NExG: Provable and Guided State Space Exploration of Neural Network Control Systems using Sensitivity Approximation

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Abstract—We propose a new technique for performing state space exploration of closed loop control systems with neural network feedback controllers. Our approach involves approximating the sensitivity of the trajectories of the closed loop dynamics. Using such an approximator and the system simulator, we present a guided state space exploration method that can generate trajectories visiting the neighborhood of a target state at a specified time. We present a theoretical framework which establishes that our method will produce a sequence of trajectories that will reach a suitable neighborhood of the target state. We provide thorough evaluation of our approach on various systems with neural network feedback controllers of different configurations. We outperform earlier state space exploration techniques and achieve significant improvement in both the quality (explainability) and performance (convergence rate). Finally, we adopt our algorithm for the falsification of a class of temporal logic specification, assess its performance, and show its potential in supplementing existing falsification algorithms.

Index Terms—Closed loop control systems, neural networks, sensitivity function, state space exploration, falsification.

I. INTRODUCTION

Design and verification of closed loop systems has become an increasingly challenging task. First, advances in hardware and software have made it easier to integrate sophisticated control algorithms in embedded systems. Second, control designers now often integrate multiple technologies and satisfy ever increasing behavioral specifications expected from complex Cyber-physical systems (CPS). Third, the non-linearity in the behaviors of the closed loop systems makes it difficult to predict the outcomes of perturbations in the state or the environment. Control design for linear systems typically involves techniques such as pole placement and computing Lyapunov functions. However, such analytical method usually do not scale well to hybrid or non-linear systems encountered in real world applications. Therefore, we have witnessed a surge in neural network based control design in recent times [38], [53]. But despite its desired utility, neural network controller, due to its characteristics and behavior, adds to the complexity of the underlying system thus making it more difficult to perform safety analysis.

In a typical work flow, the control designer designs a control algorithm and generates a few test cases to check if the specification is satisfied or violated. However, because of the increasing system complexity, these test cases often do not generalize to the system behavior at large. This is especially difficult if one has to consider all possible inter leavings of the continuous and discrete behaviors encountered by a modern CPS. Due to different sequence of mode changes, two neighboring states can potentially have divergent trajectories, thus extrapolating the behavior from one state to another becomes challenging. The problem is further exacerbated by sophisticated neural network based control algorithms. Since such neural network controllers are typically learned from a finite number of samples, a designer needs to perform additional checks for controller’s behavior outside the test suite. However, such manual validation is not practically feasible.

In some instances, the specification is mathematically expressed as a temporal logic formula that is used by an off-the-shelf falsification tool for automatically generating a trajectory that violates the specification. But such an approach has a few drawbacks. Falsification tools are primarily geared towards finding a violating trace for the given specification, not necessarily to help the designer in systematically exploring the state space. Moreover, the search for a counterexample is performed using stochastic optimization and gradient descent methods. The optimization engine generates random trajectories which would not yield much intuition for the designer about two neighboring behaviors. Second, if the control designer changes the specification during testing, the results from the previous runs may no longer be useful. Third, existing falsification tools require the specification to be provided in a temporal logic such as signal temporal logic or metric temporal logic (STL/MTL). The designer needs to understand these specification languages which despite being useful in the verification phase, may cause hindrance during the design and exploration phases.

State space exploration entails systematically generating trajectories to explore desired (or undesired) outcomes of the system. For example, for a given safety specification, a designer might like to generate test cases that are close to satisfying or violating the specification. Existing falsification tools are neither capable of obtaining such executions nor informing the control designer about the additional tests to conduct for validating safety, measuring coverage or exploring new regions. Although NeuralExplorer [29] alleviates some of these concerns by enabling the control designer to perform
systematic state space exploration, it suffers from high training time, and it lacks convergence to the true solution as well as a theoretical analysis.

In this paper, we present a technique that uses neural network approximations of sensitivity over small ranges to perform state space exploration of closed loop systems with neural network feedback controllers. The sensitivity of a closed loop system at an initial state measures the change in the system trajectory as a result of perturbing the initial state. Sensitivity can help the designer in developing an intuition about the convergence and divergence of system behaviors. Consequently, the designer can take an active role in systematically navigating the space of new test cases during control design. Thus instead of generating executions using a stochastic optimization solver for falsification, our approach explores the state space in a more systematic manner. As a result, it takes less number of iterations to generate desirable executions as illustrated in Figure 1.

Since our framework only requires system traces, it is generalizable to black-box systems in the absence of precise analytical models. Similar to other simulation driven analyses, our technique also depends on using system simulations to tap key information or properties about the system. Further, the motivation behind employing neural networks is not only driven by their power to approximate complex functions but also because hardware and software advancements have made these neural networks easy to train and deploy. We believe that such automated state space exploration is not only useful in man-machine collaborative test case generation, but also for designing safe neural network feedback functions for closed loop control systems.

This paper makes multiple contributions. (i) It presents a new state space exploration algorithm NExG, which is an extension of NeuralExplorer [29] for inverse sensitivity learned over small perturbations. (ii) It provides theoretical guarantees supported by empirical results. The paper demonstrates that NExG will converge to a neighborhood of the target point even if the learned neural network only approximates the inverse sensitivity function, and it performs much better than NeuralExplorer while requiring less computational resources. (iii) It performs extensive evaluation on 20 standard nonlinear benchmarks with up-to 6 dimensions state spaces having neural network feedback controller with multiple layers. (iv) It presents a simple inverse sensitivity based falsification algorithm for a class of temporal logic safety specifications. The evaluations exhibit that the presented falsification scheme is capable of finding a more robust falsifying trajectory in significantly less number of iterations as compared to a widely used falsification tool S-TaLiRo [4]. (v) Finally, it presents additional features of the framework such as computing set coverage and customized state space exploration.

II. RELATED WORK

Verification or Reachability analysis is typically aimed at verifying safety specification(s) of the safety critical control system. Some of the notable works in this domain are SpaceEx [23], Flow* [8], CORA [2] and HyLAA [5]. These tools use different symbolic representations such as support functions, generalized star etc. for the set of reachable states. While these techniques are useful for proving that the safety specification is satisfied, some other recent works [25], [26], [28] have explored using reachability analysis to generate counterexamples of interest.

Falsification is employed to generate executions that violate a given safety specification [15], [29] instead of proving safety. In these techniques, the required specification is expressed as a formula in temporal logic such as Metric Temporal Logic (MTL) [36] or Signal Temporal Logic (STL) [37], [42]. For a given temporal logic specification, falsification techniques use various heuristics [1], [12], [24], [46], [49], [57] in an attempt to generate trajectories that violate the specification. Two well known falsification tools are S-TaLiRo [4] and Breach [13]. Another work [6] uses symbolic reachability supplemented by trajectory splicing to scale up hybrid system falsification.

Simulation based state space exploration [10], [14] and verification [16], [21], [32] have also shown some promise by taking the advantages of symbolic and analytical techniques. Such methods either use bounds on sensitivity [21], [32] to obtain an overapproximation of the reachable set or require analytical model to perform random exploration of the state space [10]. While these techniques can bridge the gap between falsification and verification, they might still suffer due to high system dimensionality and complexity. That is, the number of required trajectories may increase exponentially with system dynamics and dimensions. C2E2 [17], and DryVR [22] are some of the well known tools in this domain.
Given the rich history of application of neural networks in control [39], [44], [45] and the recent advances in software and hardware platforms, neural networks are now being deployed in various control tasks. Consequently, many verification techniques are being developed for neural network based control systems [18], [33], [51], [54], [56] and some other domains [31], [52]. Many neural network based frameworks for learning the dynamics or their properties have been also proposed in recent times [4], [50], [48], which further underlines the need of an efficient state space exploration.

In the model checking domain, neural networks have been used for state classification [47] as well as reachability analysis by learning state density distribution [43] or reachability function in NeuReach [50]. In contrast, NExG learns sensitivity functions and is geared towards state space exploration. While NeuralExplorer [29] also learns the sensitivity functions, NExG approximates the sensitivity of closed loop control functions and is geared towards state space exploration. While NeuReach [50] uses numerical ODE solvers which generate trajectories, one of the distinguishing features of NExG is that we provide theoretical approximation error and the number of simulations generated.

Two parameters, scaling factor and correction period, are introduced in NExG to maintain the trade off between approximation error and the number of simulations generated. Another distinguishing feature is that we provide theoretical guarantees for NExG for its convergence.

III. Preliminaries

The state of the system is an element typically denoted as \( x \equiv (x_1, \ldots, x_n) \in \mathbb{R}^n \). For \( v \in \mathbb{R}^n \), let \( \|v\| \) denote the standard Euclidean norm of the vector \( v \). For \( \delta \geq 0 \), \( B_\delta(x) \equiv \{ x' \in \mathbb{R}^n | \| x - x' \| \leq \delta \} \) is the closed neighborhood around \( x \) of radius \( \delta \). We will denote the state space of the system by \( \mathbb{D} \subseteq \mathbb{R}^n \), and the dynamics of the plant as

\[
\dot{x} = f(x, u)
\]

where \( x \in \mathbb{D} \) is the state of the system and \( u \in \mathbb{R}^n \) is the input. A closed loop system is a control system where the process or the system is regulated by a feedback control action which is automatically computed as a function of system output. Suppose we use a feedback-function (also called a controller) \( g \) that is regulated by the system output, i.e. \( u = g(x) \), then have a closed loop system that satisfies

\[
\dot{x} = f(x, g(x)).
\]

We will assume that \( f \) and \( g \) are such that (1) has a unique solution \( x : \mathbb{R} \rightarrow \mathbb{D} \) satisfying \( x(0) = x_0 \) for every \( x_0 \in \mathbb{D} \). For example, by existence and uniqueness theorem for differential equations, this condition is guaranteed if \( \mathbb{D} = \mathbb{R}^n \) and both \( f \) and \( g \) are Lipschitz functions of their inputs.

Definition 1. Let \( \xi(x_0, \cdot) : [0, \infty) \rightarrow \mathbb{D} \) denote the system trajectory starting from the initial point \( x_0 \in \mathbb{D} \). In other words, \( x(t) = \xi(x_0, t) \) satisfies (1) with \( x(0) = x_0 \) for \( t \geq 0 \). Let \( \xi^{-1}(x, \cdot) : [0, \infty) \rightarrow \mathbb{D} \) denote the backward time system trajectory starting from \( x_1 \in \mathbb{D} \), so that \( x(t) = \xi^{-1}(x_1, -t) \) is a solution to (1) with \( x(0) = x_1 \) for \( t \leq 0 \).

By the uniqueness of solution to (1), given \( x_0, x_1 \in \mathbb{D} \) and \( t > 0 \) such that \( \xi(x_0, t) = x_1 \), we have the inverse relation \( \xi^{-1}(x_1, t) = x_0 \). We now adopt the definitions of sensitivity and inverse sensitivity from [29] as shown in Figure 2.

Definition 2. Given an initial state \( x_0 \), vector \( v \), and time \( t \), the sensitivity \( \Phi(x_0, v, t) \) for the system is defined as

\[
\Phi(x_0, v, t) = \xi(x_0 + v, t) - \xi(x_0, t).
\]

We extend the definition of sensitivity to backward time trajectories, denoted by inverse sensitivity, as

\[
\Phi^{-1}(x_1, v, t) = \xi^{-1}(x_1 + v, t, t) - \xi^{-1}(x_1, t).
\]

Figure 2. Visual description of the sensitivity functions \( \Phi \) and \( \Phi^{-1} \).

Informally, sensitivity is the vector difference between states starting from \( x_0 \) and \( x_0 + v \) after time \( t \); whereas, inverse sensitivity is the perturbation of the initial state required to displace the state at time \( t \) by \( v \). In this work, we will primarily focus on using the inverse sensitivity function \( \Phi^{-1} \) for performing systematic state space exploration, but an analogous analysis can also be conducted with the sensitivity function \( \Phi \).

For a smooth inverse-sensitivity function \( \Phi^{-1}(x_0, v, t) \), let \( \nabla v \Phi^{-1} \) denote its Jacobian matrix when considered a function only of its second argument \( v \). Then under smoothness assumption, we have the Taylor expansion

\[
\Phi^{-1}(x_0, v, t) = \nabla v \Phi^{-1}(x_0, 0, t)v + o(\|v\|)
\]

since \( \Phi^{-1}(x_0, 0, t) = 0 \). Therefore learning the inverse-sensitivity function for very small \( v \) is akin to learning its directional derivative in the direction \( v \).

A. Learning the inverse sensitivity function using observed trajectories

For testing the system operation on the domain \( \mathbb{D} \), one may wish to generate a finite set of trajectories. Often, these trajectories are generated using numerical ODE solvers which return system simulations sampled at a regular time step. The step size, time bound, and the number of trajectories are specified by the user. Given a sampling of a trajectory with step size \( h \), i.e., \( \xi(x_0, 0), \xi(x_0, h), \xi(x_0, 2h), \ldots, \xi(x_0, kh) \), we make a few observations. First, any prefix of this sequence is also a trajectory of a shorter duration. Hence, from a
given set of trajectories, one can truncate them to generate more trajectories having shorter duration. Second, given two trajectories starting from states \(x_0\) and \(x_0'\), we can compute the following values for the sensitivity functions:

\[
\begin{align*}
\Phi(x_0, x_0' - x_0, t) &= \xi(x_0', t) - \xi(x_0, t) = x_0' - x_t \\
\Phi^{-1}(x_t, x_t' - x_t, t) &= x_t' - x_0
\end{align*}
\]

(5) (6)

Note that we can estimate values of \(\Phi^{-1}\) based only on samples from a forward simulator \(\xi\).

Let us explain how we generate values of the function \(\Phi^{-1}(x_t, v, t)\) for small values of \(v\) in order to learn an approximator \(N_{\Phi^{-1}}(x_t, v, t)\) (or \(N_{\Phi}(x_0, v, t)\)). First, we generate a set of reference trajectories from initial states sampled uniformly at random. Then a fixed number of additional trajectories within a small neighborhood (with radius \(\|v\| \ll 1\)) of each initial state are generated. Now, we compute prefixes of the reference and its neighboring trajectories and use Equations (5) and (6) for generating tuples \((x_0, v, t, v_+)\) and \((x_t, v, t, v_-)\) such that \(v_+ = \Phi(x_0, v, t)\) and \(v_- = \Phi^{-1}(x_t, v, t)\). We use these tuples to train either a forward sensitivity approximator denoted as \(N_{\Phi}\) or an inverse sensitivity approximator \(N_{\Phi^{-1}}\). Further details on the training procedure for learning the neural networks used in this work are mentioned in Section VI-A. The training performance for various benchmark systems and neural network architectures is detailed in Section VI-A.

IV. STATE SPACE EXPLORATION USING LOCAL INVERSE SENSITIVITY APPROXIMATORS

In this section, we show how to use an inverse sensitivity approximator \(N_{\Phi^{-1}}(x_t, v, t)\) for small values of \(\|v\|\) in order to perform systematic state space exploration. State space exploration is typically aimed at finding trajectories that may satisfy or violate a given specification. We primarily concern ourselves with safety specifications where the unsafe set is specified as a convex polytopes. In this setup, we would like to find trajectories that reach the set of unsafe states at a specified time, or within a certain time interval. We begin with a sub-routine for state space exploration approach to reach a given destination. We extend this method to a set of states in a subsequent section.

A. Reaching a destination at specified time

In the course of state space exploration, the designer might want to explore the system behavior that reaches a given destination or approaches the boundary condition for safe operation. Given a domain of operation, and a sample trajectory \(\xi\), the control system designer desires to generate a trajectory that reaches a destination state \(z\) (with an error threshold of \(\delta\)) at time \(t\). Using previous notation, our goal is to find a state \(x\) such that the state \(\xi(x, t)\) lies in the \(\delta\)-neighborhood of \(z\).

A toy illustration of our the state space exploration technique with oracle access to the exact inverse sensitivity function is shown in Figure 3. Given an initial point \(x_0\), a destination \(z\), and time \(t\), we successively move the initial point in small steps in the direction specified by \(\Phi^{-1}\), so that the trajectory starting from the new initial point at time \(t\) moves closer to that target \(z\) with each step. In practice, since the exact inverse sensitivity function is unknown, we use a neural-network based approximation instead.

Formally, given an anchor trajectory starting from initial state \(x_0 \in \theta\) (typically chosen at random), we first compute the vector \(w^0 = z - x_0\) where \(x_0 = \xi(x_0, t)\). Next, we estimate the inverse sensitivity \(v_0 = N_{\Phi^{-1}}(x_0, w^0, t)\) required at \(x_0\) to move \(x_t\) towards \(z\), and then move \(x_0\) by \(\hat{v}^0\). Here, the input \(s \in (0, 1)\), called as the scaling factor, controls the magnitude of movement at each step. This process is again repeated: move the new initial state \(x_0' = x_0 + \hat{v}^0\) by the vector \(\hat{v}^1 = N_{\Phi^{-1}}(x_0', w^1, t)\), where \(w^1 = z - x_1\) and \(x_1 = \xi(x_1, t)\) is the point reached at time \(t\) by a new simulated trajectory for the system starting from initial state \(x_0'\). This process is repeated until \(x_k\) reaches a pre-specified neighborhood of \(z\).

Since \(N_{\Phi^{-1}}\) is only an approximation of \(\Phi^{-1}\), the repeated application of the former will typically compound the approximation error. Hence periodically simulating system trajectories starting from intermediate initial states – a step that we term course correction – is important to keep the exploration on track. Course correction steps not only confirm that the estimates at time \(t\) of the trajectory are indeed close to the \(z\), but they also allow our procedure to make suitable adjustments if that is not indeed the case.

Since system simulation is expensive, our framework allows for course correction to be performed as frequently as desired. The parameter \(p\) is designated as correction period because the new anchor trajectory attempts to correct the course once for every \(p\) invocations of \(N_{\Phi^{-1}}(\cdot)\). Figure 4 shows the effect of performing course corrections after every 4 steps which reduces the number of course corrections to 7 from 23 if we corrected the course at every step. Algorithm I which we call Reach Destination (abbreviated as \(RD\)), provides further details of the our procedure. After termination, algorithm

![Figure 3. Toy execution of Algorithm I](image-url)
Algorithm 1: \( \mathcal{RD} \) algorithm aims at finding a trajectory that reaches \( \delta \)-neighborhood of \( z \) at time \( t \). It estimates the inverse sensitivity at each step to perturb the initial state, generates a new simulation from perturbed state, and treats this simulation as the new anchor. \( k \) is the number of simulations generated.

\[
\begin{align*}
\text{input} & : \xi, \text{time instance: } t \leq T, \text{reference trajectory: } \xi_A, \text{destination: } z \in \mathbb{D}, \text{course corrections bound: } B, \text{function } N_{\Phi^{-1}} \text{ that approximates } \Phi^{-1}, \text{initial set: } \theta, \text{correction period: } p, \text{scaling factor: } s, \text{and threshold: } \delta. \\
\text{output} & : \text{course corrections: } k, \text{final trace: } (\xi(x_0^k, \cdot), \text{final distance: } d^k_0, \text{final relative distance: } d_r. \\
\text{0} & : x_0^0, x_t^0 \leftarrow \xi_A(0), \xi_A(t) ; \quad \text{// states at time 0 and } t \\
\text{1} & : w^0 \leftarrow z - x_0^0 ; \quad \text{// initial vector difference with } z \\
\text{2} & : d_{\text{init}} \leftarrow d_a \leftarrow \|w^0\| ; \quad \text{// initial distance} \\
\text{3} & : k \leftarrow 0; \\
\text{4} & : \text{while } (d_{\text{init}}^k > \delta) \& (k < B) \text{ do} \\
\text{5} & : \text{for } 1 \leq j \leq p \text{ do} \\
\text{6} & : \tilde{x}_j^k \leftarrow \Phi^{-1}(x_j^k, v^k, t) ; \quad \text{// predict } v^k \\
\text{7} & : \tilde{x}_j^k \leftarrow \xi(x_j^0 + \tilde{x}_j^k) ; \quad \text{// perturb } x_j^0 \\
\text{8} & : \hat{\xi}_j^k \leftarrow x_j^k + \hat{v}_j^k ; \quad \text{// progress } x_j^k \\
\text{9} & : \text{end} \\
\text{10} & : \hat{\xi}_j^k \leftarrow \hat{\xi}_j^k(t) ; \quad \text{// course correction} \\
\text{11} & : \xi_{k+1}^j \leftarrow \xi(x_j^0, \xi^k + 1) ; \quad \text{// new anchor} \\
\text{12} & : \xi_{k+1}^j \leftarrow \xi_{k+1}^j(t) ; \quad \text{// course correction} \\
\text{13} & : \xi_{k+1}^j \leftarrow x_{k+1}^j = x_{k+1}^j(t) ; \quad \text{// course correction} \\
\text{14} & : \text{end} \\
\text{15} & : \text{for } k = 0 \rightarrow k + 1 ; \quad \text{// increment corrections by 1} \\
\text{16} & : \text{end} \\
\text{17} & : \text{end} \\
\text{18} & : d_a^k \leftarrow d_a^k/d_{\text{init}} ; \quad \text{// update relative distance} \\
\text{19} & : \text{return } (k, \hat{\xi}_A, d^k_0, d_r); \\
\end{align*}
\]

Limiting the number of simulated trajectories also makes the exploration algorithm more user-friendly by saving time. Thus, we choose the number of course corrections as the primary metric for performance evaluation.

V. Theoretical Analysis of the Convergence of ReachDestination

We now discuss the convergence of Algorithm 1. As seen in Figure 3, the distance between \( x_t^k \) and the target \( z \) contracts by a factor of \( 0 < 1 - sp < 1 \) in each iteration if the exact inverse sensitivity is used. That is,

\[
\|x_t^k - z\| \leq (1 - sp)^k \|x_0^0 - z\| 
\]

Hence, the generated trajectory will reach the desired destination within an error of \( \delta \) after \( k^* \) iterations where,

\[
k^* = \left\lceil \frac{\log(\|x_0^0 - z\|/\delta)}{-\log(1 - sp)} \right\rceil.
\]

However, in the \( \mathcal{RD} \) algorithm, instead of the exact inverse sensitivity function, we only use its approximation. In this section, we show that it is possible to achieve a similar geometric rate of convergence even with an approximation. Note however that the convergence of \( \mathcal{RD} \) can fail badly in cases when the system is chaotic or the approximation error is large. To this end, we now make assumptions on the regularity of the system and the magnitude of the approximation error that will allow for performance guarantees for \( \mathcal{RD} \).

Assumption 1. Suppose there are functions \( \eta_1, \eta_2 : [0, T) \rightarrow [0, \infty) \) so that

\[
\eta_1(t)\|x - x'\| \leq \|\xi(x, t) - \xi(x', t)\| \leq \eta_2(t)\|x - x'\| \quad \text{for each } x, x' \in \mathbb{D} \text{ and } t \in [0, T].
\]

The functions \( \eta_1 \) and \( \eta_2 \), sometimes called as witnesses to the discrepancy function [16], provide worst-case bounds on how much the distance between trajectories expand or contract starting from different initial states. These functions (and their ratios) can be considered as a measure of the regularity of the system. Although in practice it may be hard to obtain the values \( \eta_1 \) and \( \eta_2 \) for the system at hand, exponential lower bound for \( \eta_1 \) and a similar upper bound for \( \eta_2 \) can be obtained using Grönwall’s inequality under a Lipschitz continuity assumption on the vector field. As shown in the following lemma, Assumption 1 also ensures that \( \Phi^{-1}(x, v, t) \) is a Lipschitz function of its inputs \( x \) and \( v \). This is important as such functions can be approximated by Neural networks of bounded depth (see e.g. [30, Theorem 4.5]).

Lemma 1. If Assumption 1 is satisfied then for any \( t \in [0, T] \)

\[
\|\Phi^{-1}(z', v', t) - \Phi^{-1}(z, v, t)\| \leq 2\|z - z'\| + \|v - v'\| / \eta_1(t)
\]

Proof. By taking \( (x, x') = (\xi^{-1}(y, t), \xi^{-1}(y', t)) \) in Assumption 1 note that \( \|\xi^{-1}(y, t) - \xi^{-1}(y', t)\| \leq \|y - y'\| / \eta_1(t) \) for any \( y, y' \in \mathbb{D} \). The Lemma now follows by suitably applying triangle inequality and the definition of \( \Phi^{-1} \).

In general, we will use the following model to measure the approximation error of \( N_{\Phi^{-1}} \). The separate roles played by
the relative error $\varepsilon_{rel}$ and the absolute error $\varepsilon_{abs}$ will become more clear in the context of Theorem 1.

**Definition 3.** $N_{a-1}$ is called an $(\varepsilon_{rel}, \varepsilon_{abs})$-approximator of $\Phi^{-1}$ up to radius $r$ and time $T$ if

$$\|N_{a-1}(x_t, v, t) - \Phi^{-1}(x_t, v, t)\| \leq \varepsilon_{rel}\|\Phi^{-1}(x_t, v, t)\| + \varepsilon_{abs}$$

for any $x_t \in \mathbb{D}$, $t \in [0, T]$ and $v \in \mathbb{R}^n$, with $\|v\| \leq r$.

We are now ready state Theorem 1 which bounds the distance between $z$ and iterate $x^k_t$ in the 4th iterations of the outer loop in $\mathcal{RD}$ when the system satisfies Assumption 1 and $N_{a-1}$ satisfies Definition 3 with sufficiently small error terms ($\varepsilon_{rel}, \varepsilon_{abs}$). To further interpret Theorem 1 note that:

1. When the additive error $\varepsilon_{abs} \approx 0$ is negligible and the relative error satisfies $\varepsilon_{rel} \in [0, \eta_1(t)\eta_2(t)^{-1}]$, Equation \ref{eqn:main} holds for any $k \in \mathbb{N}$ with $r(x)/s \approx 0$. Hence, in this case, a geometric convergence similar to that described for the toy example from above continues to hold with a slightly slower convergence rate (i.e., $-\log(1 - sp\gamma(t))$ instead of $-\log(1 - sp)$).

2. On the other hand, when $\varepsilon_{abs}$ is non-negligible (but sufficiently small so that $r(x)/s \leq r$), the last term in Equation \ref{eqn:main} cannot be ignored. In this case, if the rest of the assumptions of Theorem 1 are also satisfied, one obtains the guarantee that $\lim_{k \to \infty} d_k(k) \leq r(x)/s$. Hence if $r(x)/s < \delta$, the termination condition $x^k_t \in B_3(z)$ will eventually be satisfied whenever $k > k^* = \left\lfloor \log(\frac{r(x)/s}{\delta}) \right\rfloor / \log(1- \varepsilon_{rel}(t))$.

**Theorem 1 (Convergence of $\mathcal{RD}$).** Fix the domain $\mathbb{D} = \mathbb{R}^d$ and a time $T > 0$. Suppose

1. The system $\xi$ satisfies Assumption 1.
2. $N_{a-1}$ is an $(\varepsilon_{rel}, \varepsilon_{abs})$-approximation of $\Phi^{-1}$ for radius $r$ and time $T$, and
3. $\varepsilon_{rel}, \varepsilon_{abs} \geq 0$ values small enough so that for each $t \in [0, T]$, $\gamma(t) = 1 - \varepsilon_{rel}(t)\eta_2(t)^{-1} > 0$ and $r(x) = \varepsilon_{abs}(t)\eta_2(t)/\gamma(t) \leq r$.

Suppose the inputs $\theta \in \mathbb{D}$, $t \in [0, T]$, the correction period $p$ and the destination $z \in \mathbb{D}$ to Algorithm 1 are given and the scaling factor satisfies $s \in [r(x)/d_{init}, \min(r/d_{init}, 1/p)]$, where $d_{init} = \|x^0_0 - z\|$ and the destination $z$. Then the distance after $k$ iterations of the outer loop in Algorithm 1 satisfies the following bound

$$\|x^k_t - z\| \leq (1 - sp\gamma(t))^k d_{init} + \frac{r(x)}{s}$$

for any $k \in \mathbb{N}$.

The proof of Theorem 1 can be seen to be a plausible contraction argument. Formal details are given below.

**Proof of Theorem 1** In this proof, for mathematical clarity, we slightly change the notation for the variables used in Algorithm 1. For each $k \geq 0$, let $x_0(k), x_t(k), w(k) \text{ and } d_a(k)$ denote the values of the variables $x_0(k), x_t(k), w(k)$ and $d_a(k)$ after $k$ executions of the outer loop in Algorithm 1. Hence the equalities $w(k) = z - x_t(k), d(k) = \|w(k)\|$, and $x_t(k) = \xi(x_0(k), t)$ are satisfied for any $k \geq 0$.

Since $\theta = \mathbb{D}$, unwinding the inner loop in Algorithm 1 note

$$x_0(k + 1) = x_0(k) + \sum_{i=1}^p N_{a-1}(x_i(k) + (l - 1)s_w(w(k), sw(k), t)).$$

Let $\tilde{y}(k) = x_t(k) - x_t(k)$ denote the increment between the trajectory end points between the $k$ and $(k+1)$th iteration. Using the fact that $x_t(k) = \xi(x_0(k), t)$, note

$$\tilde{y}(k) = \xi(x_0(k), t) - \xi(x_0(k), t).$$

The quantity $\tilde{y}(k)$ approximates the true target increment given by

$$y(k) = \xi(x_0(k) + \xi^{-1}(x_t(k), sw(k), t) - \xi^{-1}(x_t(k), t) - \xi(x_0(k), t)$$

which, using Definition 3 of $\Phi^{-1}$, satisfies

$$y(k) = \xi(x_0(k) + \xi^{-1}(x_t(k), sw(k), t) - \xi^{-1}(x_t(k), t) - \xi(x_0(k), t) - x_t(k)$$

$$= x_t(k) + sw(k) - x_t(k).$$

(12)

Subtracting (13) from (12), and using the upper bound from (9)

$$\|\tilde{y}(k) - y(k)\| = \|\xi(x_0(k) + 1), t) - \xi(x_0(k) + \Phi^{-1}(x_t(k), sw(k), t)\|$$

$$\leq \eta_2(t)\|\xi(x_0(k) + 1) - x_t(k) - \Phi^{-1}(x_t(k), sw(k), t)\|$$

$$= \eta_2(t)\|\sum_{i=1}^p N_{a-1}(x_i(k) + (l - 1)s_w(w(k), sw(k), t)$$

$$- \Phi^{-1}(x_t(k), t)\|$$

$$\leq \eta_2(t)\max_{i=1,...,p} N_{a-1}(x_i(k) + (l - 1)s_w(w(k), sw(k), t)$$

$$- \Phi^{-1}(x_t(k), t).$$

(14)

where the equality is the third line is obtained by using (11) and rewriting $\Phi^{-1}(x_t(k), sw(k), t)$ as a telescoping sum. To bound the terms under the maximum in (15), we now use that $N_{a-1}$ is an $(\varepsilon_{rel}, \varepsilon_{abs})$-approximator of $\Phi^{-1}$.

By an application of Definition 3 followed by the lower bound in (9), we obtain

$$\|N_{a-1}(x, v, t) - \Phi^{-1}(x, v, t)\| \leq \varepsilon_{abs}\|\Phi^{-1}(x, v, t)\| + \varepsilon_{abs}$$

$$\leq \varepsilon_{abs}\|\xi^{-1}(x, t)\| + \varepsilon_{abs}$$

(16)

as long as $x \in \mathbb{D}$, $\|v\| \leq r$ and $t \in [0, T]$. Our assumptions imply that $sd_{init} \leq r$. Hence, whenever $\|w(k)\| \leq d_{init}$, we have

$$\|\tilde{y}(k) - y(k)\| \leq sp\|w(k)\|\varepsilon_{rel}(t)\|\xi^{-1}(t)\|^{-1} + \varepsilon_{abs}$$

(17)

We will now use the above estimate to obtain a contraction-like argument. From Equation (14) we have

$$w(k + 1) - w(k) = -x_t(k + 1) + x(k) = -\tilde{y}(k) - y(k) - \tilde{y}(k) = -sw(k) + y(k) - \tilde{y}(k).$$

Note $\|w(k)\| = \|z - x_t(k)\| = d_a(k)$, Combining the above display with Equation (17) establishes the following recursive inequality for $d_a(k)$ whenever $d_a(k) \leq d_{init}$:

$$d_a(k + 1) = \|w(k + 1)\| = \|[(1 - sp)w(k) + y(k) - \tilde{y}(k)]$$

$$\leq (1 - sp)|w(k)| + \|y(k) - \tilde{y}(k)\|$$

$$\leq (1 - sp)(1 - \varepsilon_{rel}(t))^{-1}d_a(k) + \varepsilon_{rel}(t)\varepsilon_{abs}$$

$$= (1 - sp\varepsilon_{rel}(t))d_a(k) + \varepsilon_{rel}(t)\varepsilon_{abs}$$

(18)

where we have used the assumption $sp \leq 1$ in second line, (17) in the third line, and $\gamma_2(t) = 1 - \varepsilon_{rel}(t)\|\xi^{-1}(t)\|^{-1}$ in the fourth line. From the assumed lower bound on $s$, we have $\varepsilon_{rel}(t)\varepsilon_{abs} \leq sp\gamma(t)d_{init}$, and the hence the condition
\( d_k \leq d_{init} \) continues to hold for each \( k \in \mathbb{N} \) by induction. By repeatedly applying the above inequality, we obtain

\[
d_k \leq (1 - sp_\gamma(t))^k d_0 + p_\gamma(t) \varepsilon_{ab} \sum_{i=0}^{k-1} (1 - sp_\gamma(t))^{k-1-i}
\]

\[\leq (1 - sp_\gamma(t))^k d_{init} + \frac{r_\gamma(t)}{s}.
\]

Since \( sp_\gamma(t) \in [0, 1) \), we used the formula for the infinite geometric sum to obtain the last inequality.

**A. Guidance on designing better approximators**

Theorem 1 also provides guidance on how to design good approximators to use with \( \mathcal{RD} \). For various approximators which one may consider that satisfy Definition 3 \( \varepsilon_{ab} \) will typically be non-zero. Therefore, Theorem 1 suggests that approximators with small additive error \( \varepsilon_{ab} \) will have better reachability guarantees when used within \( \mathcal{RD} \). This naturally raises the question of how to design approximators with a small additive error \( \varepsilon_{ab} \). One important aspect of this is the evaluation radius \( r > 0 \). For any given approximator \( N_{\Phi^{-1}} \), the additive error \( \varepsilon_{ab} = \varepsilon_{ab}(r) \) in Definition 3 can be considered as an increasing function of the evaluation radius \( r \). Therefore, one may hope to obtain estimators with better values of \( \varepsilon_{ab}(r) \) by evaluating for small values of the radius \( r \).

In Figure 5 we used test trajectories (i.e., system trajectories generated independently of the training data) to empirically estimate the absolute error \( \varepsilon_{ab}(r) \) for the approximator used in NeuralExplorer evaluated for various values of \( r \) on four systems. Even as \( r \to 0 \), the \( \varepsilon_{ab}(r) \) values of NeuralExplorer seem to approach a non-zero value \( \delta_0 = \lim_{r \to 0} \varepsilon_{ab}(r) > 0 \). In the light of Theorem 1, this might explain the lack of convergence of NeuralExplorer that we have observed in certain empirical examples. Indeed, as the iterates \( x_k \) in the NeuralExplorer approach the target \( z \), the error in the approximation of \( N_{\Phi^{-1}} \) might possibly be dominating the increment \( \Phi^{-1}(x_t, z - x_t, t) \) needed to proceed towards the target.

Motivated by this discussion, in this work, we introduce approximators based on neural networks \( N_{\Phi^{-1}}(x_t, v/\|v\|, t) \) that learn only the direction (and not the magnitude) of the vector \( \Phi^{-1}(x_t, v, t) \approx \nabla_v \Phi^{-1}(x_t, 0, t) v \), for small values of \( \|v\| \). By focusing only on learning the direction, we avoid numerical issues involved in learning small vectors. Intuitively, if the value \( \|\Phi^{-1}(x_t, v, t)\| \) was then known, we could use the oracle-estimator

\[
N_{\Phi^{-1}}(x_t, v, t) = \tilde{N}_{\Phi^{-1}}(x_t, v/\|v\|, t) \|\Phi^{-1}(x_t, v, t)\| \tag{19}
\]

to approximate \( \Phi^{-1}(x_t, v, t) \) for small values of \( \|v\| \). Figure 5 shows the estimate of the \( \varepsilon_{ab}(r) \) versus \( r \) plot for the oracle estimator in (19). However, note that outside a testing scenario like that in Figure 5 \( N_{\Phi^{-1}}(x_t, v, t) \) cannot be evaluated for the directional approximators. Instead, we directly use \( N_{\Phi^{-1}}(x_t, v/\|v\|, t) \) in \( \mathcal{RD} \) algorithm by the modifications mentioned in Remark 1.

**Remark 1.** As mentioned above, it may be helpful to work with directional-approximators \( \tilde{N}(x_t, v/\|v\|, t) \) for \( \Phi^{-1}(x_t, v, t) \), which learn only the direction (and not the magnitude) of the vector \( \Phi^{-1}(x_t, v, t) \).

Figure 5. Empirical values of the additive error \( \varepsilon_{ab} \) in Definition 3 (assuming \( \varepsilon_{rel} \approx 0 \)) for the approximators \( N_{\Phi^{-1}} \) learned for NeuralExplorer and NExG as a function of the evaluation radius \( r \), for four benchmark systems. Note that we have used the oracle-estimator \( N_{\Phi^{-1}} \) given by (19) to estimate the additive error of NExG, since NExG only learns a directional approximator \( \tilde{N}_{\Phi^{-1}} \).

**VI. Evaluation**

We choose a standard benchmark suite of control systems with neural feedback functions [19], [34], [35], [41] for evaluation. To be more specific, systems #10-#12 are adopted from [34], system #13 is adopted from [19] and the rest of the benchmarks are adopted from the ARCH suite [35], [41]. Considered benchmarks span 6 dimensional systems, controllers with 6-10 hidden layers and 100-300 neurons per layer (c.f. Table I). The tool along with the learned models and presented artifacts is available at https://github.com/manishgcs/NExG.

**A. Network architecture and Training**

For each benchmark, we sample a fixed number (40) of initial states chosen uniformly at random and use a given ODE solver to generate anchor trajectories from these initial states. We further generate ten additional trajectories from the states randomly sampled in the small neighborhood (\( \|v\| = 0.01 \)) of each initial state. We choose a step size (\( h = 0.01 \)). Max step (\( T \)) for each system is shown in Table I; however, a user can pick any suitable values for these parameters including the number of anchor trajectories. Our preliminary analysis shows that increasing the number of anchor trajectories from 40 to 50 slightly improves the MRE, however, this improvement comes at the expense of higher training time. These trade-offs between the amount of data required, training time,
distance between neighboring points, and accuracy of the approximation are subject to future research. Nonetheless, the evaluations presented in subsequent sections underscore the promise of our approach even when the resources are constrained. The data used for training the neural network is collected as previously described. We use 90% of the data for training and 10% for testing.

### TABLE I

Training $N_{\Phi-1}$. Each neural network feedback controller configuration is given as the number of hidden layers and the maximum of neurons per layer. Dims is the number of system variables and $T$ is simulation time bound. The training performance is measured in mean squared error (MSE) and mean relative error (MRE).

| System       | No. | Name     | Dims | NN controller config | Max steps (T) | $N_{\Phi-1}$ Training Time (min) | MSE = 0.004 | MRE = 0.5% |
|--------------|-----|----------|------|----------------------|---------------|----------------------------------|-------------|------------|
| #1 Arch1     | 5   | 6/30     | 200  | 8.0                  | 0.018         | 16.0                             |             |            |
| #2 Arch2     | 5   | 7/70     | 200  | 12.0                 | 0.038         | 14.0                             |             |            |
| #3 Arch3     | 5   | 5/60     | 200  | 10.0                 | 0.021         | 10.2                             |             |            |
| #4 Arch4     | 5   | 9/60     | 200  | 12.0                 | 0.023         | 13.0                             |             |            |
| #5 Arch5     | 5   | 7/60     | 200  | 9.0                  | 0.023         | 9.0                              |             |            |
| #6 Arch6     | 5   | 6/60     | 200  | 10.0                 | 0.021         | 10.2                             |             |            |
| #7 Arch7     | 4   | 7/60     | 200  | 9.0                  | 0.035         | 9.0                              |             |            |
| #8 Arch8     | 4   | 6/60     | 200  | 10.0                 | 0.021         | 10.2                             |             |            |
| #9 Arch9     | 3   | 6/30     | 200  | 7.0                  | 0.023         | 7.0                              |             |            |
| #10 Arch10   | 3   | 6/30     | 200  | 7.0                  | 0.018         | 7.0                              |             |            |
| #11 Arch11   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #12 Arch12   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #13 Arch13   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #14 Arch14   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #15 Arch15   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #16 Arch16   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #17 Arch17   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #18 Arch18   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #19 Arch19   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |
| #20 Arch20   | 3   | 6/30     | 200  | 8.0                  | 0.018         | 8.0                              |             |            |

**B. ReachDestination Evaluation and Features**

We analyze the performance of Algorithm [1] by picking, at every invocation of the algorithm, a random reference trajectory $\xi_A$, a time $t \in [0, T]$, and a target state $z$, reachable at time $t$ in the domain of interest. We choose them randomly to not bias the evaluation of our search procedure to a specific sub-space. The performance metrics used to evaluate various runs are number of course corrections $(k)$ and/or minimum relative distance $(d_t)$. The threshold $\delta$ is fixed as 0.004.

#### B.1 Comparison with NeuralExplorer [29]

The neural network architectures used in this work are the same as those used in NeuralExplorer. For a given $N \in \mathbb{Z}_+$, number of anchor trajectories, NeuralExplorer creates all possible $C(N, 2)$ pairs of these trajectories for training as it attempts to learn the inverse sensitivity function for any $v \in \mathbb{R}^n$ in the domain of interest. Whereas NExG focuses on learning only the direction of the inverse sensitivity. So we only sample a few random points (say, $y$) in a small neighborhood of the initial state of each anchor trajectory and generate total $y \times N$ pairs. As a consequence, we achieve up to 60% reduction in the training time. Further, the state space exploration algorithm in NeuralExplorer predicts inverse sensitivity directly for $w^k$ and course corrects at every step; whereas, NExG predicts only the direction of the inverse sensitivity vector needed to move in the direction $w^k$. Hence the NExG search is guided by additional parameters like the scaling factor $s$ and the correction period $p$. We report in Table [II] the mean values of $k$ and $d_t$ computed over 250 runs of each technique for each system. The evaluation shows that NExG has a relative error of 1-4% (with considerably fewer iterations) as compared to the relative error of 5-15% for NeuralExplorer.

#### B.2 Correction period $(p)$ and scaling factor $(s)$

We fix the tuple $\xi_A, z, t$ in each benchmark, run $\mathcal{RD}$ for $s \in \{0.01, 0.1\}$, $p \in \{1, 5, 10\}$. The evaluation results in Table [III] are presented to make some key observations and emphasize that the technique performs consistently across systems. For a fixed tuple $\xi_A, z, t$, change in the number of trajectories $(k)$ generated by $\mathcal{RD}$ is roughly inversely proportional to the change in the product $s \cdot p$. For example, first row (i.e., $s = 0.01$) in System #7 shows that the number of trajectories $(k)$ reduces from $\sim 400$ to $\sim 40$ (10 fold reduction).
when course correction is performed only once for every 10 steps instead of at every steps. This trend is observed in almost all systems for appropriate s·p values. It can also be observed that the number of course corrections (k) remains roughly the same for different (s, p) pairs as long as the product s·p is same. For e.g., the value of k for pairs (s = 0.01, p = 10) and (s = 0.1, p = 1) is ~ 40 in System #1. These results are consistent with the theoretical bound (Equation 10) that decreases geometrically in k for a fixed value of s·p.

B.3 Satisfying initial conditions: As the algorithm increments the initial state $x_0^{k+1}$ in line 9, it may happen that next $x_0^{k+1} = (x_0^k + e^k)$ is not in the initial set $\theta$, thus violating the initial constraint. We address this problem by picking an element-wise projection of $x_0^k$ in $\theta$ denoted as $\hat{x}_0^k = \text{proj}_\theta(x_0^k) \in \theta$, defined by $\hat{x}_0^k = \arg \min_{x \in \theta} ||x-x_0^k||$.

Consider System #10 with 2$n$ components of its initial set hyper-rectangle, given as $\theta = [-0.5,0.5]$. Both Figures 6(a) and 6(b) demonstrate how the course of exploration makes a detour around the initial set boundary in order to satisfy its constraints.

B.4 Customizing the state exploration algorithm: Note that the inverse sensitivity approximator $N_{\theta-1}$ is agnostic to the exact state space exploration technique. While our implementation of $\mathcal{RD}$ uses this estimator to proceed in a straight line direction towards the destination (i.e. $v^k$ has the same direction as $z-x^k$), the progress direction can also be customized. This allows for designing custom state space exploration algorithm by prioritizing trajectories along different directions at different steps. For an n-dimensional system, at every step, one might be interested in picking a direction among the 2n unit vectors $\{\pm e_i : i = 1,2,\ldots, n\}$ that are aligned with the orthonormal axes. For instance, one can choose the direction vector that is closest to $z-x^k$.

The illustration of one such axis-aligned approach is given in Figure 6(b). It emphasizes that instead of $\mathcal{RD}$, we can also use some other state space exploration algorithm that requires an inverse sensitivity approximator.

B.5 Coverage analysis: Given an initial set $\theta \subseteq \mathbb{D}$, we assess the coverage among the set of reachable states at time $t \in [0,T]$ by calculating the proportion of points in the reachable set that $\mathcal{RD}$ converges to, within a neighborhood of radius $\delta$. To obtain a convenient representation of the reachable set for an n-dimensional system, we use a polygon with faces in the 2n template directions $\{\pm e_i : i = 1,2,\ldots, n\}$. While we have used orthonormal vectors as template directions, different set of template directions can yield a less conservative approximation of the reachable set. The polygon in our experiment was obtained by starting from the destination state of random anchor trajectory $\xi_A(\cdot)$ at time t, and using a modification of $\mathcal{RD}$ to maximally perturbs the destination state in each of the template directions. This provides as many extremal points as the number of template directions, and can be used to construct the bounding polygon (e.g. see the black rectangle in Figure 7), denoted by $\tilde{Z}$, as an approximation of the reachable set. Next, to assess the coverage for $\mathcal{Z}$, we sampled 200 points from $\tilde{Z}$ uniformly at random, and examined which were the ones that $\mathcal{RD}$ could converge within a $\delta = 4 \times 10^{-3}$ neighborhood at time $t$ starting from the initial set $\theta$. As shown in Figure 7, 137 out of these 200 points were reached from $\mathcal{RD}$, with the color of the point (green or red) representing if $\mathcal{RD}$ was successful or not. For each of these points in $\tilde{Z}$, we also plot the best initial point output by $\mathcal{RD}$. Most of these red initial points (that did not reach the destination) lie on the boundary of the initial set $\theta$, suggesting that the trajectory that can possibly reach its destination might perhaps start from a state outside the given initial set.

---

### Table III

| System | $d_{init}$ | s | Course corrections k | p = 5 | p = 10 |
|--------|------------|---|----------------------|-------|--------|
| #7     | 0.39       | 0.01 | 418 83 41          |       |        |
| #17    | 0.85       | 0.01 | 550 109 54         |       |        |

---

### Figure 6

RD and its customizations can provide algorithms for state space exploration with a constrained initial set. In the figure, the inner box represents the initial set. Original RD generates smoother trajectories because it moves in the direction of the target at each step (Figure 6(a)), however RD can be customized to obtain a different state space exploration method.

### Figure 7

Measuring coverage of a reachable set in System #1. For every red colored state in the destination set, RD could not find a trajectory that reaches within its $\delta$-neighborhood at time $t$.

---

### VII. Falsification of a Safety Specification

Given system and a corresponding safety specification in either Signal or Metric Temporal Logic [36], [42], falsification is aimed at finding a system parameter or an input that violates the specification. Existing falsification schemes generate executions using some heuristics or stochastic global optimization and compute their robustness with respect to a
safety specification provided as a set of states. Robustness \((\rho \in \mathbb{R})\) is a measure that quantifies how deep is the execution within the set or how far away it is from the set. Informally, it determines the degree to which an execution satisfies \((\rho > 0)\) or violates \((\rho < 0)\) a given safety specification. Our framework can currently handle a subset of MTL formulas.

\[
\varphi := \top \ | \ p \ | \ \neg \varphi \ | \ \top \cup \varphi
\]

where \(p\) is an atomic proposition, \(I\) is a non-empty interval of \(\mathbb{R}_+\), and \(\varphi\) is a well formed MTL formula. The temporal operator \(\circ\) (eventually) is defined as \(\circ \varphi := \top \cup \varphi\). The reader can refer to [46] for robust semantics of MTL formulas.

### A. Our Falsification algorithm

We describe a simple \(\mathcal{RD}\)-based algorithm to obtain a falsifying trajectory to a given safety specification \(\neg \circ_I U\), where \(U \subseteq \mathbb{R}^n\) is the unsafe set. We generate an anchor trajectory \(\xi_A\), sample a state \(z \in U\), and choose \(I = \arg \min_{\xi \in \xi_A} ||\xi(t^k) - z||\). We then invoke \(\mathcal{RD}\) sub-routine for generating trajectories until we obtain a counterexample \((\rho^k < 0)\) to the given safety specification or bound \(I\) is exhausted, where \(\rho^k\) is the robustness of trajectory \(\xi_A\). To be precise, in the falsification run of \(\mathcal{RD}\): (i) distance \(d^k_u\) is replaced by robustness \(\rho^k\), (ii) constraint \(d^k_u > \delta\) is replaced by \(\rho^k > 0\), and (iii) an additional constraint \(x^k_t \notin U\) is added to the main while loop condition. While it may be the case that \(z\) is not reachable at time \(t\), both these parameters primarily act as anchors to guide the procedure in obtaining a falsifying execution.

### B. Evaluation of Falsification techniques

We evaluate our falsification algorithm against one of the widely used falsification platforms, S-TaLiRo [46]. Monte-Carlo sampling scheme in S-TaLiRo is sensitive to the “temperature” parameter \(\beta\), where the adaptation of \(\beta\) is performed after every fixed number of iterations provided it is unable to find a counterexample by then. We keep \(\beta = 50\) which is the default value, and we consider \(p = 2, s = 0.5\) for our \(\mathcal{RD}\)-based falsification scheme. Although adaptation parameters and mechanisms in both approaches are different, an upper bound \((B)\) on the number of trajectories is crucial to both of them. We fix \(B = 100\) for systems #1-#16 and \(B = 150\) for systems #17-#30 in S-TaLiRo. We consider \(B = 50\) for NExG as we notice that, if it can, it usually finds a trajectory of interest in notably less number of iterations. The sampling time is fixed as 0.01. We exclude cases where the initial reference trajectory \(\xi_A\) is falsifying so as to minimize the bias induced by different distributions in different schemes. For a given pair of initial configuration \(\theta\) and safety specification \(\neg \circ_I U\) in each system, we report in Table [IV] the mean of total trajectories \((k)\) generated along with mean robustness \((\rho)\) computed over 250 runs of respective techniques.

The evaluations exhibit that our algorithm not only takes a very few trajectories to converge but also the counterexample obtained is relatively more robust in most cases. Unlike NExG, the performance of S-TaLiRo seems to deteriorate further with increase in the number of system dimensions and complexity. Even in scenarios where \(\mathcal{RD}\) generates more than 10 trajectories, experiments indicate that it is able to reach the neighborhood around \(U\) within fewer iterations. This observation motivated us to attempt to integrate both frameworks. In the case of non-convergence in S-TaLiRo, its best execution can be used as the input reference trajectory for \(\mathcal{RD}\). One such instance is shown in Figure [8(a)] where S-TaLiRo is unable to find a falsifying trajectory within 100 iterations. We use its best sample as the reference \(\xi_A\) for \(\mathcal{RD}\) and find 4th trajectory to be a counterexample (Figure [8(b)]). This exercise is performed for illustration purpose i.e., at present we manually port the best sample from S-TaLiRo to NExG. One of the future tasks is to automate this integration. Additionally, our approach - as a side effect - provides intuition about the course of exploration leading to the falsifying execution unlike scattered stochastically sampled states generated in S-TaLiRo.

Another important take away from this comparison is that if S-TaLiRo fails to find a counterexample for a given specification, the user is left with a sample of trajectories generated by S-TaLiRo and the execution that comes closest to falsifying the given safety specification. Instead, in our case, the user can still access the inverse sensitivity approximator and manually (or algorithmically) probe nearby trajectories and proceed to discover a falsifying trajectory. Finally, S-TaLiRo’s implementation platform is MATLAB while our framework is implemented in Python. We do not report the wall-clock time taken by respective frameworks as performance differences are expected due to their different implementation platforms.

Figure 8. Falsification demonstrations. The red-colored box is the unsafe set and the inner while-colored box is the initial set. These demonstrations depict how NExG can potentially supplement other falsification platforms if they fail to find a falsifying execution.
TABLE IV  
Performance of falsification techniques. k is the number of simulations generated and ρ is the robustness. The parity of ρ determines whether the execution satisfies (ρ > 0) or falsifies (ρ < 0) a given safety specification, whereas its magnitude determines how robust is the execution. NEXG takes a few very iterations to find a counterexample with ρ < 0. ✓ marks the scenarios with equally (or more) robust falsifying trajectory.

| System | Initial configuration θ | Safety specification ρ | S-TaLiRo | Mean k | Mean ρ | Mean k | Mean ρ |
|--------|--------------------------|------------------------|----------|--------|--------|--------|--------|
| #1     | (0.5, 1.5)              | (0.5, 1.5)             |          | 12     | -0.01  | 3      | 0.00   |
| #2     | (0.5, 1.5)              | (0.5, 1.5)             |          | 24     | 0.006  | 3      | -0.008 |
| #3     | (0.5, 1.5)              | (0.5, 1.5)             |          | 8      | -0.024 | 3      | -0.014 |
| #4     | (0.5, 1.5)              | (0.5, 1.5)             |          | 11     | -0.008 | 3      | 0.002  |
| #5     | (0.5, 1.5)              | (0.5, 1.5)             |          | 39     | 0.001  | 3      | 0.004  |
| #6     | (0.5, 1.5)              | (0.5, 1.5)             |          | 57     | 0.004  | 3      | 0.009  |
| #7     | (0.5, 1.5)              | (0.5, 1.5)             |          | 36     | 0.008  | 9      | 0.004  |
| #8     | (0.5, 1.5)              | (0.5, 1.5)             |          | 76     | 0.005  | 22     | 0.008  |
| #9     | (0.5, 1.5)              | (0.5, 1.5)             |          | 88     | 0.01   | 5      | -0.005 |
| #10    | (0.5, 1.5)              | (0.5, 1.5)             |          | 95     | 0.03   | 3      | -0.016 |
| #11    | (0.5, 1.5)              | (0.5, 1.5)             |          | 98     | 0.058  | 6      | -0.009 |
| #12    | (0.5, 1.5)              | (0.5, 1.5)             |          | 95     | 0.009  | 4      | -0.01   |
| #13    | (0.5, 1.5)              | (0.5, 1.5)             |          | 9      | -0.002 | 6      | -0.002 |
| #14    | (0.5, 1.5)              | (0.5, 1.5)             |          | 55     | 0.002  | 8      | -0.007 |
| #15    | (0.5, 1.5)              | (0.5, 1.5)             |          | 47     | -0.002 | 9      | -0.003 |
| #16    | (0.5, 1.5)              | (0.5, 1.5)             |          | 150    | 0.10   | 15     | -0.001 |
| #17    | (0.5, 1.5)              | (0.5, 1.5)             |          | 150    | 0.81   | 14     | -0.002 |
| #18    | (0.5, 1.5)              | (0.5, 1.5)             |          | 149    | 0.11   | 9      | -0.007 |
| #19    | (0.5, 1.5)              | (0.5, 1.5)             |          | 145    | 0.14   | 34     | 0.015  |
| #20    | (0.5, 1.5)              | (0.5, 1.5)             |          |        |        |        |        |

VIII. DISCUSSION AND FUTURE WORK

In this work, we have proposed a new state space exploration technique NEXG that is an improvement over existing state space approaches. In addition to out-performing state of the art falsification techniques, our technique enables the control designer to develop custom algorithms for state space approaches. In addition to out-performing state of the art falsification technique NExG that is an improvement over existing state space approaches, in this material are those of the author(s) and do not necessarily reflect the views of the United States Air Force, National Science Foundation, or Amazon.

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