Data-driven Estimation of Forward Reachable Sets

Alex Devonport

Murat Arcak

alex_devonport@berkeley.edu

arcak@berkeley.edu

University of California, Berkeley

Berkeley, California

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1 INTRODUCTION

The computation of reachable sets is an effective way to characterize and verify the behavior of safety-critical cyber-physical systems. However, many systems of practical interest possess high-dimensional, analytically intractable, and possibly unknown dynamics, which make the computation of safe sets with formal guarantees difficult or impossible. In these cases we can employ a data-driven approach to reachability analysis instead. The data-driven approach uses a finite ensemble of sample trajectories to compute reachable set estimates which are guaranteed to achieve high accuracy in a probabilistic sense.

Unlike earlier results on data-driven reachability which incorporate data-driven elements into existing reachability approaches, e.g. [2, 5], we obtain an estimate directly from data, thus eliminating intermediate steps that may introduce conservatism, and reducing the number of assumptions imposed on the system. In addition to being applicable to any system which admits simulation, data-driven reachability is computationally straightforward: computation is typically dominated by an *a priori* known number of trajectory simulations which can be done in parallel.

We present two approaches to data-driven forward reachability analysis. The first approach uses the tools of scenario optimization to construct reachable set estimates as approximate solutions to chance-constrained optimization problems. The scenario approach can be applied to a range of estimator geometries, of which we examine p -norm balls as a special case. The second approach uses a class of polynomials derived from empirical moment matrices, whose sublevel sets act as non-convex estimates of the reachable set.

2 PROBLEM FORMULATION

We consider a general dynamical system with state transition function $\Phi : X_0 \times \mathcal{D} \rightarrow \mathbb{R}^n$ defined on an initial set $X_0 \subseteq \mathbb{R}^n$ and a set of disturbances $\mathcal{D}$ comprising disturbance signals $d : [t_0, t_1] \rightarrow \mathbb{R}^w$. We assume, if the system has inputs, that a control policy has been selected, yielding an autonomous system subject to a disturbance made up of a combination of control deviation and exogenous disturbances.

The object of forward reachability analysis is to approximate *forward reachable set*

$$R_{[t_0, t_1]} = \{\Phi(t_f; t_0, x_0, u, d) : x_0 \in X_0, u \in \mathcal{U}, d \in \mathcal{D}\},$$

that is the set of all states to which the system can transition in the time range $[t_0, t_f]$ with initial states in X_0 , inputs in $\mathcal{U}$, and disturbances in $\mathcal{D}$.

To estimate the reachable set by statistical means, we introduce probabilistic structure to the problem in the form of random variables X_0 and D defined on X_0 and $\mathcal{D}$ respectively. These, random variables in turn induce a random variable $X_1 = \Phi(X_0, D)$ on the reachable set. Let P_{X_1} denote the probability measure corresponding to X_1 . Since $P_{X_1}(R_{[t_0, t_1]}) = 1$ and $P(A) = 0$ for any set disjoint from $R_{[t_0, t_1]}$, $P_{X_1}(A)$ acts as a probabilistic measure of how well a set A acts as an approximation of $R_{[t_0, t_1]}$. With this in mind, we formulate the probabilistic version of the forward reachability problem as follows:

PROBLEM 1. *Given the transition function Φ , the random variables X_0 and D , and an accuracy level $\epsilon \in (0, 1)$, compute a compact set $\hat{R}_{[t_0, t_1]}$ such that $P_{X_1}(\hat{R}_{[t_0, t_1]}) \geq 1 - \epsilon$.*

To reduce the conservatism of the approximation, we also typically include some regularization on the volume of $\hat{R}_{[t_0, t_1]}$.

Note that, while X_0 and D may be chosen to model stochastic elements in the system, it is not necessary to do so. Indeed, the system need not be stochastic: in this case X_0 and D may be viewed as *instrumental distributions* that provide a consistent rule for collecting data from the system.

3 BOUNDING THE PROBABILISTIC ERROR

In this problem formulation, we assume that the transition function Φ is unknown: information about Φ is available only through samples $X_1^{(i)} = \Phi(x_0^{(i)}, d^{(i)})$, $i = 1, \dots, N$, where the $x_0^{(i)}$ and $d^{(i)}$ are independent and identically distributed samples from X_0 and D respectively. Our goal is to compute a set $\hat{R}_{[t_0, t_1]}$ that solves Problem 1 using only the samples $x_1^{(1)}, \dots, x_1^{(N)}$.

Since Φ is not known, it is not possible to verify that a set $\hat{R}_{[t_0, t_1]}$ solves Problem 1 by directly evaluating $P_{X_1}(\hat{R}_{[t_0, t_1]})$. We instead

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use the data $x_1^{(1)}, \dots, x_1^{(N)}$ to compute a probabilistic lower bound on $P_{X_1}(\hat{R}_{[t_0, t_1]})$ of the form

$$P_{x_1^{(1)}, \dots, x_1^{(N)}}(\hat{P}(\hat{R}_{[t_0, t_1]}) - P_{X_1}(\hat{R}_{[t_0, t_1]}) \leq \epsilon) \geq 1 - \delta, \quad (1)$$

where $\hat{P}(\hat{R}_{[t_0, t_1]}) = \sum_{i=1}^N \mathbb{1}\{x_1^{(i)} \in \hat{R}_{[t_0, t_1]}\}$ is the empirical accuracy. The bound (1) is known as a “Probably Approximately Correct” (PAC) bound: it ensures that, with probability $1 - \delta$ with respect to the samples $x_1^{(1)}, \dots, x_1^{(N)}$, the empirical accuracy approximates the true accuracy $P_{X_1}(\hat{R}_{[t_0, t_1]})$ with an error no greater than ϵ . There are several ways to derive PAC bounds for statistical estimators: we consider two approaches, one based on scenario optimization, and another which bounds the Vapnik-Chervonenkis (VC) dimension of a class of polynomial sublevel sets.

3.1 Scenario Optimization

Scenario optimization is a technique to approximately solve chance-constrained convex optimization problems, i.e. programs of the form

$$\begin{aligned} & \underset{\theta}{\text{minimize}} && J(\theta) \\ & \text{subject to} && P_Z(g(\theta, Z) \leq 0) \geq 1 - \epsilon \\ & && \theta \in \Theta, \end{aligned} \quad (2)$$

where P_Z is a probability measure corresponding to a random variable Z , $\Theta \in \mathbb{R}^{n_\theta}$ is convex and compact, and J and g are compact with respect to θ . Importantly, no restrictions are made on the random variable Z , and g need not be convex with respect to Z . Problems of this form arise in many areas of the areas of control that intersect with probability, such as collision avoidance [6] and model-predictive control [3].

Under certain conditions, the search for a solution to Problem 1 can be encoded as a program of the form (2). Specifically, consider reachable set approximations of the form $\hat{R}_{[t_0, t_1]}(\theta) = \{x \in \mathbb{R}^n : g(\theta, x) \leq 1\}$, where g is a convex function of θ , and let $\text{Vol}(\theta)$ be a convex proxy for the volume of $\hat{R}_{[t_0, t_1]}(\theta)$. Then a feasible solution θ to the program

$$\begin{aligned} & \underset{\theta}{\text{minimize}} && \text{Vol}(\theta) \\ & \text{subject to} && P_{X_1}(g(\theta, X_1) \leq 1) \geq 1 - \epsilon \\ & && \theta \in \Theta, \end{aligned} \quad (3)$$

yields a set $\hat{R}_{[t_0, t_1]}(\theta)$ which solves Problem 1.

Directly computing a solution to (3) is typically impossible, since P_{X_1} is not known. The method of *scenario optimization* replaces the probabilistic constraint $P_{X_1}(g(\theta, X_1) \leq 1) \geq 1 - \epsilon$ with the data-driven constraints $g(\theta, x_1^{(i)}) \leq 1$, $i = 1, \dots, N$, transforming the problem into an ordinary convex program. The solution $\hat{\theta}$ of this data-driven relaxation is guaranteed with probability $1 - \delta$ to be a feasible solution of (3) when the sample size N satisfies the lower bound

$$N \geq \frac{1}{\epsilon} \left(\frac{e}{e-1} \right) \left(\log \frac{1}{\delta} + n_\theta \right), \quad (4)$$

where e is the base of the natural logarithm, yielding a PAC bound of the form (1) for the reachable set estimate $\hat{R}_{[t_0, t_1]}(\hat{\theta})$.

As a concrete example of the scenario approach, consider the case where $g(x, A, b) = \|Ax - b\|_p$, where $A > 0$ and $p \geq 1$: the

reachable set approximations $\hat{R}_{[t_0, t_1]}(A, b)$ take the form of p -norm balls, for which $\text{Vol}(A, b) = -\log \det A$ acts as the volume proxy. Since A is a symmetric $n \times n$ matrix, we have $n_\theta = O(n^2)$, so the number of samples required to ensure the probabilistic accuracy of the norm ball reachable set estimate scales quadratically with the state dimension.

3.2 Christoffel Functions

We next consider reachable set estimates constructed as sublevel sets of a class of positive polynomials called empirical inverse Christoffel functions. These polynomials, and the Christoffel functions from which they are derived, are known empirically to provide good estimates of the support of random variables, and have been used in data-driven novelty detection applications [1, 4]. We show that Christoffel function-based estimates are also suitable for solving Problem 1 by deriving a PAC bound.

Given data $x_1^{(1)}, \dots, x_1^{(N)}$, the empirical inverse Christoffel function is

$$C(x) = z_k(x)^\top \left(\frac{1}{N} \sum_{i=1}^N z_k(x_1^{(i)}) z_k(x_1^{(i)})^\top \right)^{-1} z_k(x),$$

where $z_k(x)$ is the vector of monomials in n variables of degree $\leq k$ evaluated at the point x . In the Christoffel function approach, we take a sublevel set of $C(x)$ to be the reachable set estimate, namely $\hat{R}_{[t_0, t_1]} = \{x \in \mathbb{R}^n : C(x) \leq \alpha\}$, where $\alpha = \max_i C(x_1^{(i)})$. A PAC bound of the form (1) holds for this estimate for sample sizes

$$N \geq \frac{5}{\epsilon} \left(\log \frac{4}{\delta} + \binom{n+d}{n} \log \frac{40}{\epsilon} \right), \quad (5)$$

ensuring that the Christoffel function approach can solve Problem 1 with high probability with a finite sample size.

4 CONCLUSION

In addition to being useful in optimization and statistics, the techniques described in Sections 3.1 and 3.2 can also be used as tools to provide principled and computationally straightforward data-driven solutions to control-theoretic problems such as forward reachability analysis. Common to both methods is a tradeoff between estimate geometry and computational difficulty, which is made explicit by sample size bounds such as (4) and (5).

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