for some given $\rho \in (0, 1]$. Then the following statement holds with a confidence of at least $1 - \beta - \beta_s$:

If $\mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0$, then

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho.$$

Proof Denote the optimal values of the RCP and the SCP_N by \mathcal{K}^* and $\mathcal{K}_m^*(\mathcal{D})$, respectively. According to [36, Theorem 3.6], one has

$$\mathbb{P}(\mathcal{K}^* - \mathcal{K}_m^*(\mathcal{D}) \in [0, \epsilon]) \geq 1 - \beta,$$

for any $N \geq N(g(\frac{\epsilon}{L_{sp}L_x}), \beta)$, where $g(r) = r^n$ for all $r \in [0, 1]$, and L_{sp} being a Slater constant as defined in [36, equation (5)]. Since the original RCP in (8) is a min-max optimization problem, the content L_{sp} can be selected as one according to [36, Remark 3.5]. The number of decision variables in the original RCP is $Q+3$ including Q coefficients of the barrier function together with parameters \mathcal{K} , c and λ . This leads to the expression (17) for the minimum required number of samples $N(\bar{\epsilon}, \beta)$ according to [36, Eq. 3]. Now, one can readily deduce that for any $N \geq N(\bar{\epsilon}, \beta)$, we have

$$\mathbb{P}(\mathcal{K}^* \leq \mathcal{K}_m^*(\mathcal{D}) + \epsilon) \geq 1 - \beta. \quad (18)$$

On the other hand, due to the particular selection of \hat{N} and β_s according to Theorem 2, we know that (15) holds. Therefore,

$$\mathbb{P}(\mathcal{K}_m^*(\mathcal{D}) \leq \mathcal{K}^*(\mathcal{D})) \geq 1 - \beta_s. \quad (19)$$

Define the events $\mathcal{A} := \{\mathcal{D} \mid \mathcal{K}^* \leq \mathcal{K}_m^*(\mathcal{D}) + \epsilon\}$, $\mathcal{B} := \{\mathcal{D} \mid \mathcal{K}_m^*(\mathcal{D}) \leq \mathcal{K}^*(\mathcal{D})\}$, and $\mathcal{C} := \{\mathcal{D} \mid \mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0\}$, where $\mathbb{P}(\mathcal{A}) \geq 1 - \beta$ and $\mathbb{P}(\mathcal{B}) \geq 1 - \beta_s$. It is easy to see from the chain of inequalities

$$\mathcal{K}^* \leq \mathcal{K}_m^*(\mathcal{D}) + \epsilon \leq \mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0,$$

that $\mathcal{A} \cap \mathcal{B} \cap \mathcal{C} \neq \emptyset$ implies $\mathcal{K}^* \leq 0$. For a particular dataset $\mathcal{D} \in \mathcal{C}$, it will belong to $\mathcal{A} \cap \mathcal{B}$ with a probability of at least $1 - \beta - \beta_s$:

$$\mathbb{P}(\mathcal{A} \cap \mathcal{B}) \geq 1 - \mathbb{P}(\mathcal{A}^c) - \mathbb{P}(\mathcal{B}^c) \geq 1 - \beta - \beta_s.$$

Therefore, $\mathcal{A} \cap \mathcal{B} \cap \mathcal{C} \neq \emptyset$ and in turn $\mathcal{K}^* \leq 0$ with a probability of at least $1 - \beta - \beta_s$. This completes the proof since non-positiveness of \mathcal{K}^* ensures with a confidence of at least $1 - \beta - \beta_s$ safety of the system with a lower bound of $(1 - \rho)$.

Remark 5 The barrier function constructed based on the finite number of samples according to the above theorem together with the obtained parameters c and λ satisfies the conditions (3)-(5) in Definition 3 with a confidence of at least $1 - \beta - \beta_s$.

Remark 6 Note that the constraint g_4 in (8) enforces the constraint $\mathbb{P}(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho$ for a given ρ . When ρ is not fixed, one can eliminate this constraint from the optimization and guarantee directly the following inequality

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \frac{1 + c^* \mathcal{H}}{\lambda^*},$$

where c^* and λ^* are the optimal values of the $\text{SCP}_{N, \hat{N}}$. This increases the likelihood of getting a feasible optimization and gives the best possible lower bound on the safety probability.

For the sake of clarity, we present the steps required for applying Theorem 4 in Algorithm 1.

Algorithm 1: Safety verification of an unknown dt-SS $\mathcal{S} = (X, V_w, w, f)$ using collected data.

- Input:** $\beta \in [0, 1]$, $\beta_s \in [0, 1]$, $\rho \in (0, 1]$, $\delta \in \mathbb{R}^+$, $L_x \in \mathbb{R}^+$, $\hat{M} \in \mathbb{R}^+$, and the degree of barrier certificate
- 1: Compute the number of samples $\hat{N} \geq \hat{M} / (\delta^2 \beta_s)$ for the empirical approximation (Theorem 2)
 - 2: Choose $\epsilon \in [0, 1]$ such that $\epsilon \leq L_x$ and set $\bar{\epsilon} = (\epsilon / L_x)^n$, where n is the dimension of X
 - 3: Compute the minimum number of samples as $N(\bar{\epsilon}, \beta)$ according to (17)
 - 4: Select a probability measure \mathbb{P} for the state set X
 - 5: Collect $N \hat{N}$ state pairs from the system

$$\mathcal{D} = \{(x_i, x_{ij}^+) \in X^2, x_{ij}^+ = f(x_i, w_{ij})\}_{i,j}$$

- 6: Solve $\text{SCP}_{N, \hat{N}}$ in (11) with \mathcal{D} and obtain the optimal solution $\mathcal{K}^*(\mathcal{D})$
- Output:** If $\mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0$, then $\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho$ with a confidence of at least $1 - \beta - \beta_s$.
-

Remark 7 Theorem 4 provides a connection between the optimal values of $\text{SCP}_{N, \hat{N}}$ and that of the original RCP in (8), and accordingly, provides a lower bound for the probability of safety for an unknown system with a confidence of at least $1 - \beta - \beta_s$. According to [36, Lemma 3.2], one can improve the confidence to $1 - \beta_s$ by making all the constraints of $\text{SCP}_{N, \hat{N}}$ more conservative with an amount of $L_x \epsilon^{\frac{1}{n}}$. Although this will improve the confidence, it will lead to very conservative constraints and much less likelihood of getting $\mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0$.

Both Theorem 4 and Algorithm 1 require knowing (an upper bound for) Lipschitz constant L_x . The following lemma shows how to get this constant for quadratic barrier certificates and systems with additive noises. A similar reasoning can be used for other polynomial-type barrier certificates by casting them as quadratic functions of monomials.

Lemma 1 Consider a nonlinear system with additive noise

$$x(t+1) = f_a(x(t)) + w(t), \quad t \in \mathbb{N}_0, \quad (20)$$

and a bounded state set X such that $\|x\| \leq \mathcal{L}$ for all $x \in X$. Without loss of generality, we assume that the mean of noise is zero. Let $\|f_a(x)\| \leq L_1\|x\| + L_2$ and $\|\mathbf{J}_x\| \leq \hat{\mathcal{L}}$ for some $L_1, L_2, \hat{\mathcal{L}} \geq 0, \forall x \in X$, where \mathbf{J}_x is the Jacobian matrix of $f_a(x)$. Given a quadratic barrier function $x^T \mathbf{P} x$ with a symmetric positive definite matrix \mathbf{P} , the Lipschitz constant L_x can be upper-bounded by

$$2\|\mathbf{P}\|(L_1\mathcal{L}\hat{\mathcal{L}} + L_2\hat{\mathcal{L}} + \mathcal{L}).$$

Remark 8 Note that according to the above lemma, computing the upper bound for Lipschitz constant L_x depends on $\|\mathbf{P}\|$. On the other hand, computing the entries of \mathbf{P} depends on Lipschitz constant L_x . In order to tackle this circulatory issue, we consider an upper bound for $\|\mathbf{P}\|$ and enforce it as an additional constraint while solving the SCP in (11). If there is no solution with the selected upper bound, we iteratively increase the upper bound until we find a solution or a predefined maximum number of iterations is reached. Increasing the upper bound will result in higher number of samples required according to (17).

Proof We first compute the Lipschitz constant of g_5 in (5) as

$$L_{x_5} = \max \left\{ \left\| \frac{\partial g_5(x)}{\partial x} \right\|, x \in X, \|x\| \leq \mathcal{L} \right\},$$

where

$$\begin{aligned} g_5(x) &= \mathbb{E}[(f^T(x(t)) + w^T(t))\mathbf{P}(f(x(t)) + w(t)) \\ &\quad - x^T(t)\mathbf{P}x(t) - c \\ &= f^T(x(t))\mathbf{P}f(x(t)) - x^T(t)\mathbf{P}x(t) + \mathbb{E}[w^T(t)\mathbf{P}w(t)] - c. \end{aligned}$$

By considering $\mathbf{J}_x = [\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}]$, one has

$$\begin{aligned} L_{x_5} &= \max_x \|2(f(x(t)))^T \mathbf{P} \mathbf{J}_x - x^T(t)\mathbf{P}\| \\ &\leq \max_x 2\|f(x(t))^T\| \|\mathbf{P}\| \|\mathbf{J}_x\| + 2\|x^T(t)\| \|\mathbf{P}\| \\ &\leq 2(L_1\mathcal{L} + L_2)\|\mathbf{P}\|\hat{\mathcal{L}} + 2\mathcal{L}\|\mathbf{P}\| \\ &= 2\|\mathbf{P}\|(L_1\mathcal{L}\hat{\mathcal{L}} + L_2\hat{\mathcal{L}} + \mathcal{L}). \end{aligned}$$

Similarly, one can readily deduce that $L_{x_1} = L_{x_2} = L_{x_3} = 2\mathcal{L}\|\mathbf{P}\|$, and $L_{x_4} = 0$. Then $L_x = \max(L_{x_1}, L_{x_2}, L_{x_3}, L_{x_4}, L_{x_5}) = 2\|\mathbf{P}\|(L_1\mathcal{L}\hat{\mathcal{L}} + L_2\hat{\mathcal{L}} + \mathcal{L})$, which completes the proof. \square

Remark 9 If the underlying dynamics is affine in the form of $x(t+1) = Ax(t) + B + w(t)$ with $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times 1}$, we can set $L_1 = \hat{L}$ as an upper bound on $\|A\|$ and L_2 as an upper bound on $\|B\|$.

5 Data-Driven Controller Synthesis

In this section, we study the problem of synthesizing a controller for an unknown stochastic control system using data to satisfy safety specifications. Our approach is to use *control barrier certificates*, fix a parameterized set of controllers, and design the parameters using an SCP. The stochastic control system is defined next.

Definition 4 A discrete-time stochastic control system (dt-SCS) is a tuple $\mathcal{S}_u = (X, U, V_w, w, f)$, where X, V_w, w are as in Definition 1, $U \subset \mathbb{R}^m$ is the input set, and $f : X \times U \times V_w \rightarrow X$ is the state transition map. The evolution of the state is according to equation

$$\mathcal{S}_u : x(t+1) = f(x(t), u(t), w(t)), \quad t \in \mathbb{N}_0. \quad (21)$$

We assume that the map f and distribution of w is unknown but we can gather data (x_i, u_i, x_i^+) by initializing the system at x_i , applying the input u_i , and observing the next state of the system x_i^+ . The collected dataset is

$$\mathcal{D}_u := \left\{ (x_i, u_i, f(x_i, u_i, w_j)) \right\}_{i,j} \subset X \times U \times X. \quad (22)$$

Now, we state the main problem we are interested to solve here.

Problem 2 Consider an unknown dt-SCS \mathcal{S}_u as in Definition 4, with a safety specification Ψ specified by the initial set X_{in} , unsafe set X_u , and time horizon \mathcal{H} . Using a dataset \mathcal{D}_u of the form (22), find a controller $k : X \rightarrow U$ together with a constant $\rho \in [0, 1)$ and confidence $(1 - \beta) \in [0, 1]$ such that \mathcal{S}_u under this controller satisfies Ψ with a probability of at least $(1 - \rho)$, *i.e.*,

$$\mathbb{P}_w^k(\mathcal{S}_u \models_{\mathcal{H}} \Psi) \geq 1 - \rho, \quad \forall x(0) \in X_{in},$$

with a confidence $1 - \beta$. Moreover, establish a connection between the required size of \mathcal{D}_u and the confidence $1 - \beta$.

Similar to the verification problem discussed in the previous sections, we use the notion of control barrier certificates with a parameterized set of controllers [22] to get a characterization of the controller together with the lower bound on the safety probability.

Definition 5 Given a dt-SCS $\mathcal{S}_u = (X, U, V_w, w, f)$ with $U \subset \mathbb{R}^m$, initial set $X_{in} \subset X$, and unsafe set $X_u \subset X$, a function $B_u : X \rightarrow \mathbb{R}_0^+$ is called a control barrier

certificate (CBC) for \mathcal{S}_u if there exist constants $\lambda > 1$, $c \geq 0$, and functions $\mathcal{P}_\ell(x)$, $\ell \in \{1, 2, \dots, m\}$, such that

$$\mathbf{B}_u(x) \leq 1, \quad \forall x \in X_{in}, \quad (23)$$

$$\mathbf{B}_u(x) \geq \lambda, \quad \forall x \in X_u, \quad (24)$$

$$\mathbb{E} \left[\mathbf{B}_u(f(x, u, w)) \mid x, u \right] + \sum_{\ell=1}^m (u_\ell - \mathcal{P}_\ell(x)) \leq \mathbf{B}_u(x) + c$$

$$\forall x \in X, \forall u = [u_1; \dots; u_m] \in U. \quad (25)$$

Theorem 5 A CBC $\mathbf{B}_u(x)$ as in Definition 5 guarantees that

$$\mathbb{P}_w^k(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho, \quad \forall x(0) \in X_{in},$$

under the controller $k(x) = [\mathcal{P}_1(x); \mathcal{P}_2(x); \dots; \mathcal{P}_m(x)]$, where $\rho = (1 + c\mathcal{H})/\lambda$ with \mathcal{H} being the time horizon of the safety specification.

Let us consider polynomial-type CBC and controllers. The CBC \mathbf{B}_u is a polynomial of degree $k \in \mathbb{N}_0$ as

$$\mathbf{B}_u(b, x) = \sum_{\iota_1=0}^k \dots \sum_{\iota_n=0}^k b_{\iota_1, \dots, \iota_n} (x_1^{\iota_1} \dots x_n^{\iota_n}), \quad (26)$$

with $b_{\iota_1, \dots, \iota_n} = 0$ for $\iota_1 + \dots + \iota_n > k$. The number of coefficients of this CBC is denoted by Q . Polynomial \mathcal{P}_ℓ has the following form for some $k' \in \mathbb{N}_0$:

$$\mathcal{P}_\ell(p^\ell, x) = \sum_{\iota_1=0}^{k'} \dots \sum_{\iota_n=0}^{k'} p_{\iota_1, \dots, \iota_n}^\ell (x_1^{\iota_1} \dots x_n^{\iota_n}), \quad (27)$$

with $p_{\iota_1, \dots, \iota_n}^\ell = 0$ for $\iota_1 + \dots + \iota_n > k'$.

The overall number of all coefficients of m polynomials $\mathcal{P}_\ell(p^\ell, x)$ is denoted by \mathcal{P} . We also assume that the input set U is a polytope of the form

$$U = \{u \in \mathbb{R}^m \mid \mathcal{A}u \leq \mathbf{b}\}, \quad (28)$$

for some $\mathcal{A} \in \mathbb{R}^{q \times m}$ and $\mathbf{b} \in \mathbb{R}^{q \times 1}$. Under these assumptions, the inequalities in Definition 5 and Theorem 5 can be written as an RCP:

$$\text{RCP} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z g_z(x, u, d) \leq 0, \\ & z \in \{1, 2, \dots, 5 + q\}, \forall x \in X, \forall u \in U, \\ & d = [\mathcal{K}; \lambda; c; b_{\iota_1, \dots, \iota_n}; p_{\iota_1, \dots, \iota_n}^\ell], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \end{cases} \quad (29)$$

where

$$\begin{aligned}
g_1(x, d) &= -\mathbf{B}_u(b, x) - \mathcal{K}, \\
g_2(x, d) &= \mathbf{B}_u(b, x) \mathbb{1}_{X_{in}}(x) - 1 - \mathcal{K}, \\
g_3(x, d) &= -\mathbf{B}_u(b, x) \mathbb{1}_{X_u}(x) - \lambda - \mathcal{K}, \\
g_4(x, d) &= \frac{1 + c\mathcal{H}}{\rho} - \lambda - \mathcal{K}, \\
g_5(x, u, d) &= \mathbb{E} \left[\mathbf{B}_u(b, f(x, u, w)) \mid x, u \right] + \sum_{\ell=1}^m (u_\ell - \mathcal{P}_\ell(p^\ell, x)) \\
&\quad - \mathbf{B}_u(b, x) - c - \mathcal{K}, \\
[g_6(x, d); \dots; g_{5+q}(x, d)] &= \mathcal{A} [\mathcal{P}_1(p^1, x); \dots; \mathcal{P}_m(p^m, x)] - \\
&\quad \mathbf{b} - \mathcal{K} \mathbf{1}_{q \times 1}.
\end{aligned} \tag{30}$$

Note that the last inequality in (30) encodes the fact that the control input should be inside the set U specified by the polytope (28).

The constrained in the RCP is always feasible. A solution can be constructed as follows. Set the coefficients of $\mathbf{B}_u(b, x)$ and $\mathcal{P}_\ell(p^\ell, x)$ equal to zero, $c = 0$, $\lambda = 2$, and $u_\ell = \mathcal{P}_\ell(p^\ell, x) \forall \ell \in \{1, \dots, m\}$. Also select \mathcal{K} large enough such that $\mathcal{K} \geq \frac{1}{\rho} - 2$ together with $\mathcal{K} \mathbf{1}_{m \times 1} \geq -\mathbf{b}$.

The RCP in (29) is in general hard to solve since the map f and the probability measure \mathbb{P}_w are unknown. Hence, similar to the verification approach discussed in Section 3, we assign a probability distribution to both state and input sets, and collect N i.i.d pairs (x_i, u_i) from this assigned distribution, and replace the robust quantifiers $\forall x \in X$ and $\forall u \in U$ with $\forall x_i \in X$ and $\forall u_i \in U, i \in \{1, \dots, N\}$, respectively. This results in a scenario convex program called SCP_N , which is not presented here for the sake of brevity.

To address the issue of unknown f and \mathbb{P}_w , the expectation in g_5 is replaced with its empirical approximation by sampling \hat{N} i.i.d. values $w_j, j \in \{1, \dots, \hat{N}\}$, from \mathbb{P}_w for each pair of (x_i, u_i) , which results in the following scenario convex program denoted by $\text{SCP}_{N, \hat{N}}$:

$$\text{SCP}_{N, \hat{N}} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z \bar{g}_z(x_i, u_i, d) \leq 0, \\ & z \in \{1, 2, \dots, 5 + q\}, \\ & \forall x_i \in X, \forall u_i \in U, \forall i \in \{1, \dots, N\}, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_m}; p_{t_1, \dots, t_m}^\ell], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \end{cases} \tag{31}$$

where $\bar{g}_z := g_z$ for all $z \in \{1, 2, \dots, 5 + q\} \setminus \{5\}$, and

$$\begin{aligned} \bar{g}_5(x_i, u_i, d) &= \frac{1}{\hat{N}} \sum_{j=1}^{\hat{N}} \mathbf{B}_u(b, f(x_i, u_i, w_j)) + \\ &\sum_{\ell=1}^m (u_{i_\ell} - \mathcal{P}_\ell(p^\ell, x_i)) - \mathbf{B}_u(b, x_i) - c + \delta_u - \mathcal{K}. \end{aligned} \quad (32)$$

Using empirical approximation introduces an error which is demonstrated by δ_u in the above optimization problem. We denote by $\hat{\mathbf{B}}_u(b, x | \mathcal{D}_u)$ the constructed control barrier certificate with coefficients computed by solving the $\text{SCP}_{N, \hat{N}}$.

Remark 10 Similar to Theorem 2, under the assumption

$$\text{Var}(\mathbf{B}_u(b, f(x, u, w))) \leq \hat{M}_u,$$

for some $\hat{M}_u > 0$, a desired confidence $\beta_s \in (0, 1]$, and an error δ_u , one has

$$\mathbb{P}_w^k \left(\hat{\mathbf{B}}_u(b, x | \mathcal{D}_u) \models \text{SCP}_N \right) \geq 1 - \beta_s, \quad (33)$$

provided that $\hat{N} \geq \frac{\hat{M}_u}{\delta_u^2 \beta_s}$.

To provide the main results here, we need the following assumption.

Assumption Function g_5 is Lipschitz continuous with respect to (x, u) with Lipschitz constant L_5 . Functions $g_1, g_2, g_3, g_6, \dots, g_{5+q}$ are also Lipschitz continuous with respect to x with Lipschitz constants $L_1, L_2, L_3, L_6, \dots, L_{5+q}$, respectively. Let us denote the maximum of all these Lipschitz constants by $L_{x,u}$.

Now, we have all the ingredients to propose the main results here.

Theorem 7 Consider an unknown dt-SCS as in Definition 4 and a safety specification Ψ . Let Assumption 6 hold with constant $L_{x,u}$. Suppose that $\mathcal{K}^*(\mathcal{D}_u)$ is the optimal objective value of $\text{SCP}_{N, \hat{N}}$ in (31) for \hat{N} selected based on Remark (10) with confidence of $1 - \beta_s$, and $N \geq N(\bar{\epsilon}, \beta)$, where

$$N(\bar{\epsilon}, \beta) := \min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^{Q+\mathcal{P}+2} \binom{N}{i} \bar{\epsilon}^i (1 - \bar{\epsilon})^{N-i} \leq \beta \right\}, \quad (34)$$

$\epsilon, \beta \in [0, 1]$ with $\epsilon \leq L_{x,u}$, $\bar{\epsilon} := (\frac{\epsilon}{L_{x,u}})^{n+m}$, Q is the number of coefficients of polynomial of control barrier certificate, and \mathcal{P} is the overall number of coefficients of polynomials $\mathcal{P}_\ell(p^\ell, x)$ for m inputs. Now the following statement is valid with a confidence of at least $1 - \beta - \beta_s$: for a given $\rho \in (0, 1]$, if $\mathcal{K}^*(\mathcal{D}_u) + \epsilon \leq 0$ then the system \mathcal{S}_u together with the constructed input

$$\mathbf{k} := [\mathcal{P}_1(p^1, x); \dots; \mathcal{P}_m(p^m, x)],$$

for which coefficients $p^\ell, \ell \in \{1, \dots, m\}$, are obtained from the solution of $\text{SCP}_{N, \hat{N}}$, is safe within the time horizon \mathcal{H} with a probability of at least $1 - \rho$, i.e.

$$\mathbb{P}_w^k(\mathcal{S}_u \models_{\mathcal{H}} \Psi) \geq 1 - \rho. \quad (35)$$

Proof The proof is similar to the proof of Theorem 4 by replacing \mathcal{D} and \mathbb{P}_w with \mathcal{D}_u and \mathbb{P}_w^p for the RCP (29) and its associated SCPs. The number of coefficients is $Q + \mathcal{P} + 3$ where \mathcal{P} is the overall number of coefficients of m polynomials defining the controller, which results in the new bound in (34). \square

Remark 11 The control barrier certificate and the controller constructed based on the finite number of samples according to the above theorem together with the obtained optimal parameters c and λ satisfy conditions (23)-(25) in Lemma 5 with a confidence of at least $1 - \beta - \beta_s$.

Remark 12 When ρ is not fixed, one can eliminate constraint g_4 from (29) and directly provide the following inequality

$$\mathbb{P}_w^p(\mathcal{S}_u \models_{\mathcal{H}} \Psi) \geq 1 - \frac{1 + c^* \mathcal{H}}{\lambda^*},$$

in which c^* and λ^* are the optimal solutions of $\text{SCP}_{N,\hat{N}}$ in (31). This increases the likelihood of getting a feasible solution and gives the best possible lower bound on the safety probability for \mathcal{S}_u .

Algorithm 2: Data-driven synthesis for safety specification on an unknown dt-SCS $\mathcal{S}_u = (X, U, V_w, w, f)$.

- Input:** $\beta \in [0, 1], \beta_s \in (0, 1], \rho \in (0, 1], \delta_u \in \mathbb{R}^+, L_{x,u} \in \mathbb{R}^+, \hat{M}_u \in \mathbb{R}^+$, degree of the barrier certificate, and degree of the polynomial functions for the controller
- 1: Compute the number of samples $\hat{N} \geq \hat{M}/(\delta_u^2 \beta_s)$ for the empirical approximation (Remark 10)
 - 2: Choose $\epsilon \in [0, 1]$ such that $\epsilon \leq L_{x,u}$ and set $\bar{\epsilon} = (\epsilon/L_{x,u})^{n+m}$, where n is the dimension of X and m is the dimension of U
 - 3: Compute the minimum number of samples as $N(\bar{\epsilon}, \beta)$ according to (34)
 - 4: Select a probability measure \mathbb{P} for the state-input space (X, U)
 - 5: Collect $N \hat{N}$ tuples from the system
 $\mathcal{D}_u := \{(x_i, u_i, x'_{ij}) \in X \times U \times X, x'_{ij} = f(x_i, u_i, w_{ij})\}_{i,j}$
 - 6: Solve $\text{SCP}_{N,\hat{N}}$ in (31) with \mathcal{D}_u and obtain the optimal solution $\mathcal{K}^*(\mathcal{D}_u)$
- Output:** If $\mathcal{K}^*(\mathcal{D}_u) + \epsilon \leq 0$, then $\mathbb{P}_w^k(\mathcal{S}_u \models_{\mathcal{H}} \Psi) \geq 1 - \rho$ with a confidence of at least $1 - \beta - \beta_s$, and controller polynomials $\mathcal{P}_\ell(p^\ell, x)$, for all $\ell \in \{1, \dots, m\}$.
-

Next lemma provides an upper bound for Lipschitz constant $L_{x,u}$, which is required in Theorem 7, in the case that the system is affected by an additive noise.

Lemma 2 Consider a nonlinear dt-SCS as in Definition 4 which is affected by an additive noise as the following:

$$x(t+1) = f_a(x(t), u(t)) + w(t), \quad (36)$$

and a bounded state set X and input set U such that $\|x\| \leq \mathcal{L}_x$ for all $x \in X$, and $\|u\| \leq \mathcal{L}_u$ for all $u \in U$. Without loss of generality, we assume that the mean of the noise is zero. Let $\|f_a(x, u)\| \leq L_1\|x\| + L_2\|u\| + L_3$, $\|\mathbf{J}_x\| \leq \hat{\mathcal{L}}_x$, and $\|\mathbf{J}_u\| \leq \hat{\mathcal{L}}_u$, for some $\mathcal{L}_x, \mathcal{L}_u, L_1, L_2, L_3, \hat{\mathcal{L}}_x, \hat{\mathcal{L}}_u \geq 0$, where \mathbf{J}_x and \mathbf{J}_u are Jacobian matrices of $f_a(x, u)$ with respect to x and u , respectively. Given a quadratic barrier function $x^T \mathbf{P} x$, and a set of quadratic functions $x^T \mathbf{P}_\ell x$, $\ell \in \{1, \dots, m\}$, representing each of $\mathcal{P}_\ell(p^\ell, x)$ with symmetric matrices \mathbf{P} and \mathbf{P}_ℓ , the Lipschitz constant $\mathcal{L}_{x,u}$ can be upper-bounded by $\sqrt{\mathcal{L}_x^2 + \mathcal{L}_u^2}$, where

$$\begin{aligned} \mathcal{L}_x &= 2\mathcal{L}_x L_1 \hat{\mathcal{L}}_x \|\mathbf{P}\| + 2\mathcal{L}_u L_2 \hat{\mathcal{L}}_x \|\mathbf{P}\| + 2L_3 \hat{\mathcal{L}}_x \|\mathbf{P}\| \\ &\quad + \mathcal{L}_x \|\mathbf{P}\| + \mathcal{L}_x \sum_{\ell=1}^m \|\mathbf{P}_\ell\|, \\ \mathcal{L}_u &= 2\mathcal{L}_x L_1 \hat{\mathcal{L}}_u \|\mathbf{P}\| + 2\mathcal{L}_u L_2 \hat{\mathcal{L}}_u \|\mathbf{P}\| + 2L_3 \hat{\mathcal{L}}_u \|\mathbf{P}\| + \sqrt{m}. \end{aligned} \quad (37)$$

Proof We first compute the Lipschitz constant regarding $g_5(x, u, d)$ in (30), where

$$\begin{aligned} g_5(x, u, d) &= \mathbb{E}[(f^T(x(t), u(t)) + w^T(t))\mathbf{P}(f(x(t), u(t)) + \\ &\quad w(t))] + \sum_{\ell=1}^m (u_\ell - \mathcal{P}_\ell(p^\ell, x)) - x^T(t)\mathbf{P}x(t) - c. \end{aligned}$$

Considering $\mathbb{E}[w(t)] = 0$, we compute the upper bounds for Lipschitz constant with respect to x and u separately denoted by \mathcal{L}_{5_x} and \mathcal{L}_{5_u} , respectively. We define $\mathbf{J}_x = [\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}]$ and $\mathbf{J}_u = [\frac{\partial f}{\partial u_1}, \dots, \frac{\partial f}{\partial u_m}]$ as Jacobian matrices with respect to x and u , respectively.

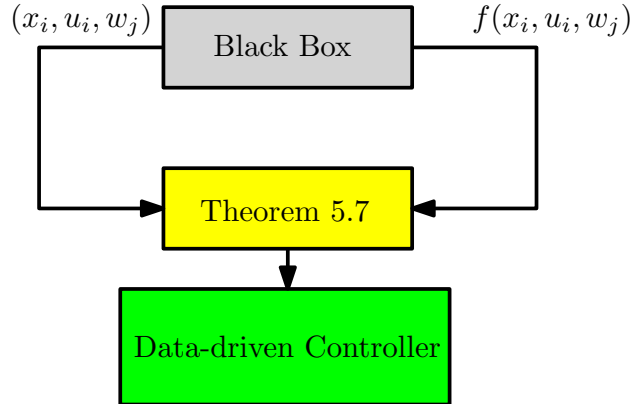


Fig. 3 A schematic overview of the data-driven synthesis presented in Section 5.

$$\begin{aligned}
 L_{5_x} &= \max_{x,u} \left\| \frac{\partial g_5(x,u,d)}{\partial x} \right\| = \max_{x,u} \|2(f(x(t), u(t))^T \mathbf{P} \mathbf{J}_x \\
 &\quad - x^T(t) \mathbf{P} - x^T(t) \sum_{\ell=1}^m \mathbf{P}_\ell\| \\
 &\leq 2\mathcal{L}_x L_1 \hat{L}_x \|\mathbf{P}\| + 2\mathcal{L}_u L_2 \hat{L}_x \|\mathbf{P}\| + 2L_3 \hat{L}_x \|\mathbf{P}\| + \\
 &\quad \mathcal{L}_x \|\mathbf{P}\| + \mathcal{L}_x \sum_{\ell=1}^m \|\mathbf{P}_\ell\|,
 \end{aligned}$$

and accordingly,

$$\begin{aligned}
 L_{5_u} &= \max_{x,u} \left\| \frac{\partial g_5(x,u,d)}{\partial u} \right\| \\
 &= \|2(f(x(t), u(t))^T \mathbf{P} \mathbf{J}_u + \mathbf{1}_m\| \\
 &\leq 2\mathcal{L}_x L_1 \hat{L}_u \|\mathbf{P}\| + 2\mathcal{L}_u L_2 \hat{L}_u \|\mathbf{P}\| + 2L_3 \hat{L}_u \|\mathbf{P}\| + \sqrt{m}.
 \end{aligned}$$

Now it can be deduced that

$$L_5 \leq \sqrt{L_{5_x}^2 + L_{5_u}^2}.$$

Similar to the proof of Lemma 1, it is straightforward to compute the upper bounds of Lipschitz constants for other constraints in (30) and show that the computed upper bound is greater than all of them. We ignore this part for the sake of brevity. Then, $L_{x,u} \leq \max(L_i, i \in \{1, 2, \dots, 5 + q\} \setminus \{4\}) = \sqrt{L_{5_x}^2 + L_{5_u}^2}$ which is equivalent to $\sqrt{\mathcal{L}_x^2 + \mathcal{L}_u^2}$ with \mathcal{L}_x and \mathcal{L}_u as in (37). \square

6 Data-driven Barrier Certificates for Non-convex Setting

In this section, we extend the proposed result in Section 4 to a case of having non-convex constraints. We modify the constraint (5) in Definition 3 as follows:

$$\mathbb{E} \left[\mathbf{B}(f(x, w)) \mid x \right] \leq \kappa \mathbf{B}(x) + c, \quad \forall x \in X, \quad (38)$$

where $\kappa \in (0, 1)$.

According to the fundamental results in [40], choosing κ in the interval $(0, 1)$ provides a better lower bound for the probability of safety satisfaction in (6), namely:

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho,$$

with

$$\rho = \begin{cases} 1 - (1 - \frac{1}{\lambda})(1 - \frac{c}{\lambda}) & \text{if } \lambda \geq \frac{c}{\kappa} \\ \frac{1}{\lambda}(1 - \kappa)^{\mathcal{H}} + \frac{c}{\kappa\lambda}(1 - (1 - \kappa)^{\mathcal{H}}) & \text{if } \lambda < \frac{c}{\kappa}, \end{cases} \quad (39)$$

where parameters c , λ , and \mathcal{H} are the same as in Definition (3). Another advantage of choosing κ in the interval $(0, 1)$ is that this new formulation can be utilized in the context of compositionality and interconnected systems [41, 42].

Replacing the last condition of RCP in (9) with the modified constraint in (38) leads to the following optimization problem which is not convex anymore:

$$\text{RP} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z (g_z(x, d)) \leq 0, z \in \{1, \dots, 4\}, \forall x \in X, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_n}; \kappa], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \kappa \in (0, 1), \end{cases} \quad (40)$$

in which,

$$\begin{aligned} g_1(x, d) &= -\mathbf{B}(b, x) - \mathcal{K}, \\ g_2(x, d) &= \mathbf{B}(b, x) \mathbb{1}_{X_{in}}(x) - 1 - \mathcal{K}, \\ g_3(x, d) &= -\mathbf{B}(b, x) \mathbb{1}_{X_u}(x) + \lambda - \mathcal{K}, \\ g_4(x, d) &= \mathbb{E}[\mathbf{B}(f(x, w)) \mid x] \leq \kappa \mathbf{B}(x) + c, \quad \forall x \in X. \end{aligned} \quad (41)$$

The non-convexity comes from the multiplication of κ and coefficients of barrier function $\mathbf{B}(b, x_i)$ in (38). With the same reasoning in Section (3), solving the above RP is not straightforward generally. Therefore, we construct an SP by taking samples and then connect the solution of the obtained scenario programming to the safety of the stochastic system in (1). By collecting i.i.d. samples x_i , $i \in \{1, \dots, N\}$, from an assigned probability distribution over the state set, and approximating the expectation term in (38) results in a non-convex programming as the following:

$$\text{SP}_{N, \hat{N}} : \begin{cases} \min_d & \mathcal{K} \\ \text{s.t.} & \max_z \bar{g}_z(x_i, d) \leq 0, \forall i \in \{1, \dots, N\}, \\ & z \in \{1, \dots, 4\}, \\ & d = [\mathcal{K}; \lambda; c; b_{t_1, \dots, t_n}; \kappa], \\ & \mathcal{K} \in \mathbb{R}, \lambda > 1, c \geq 0, \kappa \in (0, 1), \end{cases} \quad (42)$$

where $\bar{g}_z := g_z$ for all $z \in \{1, 2, 3\}$ and

$$\bar{g}_4(x_i, d) = \frac{1}{\hat{N}} \sum_{j=1}^{\hat{N}} \mathbf{B}(b, f(x_i, w_j)) - \kappa \mathbf{B}(b, x_i) - c + \delta - \mathcal{K}. \quad (43)$$

Note that in this new scenario programming, we eliminated the constraint that forces a fixed probability lower bound $1 - \rho$ on the safety of the stochastic system, namely, g_4 in (9). Instead, we are interested in providing the tightest possible lower bound of the safety probability according to Remark 6. The main issue underlying here is that by considering $\kappa \in (0, 1)$, the obtained scenario program is not convex anymore due to bilinearity between coefficients of the barrier certificate and κ as decision variables,

and accordingly, one cannot naively utilize the results proposed in Theorems 4. Hence, one cannot solve the SP in (42) by simply applying bisection over κ , while still utilizing the proposed results in the previous sections.

Now we state the main problem we aim to address in this section.

Problem 3 Consider an unknown dt-SS \mathcal{S} as in Definition 1. Compute the largest lower bound $(1 - \rho) \in [0, 1]$ on the probability of satisfying Ψ , i.e.,

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho,$$

according to (39) together with a confidence $(1 - \beta) \in [0, 1]$ using a dataset \mathcal{D} of the form (2). Moreover, establish a connection between the required size of dataset \mathcal{D} , the cardinality of the set from which the parameter κ is selected, and the desired confidence $1 - \beta$.

In the next theorem, we present our solution to Problem 3 by proposing a new confidence bound which is always valid even for the non-convex scenario program in (42).

Theorem 8 Consider an unknown dt-SS as in (1) together with the safety specification Ψ . Let M be the cardinality of a finite set from which κ takes value. Suppose that Assumption 3 holds for the RP in (40) with $L_x := \max(L_{x_1}, L_{x_2}, L_{x_3}, L_{x_4})$, where $L_{x_i}, i \in \{1, \dots, 4\}$, is an upper bound on the Lipschitz constant of the i^{th} constraint in (40). Assume \hat{N} is selected for the $SP_{N, \hat{N}}$ similar to Theorem 2 in order to provide confidence $1 - \beta_s$. Define the number of samples $N \geq N(\bar{\epsilon}, \beta)$, with

$$N(\bar{\epsilon}, \beta) := \min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^{Q+2} \binom{N}{i} \bar{\epsilon}^i (1 - \bar{\epsilon})^{N-i} \leq \frac{\beta}{M} \right\}, \quad (44)$$

where $\epsilon, \beta \in [0, 1]$ with $\epsilon \leq L_x$, $\bar{\epsilon} := (\frac{\epsilon}{L_x})^n$, and Q is the number of coefficients of barrier certificate. Suppose $\mathcal{K}^*(\mathcal{D})$ is the optimal value of the optimization problem in (42) using \hat{N} and N . Then the following statement holds with a confidence of at least $1 - \beta - \beta_s$: If $\mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0$ then

$$\mathbb{P}_w(\mathcal{S} \models_{\mathcal{H}} \Psi) \geq 1 - \rho^*, \quad (45)$$

where ρ^* is computed as in (39) using optimal solutions of $SP_{N, \hat{N}}$, namely, c^* , λ^* , and κ^* . More importantly, with a confidence of at least $1 - \beta - \beta_s$, $B(b^*, x)$ is a barrier certificate for \mathcal{S} , satisfying (3), (4), and (38), where b^* is the optimal solution of $SCP_{N, \hat{N}}$.

Proof Denote the optimal values of the RP and its equivalent scenario programming before the empirical approximation of the expectation term in g_4 , namely, SP_N , by \mathcal{K}^* and $\mathcal{K}_m^*(\mathcal{D})$, respectively. According to [36, Theorem 4.3], one has

$$\mathbb{P}(\mathcal{K}^* - \mathcal{K}_m^*(\mathcal{D}) \in [0, \epsilon]) \geq 1 - \beta,$$

for any $N \geq \tilde{N}(\bar{\epsilon}_1, \dots, \bar{\epsilon}_M, \beta)$, where

$$\begin{aligned} \tilde{N}(\bar{\epsilon}_1, \dots, \bar{\epsilon}_M, \beta) := \\ \min \left\{ N \in \mathbb{N} \mid \sum_{z=1}^M \sum_{i=0}^{d-1} \binom{N}{i} \bar{\epsilon}_z^i (1 - \bar{\epsilon}_z)^{N-i} \leq \beta \right\}, \end{aligned}$$

$\bar{\epsilon}_z = (\frac{\epsilon_z}{\mu_x})^n$, $z \in \{1, \dots, M\}$, M is the cardinality of the set from which κ is selected, and d is the number of decision variables. By choosing $\bar{\epsilon}_z := \bar{\epsilon}$ and $d := Q + 3$, one sets the inequality in (44) regarding the number of samples. On the other hand, due to the particular selection of \tilde{N} and β_s similar to Theorem 2, it can be deduced that

$$\mathbb{P}_w \left(\hat{\mathbf{B}}(b, x \mid \mathcal{D}) \models \text{SP}_N \right) \geq 1 - \beta_s,$$

where $\hat{\mathbf{B}}(b, x \mid \mathcal{D})$ is the barrier function whose coefficients are the optimal solution of SP_N . Therefore, we have

$$\mathbb{P} \left(\mathcal{K}_m^*(\mathcal{D}) \leq \mathcal{K}^*(\mathcal{D}) \right) \geq 1 - \beta_s. \quad (46)$$

By defining events $\mathcal{A} := \{\mathcal{D} \mid \mathcal{K}^* \leq \mathcal{K}_m^*(\mathcal{D}) + \epsilon\}$, $\mathcal{B} := \{\mathcal{D} \mid \mathcal{K}_m^*(\mathcal{D}) \leq \mathcal{K}^*(\mathcal{D})\}$, and $\mathcal{C} := \{\mathcal{D} \mid \mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0\}$, where $\mathbb{P}(\mathcal{A}) \geq 1 - \beta$ and $\mathbb{P}(\mathcal{B}) \geq 1 - \beta_s$, it is easy to conclude using the same reasoning as in the second part of proof of Theorem (4) that

$$\mathbb{P}(\mathcal{K} \leq 0) \geq 1 - \beta - \beta_s,$$

which ensures safety of the stochastic system with a lower bound $1 - \rho$ and a confidence at least $1 - \beta - \beta_s$. \square

7 Numerical Examples

7.1 Temperature verification for three rooms

Consider a temperature regulation problem for three rooms characterized by the following discrete-time stochastic system:

$$\begin{aligned} T_1(t+1) &= (1 - \tau_s(\alpha + \alpha_e))T_1(t) + \tau_s\alpha T_2(t) + \\ &\quad \tau_s\alpha_e T_e + w_1(t) \\ T_2(t+1) &= (1 - \tau_s(2\alpha + \alpha_e))T_2(t) + \tau_s\alpha(T_1(t) + T_3(t)) + \\ &\quad \tau_s\alpha_e T_e + w_2(t) \\ T_3(t+1) &= (1 - \tau_s(\alpha + \alpha_e))T_3(t) + \tau_s\alpha T_2(t) + \\ &\quad \tau_s\alpha_e T_e + w_3(t), \end{aligned} \quad (47)$$

where $T_1(t)$, $T_2(t)$, and $T_3(t)$ are temperatures of three rooms, respectively. Terms $w_1(t)$, $w_2(t)$, and $w_3(t)$ are additive zero-mean Gaussian noises with standard deviations of 0.01, which model the environmental uncertainties. Parameter $T_e = 10^\circ\text{C}$ is the ambient temperature. Constants $\alpha_e = 8 \times 10^{-3}$ and $\alpha = 6.2 \times 10^{-3}$ are heat exchange coefficients between rooms and the ambient, and individual rooms, respectively. The model for each room is adapted from [43] discretized by $\tau_s = 5$ minutes. Let us consider the regions of interest for each room as $X_{in} = [17^\circ\text{C}, 18^\circ\text{C}]$, $X_u = [29^\circ\text{C}, 30^\circ\text{C}]$, and $X = [17^\circ\text{C}, 30^\circ\text{C}]$. We assume the model of the system and the distribution of the noise are unknown. The main goal is to verify whether the temperature of each room remains in the comfort zone $[17, 29]$ for the time horizon $\mathcal{H} = 3$ which is equivalent to 15 minutes, with a priori confidence of 99%.

Let us consider a barrier certificate with degree $k = 2$ in the polynomial form as $[T_1; T_2; T_3]^T P [T_1; T_2; T_3] = b_0 T_1^2 + b_1 T_2^2 + b_2 T_3^2 + b_3 T_1 T_2 + b_4 T_1 T_3 + b_5 T_2 T_3 + b_6 T_1 + b_7 T_2 + b_8 T_3 + b_9$, where

$$P = \begin{bmatrix} b_0 & \frac{b_3}{2} & \frac{b_4}{2} & \frac{b_6}{2} \\ \frac{b_3}{2} & b_1 & \frac{b_5}{2} & \frac{b_7}{2} \\ \frac{b_4}{2} & \frac{b_5}{2} & b_2 & \frac{b_8}{2} \\ \frac{b_6}{2} & \frac{b_7}{2} & \frac{b_8}{2} & b_9 \end{bmatrix}. \quad (48)$$

According to Algorithm 1, we first choose the desired confidence values β and β_s as 0.005. The value of empirical approximation error is selected as $\delta = 0.05$. We choose $\rho = 0.2$ and $\epsilon = 0.29$. By having $\|x\| \leq \mathcal{L} = \sqrt{3} \times 30$, $L \leq 1.5$, $\hat{L} \leq 0.95$, and enforcing $\|P\| \leq 0.115$, the Lipschitz constant can be computed as 28.98. Hence $\bar{\epsilon} = \left(\frac{0.29}{28.98}\right)^3 = 1.002 \times 10^{-6}$ and the minimum number of samples needed for $\text{SCP}_{N, \hat{N}}$ in (11) is computed using (17) as

$$\min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^{12} \binom{N}{i} (1.002 \times 10^{-6})^i \left(1 - (1.002 \times 10^{-6})\right)^{N-i} \leq 0.005 \right\} = 24120872.$$

By enforcing $\hat{M} = 0.001$, the required number of samples for the approximation of the expected value in (11) is computed as $\hat{N} = 80$. Now, we solve the scenario problem $\text{SCP}_{N, \hat{N}}$ with the acquired values for N and \hat{N} which gives us the optimal objective value $\mathcal{K}^*(\mathcal{D})$ as -0.2907 .

Since $\mathcal{K}^*(\mathcal{D}) + \epsilon = -0.0007 \leq 0$, according to Theorem 4, one can conclude:

$$\mathbb{P}_w(\mathcal{S} \models_3 \Psi) \geq 1 - \rho = 0.80,$$

with a confidence of at least $1 - \beta - \beta_s = 0.99$. The barrier certificate constructed from solving $\text{SCP}_{N, \hat{N}}$ is as follows:

$$\begin{aligned} \hat{B}(b, T_1, T_2, T_3 | \mathcal{D}) = & 0.0573T_1^2 + 0.0745T_2^2 + 0.0589T_3^2 \\ & - 0.0671T_1T_2 - 0.0306T_1T_3 - 0.0688T_2T_3 - \\ & - 0.1319T_1 - 0.1332T_2 - 0.1294T_3 - 0.0063. \end{aligned} \quad (49)$$

The computed optimal values for c and λ are 0.2250 and 8.6653, respectively. The scatter plot of the obtained barrier certificate is illustrated in Fig. 4. As can be seen in this figure, the barrier certificate has less values in the initial set while it has larger values in the unsafe region.

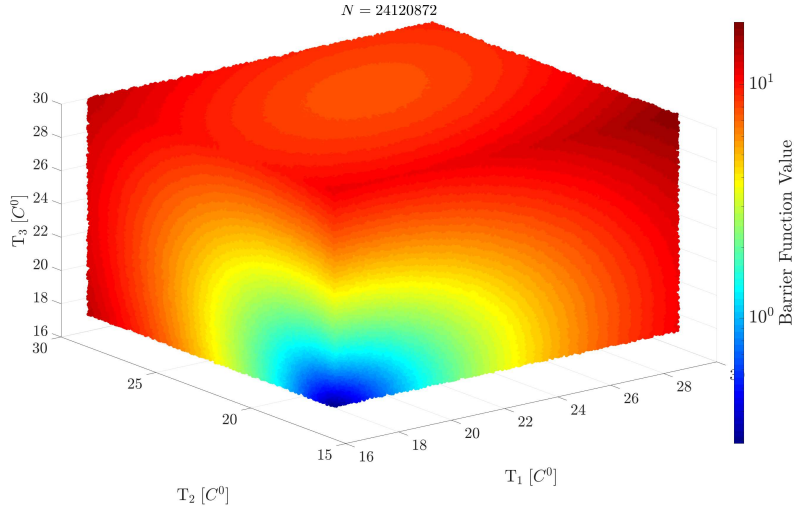


Fig. 4 Scatter plotting of the barrier certificate indicating portions of the state set where the inequalities in (11) are enforced for 24120872 sampled data.

7.2 Lane keeping system

Lane keeping assist system is a future development of the modern lane departure warning system embedded in the current vehicles. This system usually assists the driver through electronic assistance with the steering force. The characteristics of this support depends on the distance of the vehicle from the edge of the lane among other factors such as uncertainties[44]. One of the key challenges in such assisting systems is verifying the obtained performance which can be defined as a safety problem.

In this subsection, it is supposed that the model of the vehicle and the distribution of noise are unknown, and one only has access to a finite number of samples. This unknown system is characterized by a simplified kinematic single-track model of

BMW320i which is adapted from [45] by discretization of the model and adding noise to imitate the uncertainties.

The nonlinear stochastic difference equation is as follows:

$$\begin{aligned} x(t+1) &= x(t) + \tau_s v \cos(\psi(t)) + w_1(t) \\ \mathcal{S} : y(t+1) &= y(t) + \tau_s v \sin(\psi(t)) + w_2(t) \\ \psi(t+1) &= \psi(t) + \frac{\tau_s v}{l_r} \sin(\psi(t)) + w_3(t), \end{aligned} \quad (50)$$

where $\psi = \frac{l_r}{l_r + l_f} \tan^{-1}(\delta_f)$ with $\delta_f = 5$ degrees as the steering angle. Parameters $l_r = 1.384$ and $l_f = 1.384$ are the distances between the center of gravity of the vehicle to the rear and front axles, respectively. Variables x , y , and ψ denote horizontal movement, vertical movement, and the heading angle, respectively. This system is considered to be affected by zero-mean additive noises w_1 , w_2 , and w_3 which are related to uncertainties of position x , position y , and the heading angle ψ with standard deviation of 0.01, 0.01, and 0.001 respectively. Other parameters are the sampling time ($\tau_s = 0.1s$), and the velocity ($v = 5m/s$).

The state set is considered as $X = [1, 10] \times [-7, 7] \times [-0.05, 0.05]$. The regions of interest are $X_{in} = [1, 2] \times [-0.5, 0.5] \times [-0.005, 0.005]$, $X_{u1} = [1, 10] \times [-7, -6] \times [-0.05, 0.05]$, and $X_{u2} = [1, 10] \times [6, 7] \times [-0.05, 0.05]$. Now, the goal is to verify if the vehicle does not enter the unsafe regions of the lane for the time horizon of $\mathcal{H} = 3$ or equivalently $0.3s$ with a desired confidence of 90%.

We consider a barrier certificate of degree $k = 2$ in the polynomial form as $[x; y; \psi]^T P[x; y; \psi] = b_0 x^2 + b_1 y^2 + b_2 \psi^2 + b_3 xy + b_4 x\psi + b_5 y\psi + b_6 x + b_7 y + b_8 \psi + b_9$, where the matrix P is as in (48).

We follow Algorithm 1 to find the barrier certificate and providing a probabilistic guarantee on the safety of stochastic system. First, the desired confidences β and β_s are chosen as 0.095 and 0.005, respectively. We also select the empirical approximation error $\delta = 0.02$. The desired lower bound of safety probability is selected as $1 - \rho = 0.80$. By having $\|x\| \leq \mathcal{L} = \sqrt{10^2 + 7^2 + 0.05^2} = 12.21$, $L \leq 1.4$, $\hat{L} \leq 1$, and enforcing $\|P\| \leq 0.5$, the Lipschitz constant can be computed as 29.3. By fixing $\epsilon = 0.35$, $\bar{\epsilon}$ can be computed as $(\frac{0.35}{29.3})^3 = 1.7 \times 10^{-6}$. In order to reduce the number of required samples, we set some coefficients of the barrier certificate equal to zero ($b_0 = b_3 = b_6 = b_7 = b_8 = 0$). Now the minimum number of samples needed to solve $SCP_{N, \hat{N}}$ in (11) is computed using (17) as

$$\min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^7 \binom{N}{i} (1.7 \times 10^{-6})^i (1 - 1.7 \times 10^{-6})^{N-i} \leq 0.0950 \right\} = 6965301.$$

By enforcing $\hat{M} = 0.006$, the required number of samples for the approximation of the expected value in (11) is computed as $\hat{N} = 3000$. Now, we solve the scenario problem $SCP_{N, \hat{N}}$ with the obtained values of N and \hat{N} which gives us the optimal objective value $\mathcal{K}^*(\mathcal{D})$ as -0.3877 .

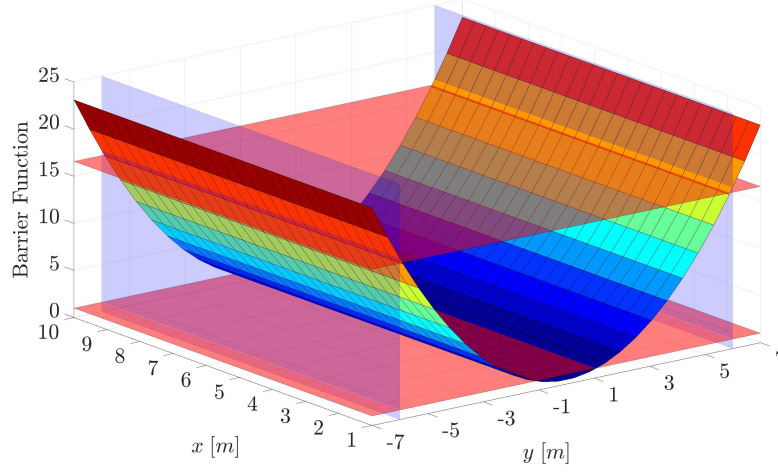


Fig. 5 Surface plot of the barrier certificate $B(x, y, \psi)$ with respect to x and y for fixed $\psi = 0$.

According to Theorem 4, since $\mathcal{K}^*(\mathcal{D}) + \epsilon \leq 0$, one can deduce that

$$\mathbb{P}_w(\mathcal{S} \models_3 \Psi) \geq 1 - \rho = 0.80,$$

with a confidence of at least $1 - \beta - \beta_s = 90\%$. The barrier certificate constructed from solving $\text{SCP}_{\mathcal{N}, \mathcal{N}}$ is represented as:

$$\begin{aligned} \hat{B}(b, x, y, \psi \mid \mathcal{D}) = & 0.4628y^2 - 0.3825\psi^2 - 0.0676x\psi \\ & - 0.2927y\psi + 0.4256. \end{aligned} \quad (51)$$

The optimal values of c and λ are 0.74 and 16.58, respectively.

The surface plot of the barrier certificate $B(x, y, \psi) = \hat{B}(b, x, y, \psi \mid \mathcal{D})$ with respect to x and y for a fixed value of $\psi = 0$ is depicted in Fig. 5. The blue transparent planes separate unsafe region on y , while the lower and upper red transparent planes demonstrate the thresholds in constraints (3) and (4), respectively. Satisfaction of the first and second condition of barrier certificate in Definition 3 can be observed in Fig. 5. The satisfaction of the third condition is illustrated in Fig. 6.

7.3 Synthesizing a temperature controller

Consider a temperature regulation problem for a room using a heater characterized by

$$\mathcal{S}_u : T(t+1) = T(t) + \tau_s (\alpha_e (T_e - T(t)) + \alpha_h (T_h - T(t))u(t)) + w(t), \quad (52)$$

where $w(t)$ is a zero-mean Gaussian noise with standard deviation of 0.05. Parameters are $T_e = 15$, $T_h = 45$, $\alpha_e = 8 \times 10^{-3}$, $\alpha_h = 3.6 \times 10^{-3}$, and $\tau_s = 5$. Regions of interest are defined as $X_{in} = [22^\circ\text{C}, 23^\circ\text{C}]$, $X_u = [27^\circ\text{C}, 30^\circ\text{C}]$, and $X = [22^\circ\text{C}, 30^\circ\text{C}]$. We assume that the model of the system and the distribution of the noise are unknown. The main goal is to design a controller that forces the temperature to remain in the comfort zone [22, 27] for the time horizon $\mathcal{H} = 9$, which is equivalent to 45 minutes, with a priori confidence of 95%.

Let us fix a control barrier certificate with degree $k = 4$ in the polynomial form as $T^T P T = b_0 T^4 + b_1 T^3 + b_2 T^2 + b_3 T + b_4$ with $b_0, b_1, b_2, b_3, b_4 \in \mathbb{R}$. The structure of the controller is considered to be a polynomial of degree $k' = 4$ as $u(p^1, T) = T^T P_u T = p_0 T^4 + p_1 T^3 + p_2 T^2 + p_3 T + p_4$. Matrices P and P_u can be represented as:

$$P = \begin{bmatrix} b_0 & \frac{b_1}{2} & \frac{b_2}{3} \\ \frac{b_1}{2} & \frac{b_2}{3} & \frac{b_3}{2} \\ \frac{b_2}{3} & \frac{b_3}{2} & b_4 \end{bmatrix}, P_u = \begin{bmatrix} p_0 & \frac{p_1}{2} & \frac{p_2}{3} \\ \frac{p_1}{2} & \frac{p_2}{3} & \frac{p_3}{2} \\ \frac{p_2}{3} & \frac{p_3}{2} & p_4 \end{bmatrix}. \quad (53)$$

According to Algorithm 2, we first choose the desired confidences β and β_s as 0.005 and 0.045, respectively. We also select the approximation error $\delta = 0.05$. The Lipschitz constant $L_{x,u}$ can be computed using Lemma 2. By having $\|x\| \leq \mathcal{L} = 30$, $L \leq 1.1$, $\hat{L} \leq 1$, $\hat{L}_u \leq 1$ and enforcing $\|P\| \leq 0.5$, and $\|P_u\| \leq 0.05$, the Lipschitz

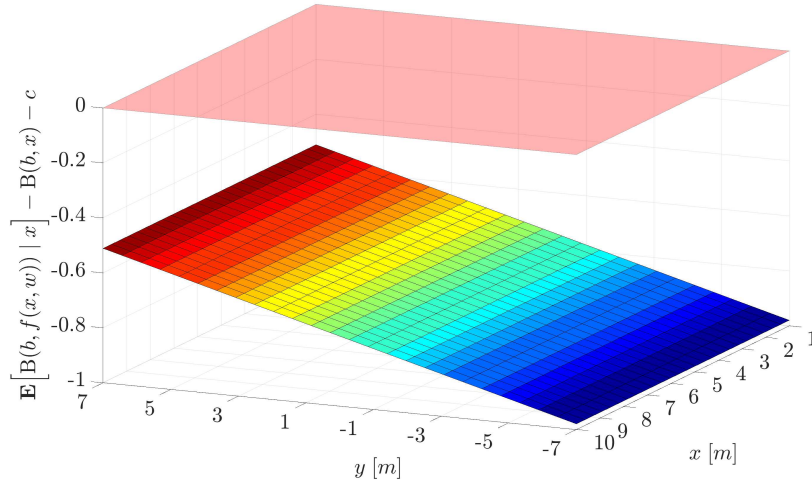


Fig. 6 Satisfaction of the third condition in Definition 3 (for $\psi = 0$) $B(x, y, \psi)$ based on collected data.

constant can be computed as 60.05. By fixing $\epsilon = 0.21$, $\bar{\epsilon}$ can be computed as $(\frac{\epsilon}{L^x})^2 = 1.2 \times 10^{-5}$. Now the minimum number of samples needed for $\text{SCP}_{N,\hat{N}}$ in (31) is computed using (34) as

$$\min \left\{ N \in \mathbb{N} \mid \sum_{i=0}^{12} \binom{N}{i} (1.2 \times 10^{-5})^i (1 - 1.2 \times 10^{-5})^{N-i} \leq 0.005 \right\} = 3838948.$$

By considering $\hat{M} = 6$, the required number of samples for the approximation of the expected value in (11) is computed as $\hat{N} = 53334$. Now, we solve the scenario problem $\text{SCP}_{N,\hat{N}}$ with the computed values for N and \hat{N} which gives us the optimal objective value $\mathcal{K}^*(\mathcal{D}_u)$ as -0.2163 .

According to Theorem 7, since $\mathcal{K}^*(\mathcal{D}_u) + \epsilon = -0.0063 \leq 0$, one has:

$$\mathbb{P}_w^p(\mathcal{S} \models \Psi) \geq 1 - \rho = 0.80,$$

with a confidence of at least $1 - \beta - \beta_s = 95\%$. The computed values for λ and c are 44.76 and 0.87, respectively. The control barrier certificate constructed from solving $\text{SCP}_{N,\hat{N}}$ is:

$$\hat{\mathbf{B}}_u(b, T \mid \mathcal{D}_u) = 0.0029 T^4 - 0.1291 T^3 + 1.4357 T^2 + 0.1652 T - 0.0012.$$

The obtained controller is:

$$\mathcal{P}_1(p^1, T \mid \mathcal{D}_u) = -4.45 \times 10^{-6} T^4 - 7.27 \times 10^{-5} T^3 + 0.0097 T^2 - 0.0976 T - 0.0031.$$

8 Conclusion

We proposed a formal verification and synthesis procedure for discrete-time continuous-space stochastic systems with unknown dynamics against safety specifications. Our approach is based on the notion of barrier certificate and uses sampled trajectories of the unknown system. We first casted the computation of the barrier certificate as a robust convex program (RCP) and approximated its solution with a scenario convex program (SCP) by replacing the unknown dynamics with the sampled trajectories. We then established that the optimal solution of the SCP gives a feasible solution for the RCP with a given confidence, and formulated a lower bound on the required number of samples. Our approach provided a lower bound on the safety probability of the stochastic unknown system when the number of sampled data is larger than a specific lower bound that depends on the desired confidence.

We extended the results to a class of non-convex barrier-based safety problems and showed the applicability of our proposed approach using three case studies.

References

1. Y. Kesten, A. Pnueli, and L. Raviv, “Algorithmic verification of linear temporal logic specifications,” in *International Colloquium on Automata, Languages, and Programming*. Springer, 1998, pp. 1–16.
2. A. Girard, “Reachability of uncertain linear systems using zonotopes,” in *International Workshop on Hybrid Systems: Computation and Control*. Springer, 2005, pp. 291–305.
3. C. Baier and J.-P. Katoen, *Principles of Model Checking*. MIT Press, 2008.
4. P. Tabuada, *Verification and Control of Hybrid Systems: A Symbolic Approach*. Springer, 2009. [Online]. Available: <http://books.google.nl/books?id=1ExhrqtzIYwC>
5. C. Belta, B. Yordanov, and E. A. Gol, *Formal methods for discrete-time dynamical systems*. Springer, 2017, vol. 15.
6. M. Lahijanian, S. B. Andersson, and C. Belta, “Formal verification and synthesis for discrete-time stochastic systems,” *IEEE Transactions on Automatic Control*, vol. 60, no. 8, pp. 2031–2045, Aug 2015.
7. R. Majumdar, K. Mallik, and S. Soudjani, “Symbolic controller synthesis for Büchi specifications on stochastic systems,” in *Proceedings of the 23rd International Conference on Hybrid Systems: Computation and Control*, 2020, pp. 1–11.
8. M. Svoreňová, J. Křetínský, M. Chmelík, K. Chatterjee, I. Černá, and C. Belta, “Temporal logic control for stochastic linear systems using abstraction refinement of probabilistic games,” *Nonlinear Analysis: Hybrid Systems*, vol. 23, pp. 230 – 253, 2017.
9. M. Zamani, P. M. Esfahani, R. Majumdar, A. Abate, and J. Lygeros, “Symbolic control of stochastic systems via approximately bisimilar finite abstractions,” *IEEE Transactions on Automatic Control*, vol. 59, no. 12, pp. 3135–3150, 2014.
10. S. Haesaert and S. Soudjani, “Robust dynamic programming for temporal logic control of stochastic systems,” *IEEE Transactions on Automatic Control*, vol. 66, no. 6, pp. 2496–2511, 2020.
11. S. Soudjani and A. Abate, “Adaptive and sequential gridding procedures for the abstraction and verification of stochastic processes,” *SIAM Journal on Applied Dynamical Systems*, vol. 12, no. 2, pp. 921–956, 2013.
12. S. Soudjani, C. Gevaerts, and A. Abate, “FAUST²: Formal abstractions of uncountable-state stochastic processes,” in *TACAS’15*, ser. Lecture Notes in Computer Science. Springer, 2015, vol. 9035, pp. 272–286.
13. M. Zamani, I. Tkachev, and A. Abate, “Towards scalable synthesis of stochastic control systems,” *Discrete Event Dynamic Systems*, vol. 27, no. 2, pp. 341–369, 2017.
14. S. Soudjani, A. Abate, and R. Majumdar, “Dynamic Bayesian networks as formal abstractions of structured stochastic processes,” in *26th International Conference on Concurrency Theory*. Schloss Dagstuhl, 2015, pp. 169–183.
15. S. Prajna and A. Jadbabaie, “Safety verification of hybrid systems using barrier certificates,” in *International Workshop on Hybrid Systems: Computation and Control*. Springer, 2004, pp. 477–492.
16. L. Zhang, Z. She, S. Ratschan, H. Hermanns, and E. M. Hahn, “Safety verification for probabilistic hybrid systems,” in *International Conference on Computer Aided Verification*. Springer, 2010, pp. 196–211.
17. Z. Yang, M. Wu, and W. Lin, “An efficient framework for barrier certificate generation of uncertain nonlinear hybrid systems,” *Nonlinear Analysis: Hybrid Systems*, vol. 36, p. 100837, 2020.
18. U. Borrmann, L. Wang, A. D. Ames, and M. Egerstedt, “Control barrier certificates for safe swarm behavior,” *IFAC-PapersOnLine*, vol. 48, no. 27, pp. 68–73, 2015.

19. S. Prajna, A. Jadbabaie, and G. J. Pappas, "A framework for worst-case and stochastic safety verification using barrier certificates," *IEEE Transactions on Automatic Control*, vol. 52, no. 8, pp. 1415–1428, 2007.
20. L. Wang, A. D. Ames, and M. Egerstedt, "Safety barrier certificates for collisions-free multi-robot systems," *IEEE Transactions on Robotics*, vol. 33, no. 3, pp. 661–674, 2017.
21. C. Sloth, G. J. Pappas, and R. Wisniewski, "Compositional safety analysis using barrier certificates," in *Proceedings of the 15th ACM international conference on Hybrid Systems: Computation and Control*, 2012, pp. 15–24.
22. P. Jagtap, S. Soudjani, and M. Zamani, "Formal synthesis of stochastic systems via control barrier certificates," *IEEE Transactions on Automatic Control*, pp. 1–1, 2020.
23. J. Coulson, J. Lygeros, and F. Dorfler, "Distributionally robust chance constrained data-enabled predictive control," *IEEE Transactions on Automatic Control*, 2021.
24. J. Berberich, J. Köhler, M. A. Müller, and F. Allgower, "Data-driven model predictive control with stability and robustness guarantees," *IEEE Transactions on Automatic Control*, 2020.
25. P. Tabuada and L. Fraile, "Data-driven stabilization of SISO feedback linearizable systems," *arXiv preprint arXiv:2003.14240*, 2020.
26. J. Kenanian, A. Balkan, R. M. Jungers, and P. Tabuada, "Data driven stability analysis of black-box switched linear systems," *Automatica*, vol. 109, p. 108533, 2019.
27. Z. Wang and R. M. Jungers, "Data-driven computation of invariant sets of discrete time-invariant black-box systems," *arXiv:1907.12075*, 2019.
28. V. B. Wijesuriya and A. Abate, "Bayes-adaptive planning for data-efficient verification of uncertain Markov decision processes," in *International Conference on Quantitative Evaluation of Systems*. Springer, 2019, pp. 91–108.
29. S. Sadraddini and C. Belta, "Formal guarantees in data-driven model identification and control synthesis," in *Proceedings of the 21st International Conference on Hybrid Systems: Computation and Control (part of CPS Week)*, 2018, pp. 147–156.
30. A. Salamati, S. Soudjani, and M. Zamani, "Data-driven verification under signal temporal logic constraints," *21st IFAC World Congress*, 2020.
31. A. Robey, H. Hu, L. Lindemann, H. Zhang, D. V. Dimarogonas, S. Tu, and N. Matni, "Learning control barrier functions from expert demonstrations," in *2020 59th IEEE Conference on Decision and Control (CDC)*. IEEE, 2020, pp. 3717–3724.
32. S. Han, U. Topcu, and G. J. Pappas, "A sublinear algorithm for barrier-certificate-based data-driven model validation of dynamical systems," in *54th IEEE conference on decision and control (CDC)*, 2015, pp. 2049–2054.
33. P. Jagtap, G. J. Pappas, and M. Zamani, "Control barrier functions for unknown nonlinear systems using gaussian processes," in *2020 59th IEEE Conference on Decision and Control (CDC)*. IEEE, 2020, pp. 3699–3704.
34. G. C. Calafiore and M. C. Campi, "The scenario approach to robust control design," *IEEE Transactions on automatic control*, vol. 51, no. 5, pp. 742–753, 2006.
35. T. Kanamori and A. Takeda, "Worst-case violation of sampled convex programs for optimization with uncertainty," *Journal of Optimization Theory and Applications*, vol. 152, no. 1, pp. 171–197, 2012.
36. P. M. Esfahani, T. Sutter, and J. Lygeros, "Performance bounds for the scenario approach and an extension to a class of non-convex programs," *IEEE Transactions on Automatic Control*, vol. 60, no. 1, pp. 46–58, 2014.
37. A. Salamati, A. Lavaei, S. Soudjani, and M. Zamani, "Data-driven safety verification of stochastic systems," *7th IFAC Conference on Analysis and Design of Hybrid Systems*, 2021.
38. M. Hernández, "Chebyshev's approximation algorithms and applications," *Computers & Mathematics with Applications*, vol. 41, no. 3-4, pp. 433–445, 2001.
39. S. Soudjani and R. Majumdar, "Concentration of measure for chance-constrained optimization," *IFAC-PapersOnLine*, vol. 51, no. 16, pp. 277–282, 2018.
40. H. J. Kushner, "Stochastic stability and control," Brown Univ Providence RI, Tech. Rep., 1967.
41. M. Zamani and M. Arcaç, "Compositional abstraction for networks of control systems: A dissipativity approach," *IEEE Trans. Control Network Syst.*, vol. 5, no. 3, pp. 1003–1015, 2018.

42. A. Swikir and M. Zamani, “Compositional synthesis of symbolic models for networks of switched systems,” *IEEE Control Syst. Lett.*, vol. 3, no. 4, pp. 1056–1061, 2019.
43. A. Girard, G. Gössler, and S. Mouelhi, “Safety controller synthesis for incrementally stable switched systems using multiscale symbolic models,” *IEEE Transactions on Automatic Control*, vol. 61, no. 6, pp. 1537–1549, 2016.
44. V. der Automobilindustrie, “Lane keeping assist systems,” <https://www.vda.de/en/topics/safety-and-standards/lkas/lane-keeping-assist-systems.html>, 2020.
45. M. Althoff, M. Koschi, and S. Manzinger, “Commonroad: Composable benchmarks for motion planning on roads,” in *2017 IEEE Intelligent Vehicles Symposium (IV)*. IEEE, 2017, pp. 719–726.