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Stochastic Neural Simulation Relations for Control Transfer

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Abstract

This paper explores a neurosymbolic approach to probabilistic transfer of control logic from a source stochastic control system to a target system while ensuring approximately equivalent behavioral guarantees in both domains. Traditional methods struggle with this problem due to the absence of a complete characterization of behavioral specifications, which prevents a direct formulation in terms of loss functions. To address this challenge, we leverage the concept of stochastic simulation relations to establish probabilistic observational equivalence between the behaviors of two (black-box) stochastic systems. These functions ensure that the outputs of both systems, equipped with their respective controllers, remain probabilistically close over time. By parameterizing stochastic simulation functions with neural networks, we introduce the notion of *stochastic neural simulation functions*, enabling a data-driven mechanism to transfer any synthesized controller—along with its proof of correctness—without requiring explicit specification of behavioral constraints. This neurosymbolic integration combines the scalability of neural methods with the formal guarantees of symbolic approaches, bridging the gap between learning-based control synthesis and formal verification. Compared to prior methods, our approach eliminates the need for a closed-loop mathematical model and explicit requirement specifications for both the source and target systems, while providing probabilistic guarantees over an infinite horizon. We also introduce validity conditions that, when satisfied, ensure the closeness of the outputs of two systems equipped with their corresponding controllers, removing the need for post-facto verification. We demonstrate the effectiveness of our approach through four case studies, highlighting its potential to advance scalable, formally grounded, and transferable control synthesis.

1. Introduction

Symbolic approaches to control design (Rungger and Zamani, 2016) have long been developed for safety-critical systems, where a carefully constructed abstract model enables the formal synthesis of controllers with provable guarantees over the original system. However, constructing such symbolic models demands significant computational effort, posing a major barrier to their widespread adoption. Recently, neural networks have been proposed for controller synthesis, offering various correctness guarantees (Abate et al., 2022). However, these guarantees often require exhaustive state-space exploration, which limits scalability. *Transfer learning* presents a promising alternative for applying neural approaches to control synthesis. By leveraging control logic from a *source system*, it enables the adaptation of controllers to a *target system*, guided by carefully designed loss functions. Since symbolic approaches are computationally feasible for smaller systems, integrating transfer learning with formal guarantees can facilitate an effective, principled, and scalable neurosymbolic approach to control design. In this paper, we propose a general framework for this integration based on stochastic simulation functions.

Transfer Learning. Humans innately exhibit remarkable capabilities in transferring expertise across different tasks, often performing significantly better in one task after learning a related one (Kendler, 1995). *Transfer learning* is a sub-field of artificial intelligence (AI) that focuses on developing similar capabilities for machine learning problems; aimed towards improving learning speed, efficiency, and data requirements. Unlike conventional learning algorithms, which typically focus on individual tasks, transfer learning approaches focus on leveraging knowledge acquired from one or multiple *source* domains to improve learning in a related *target* domain (Weiss et al., 2016). Recently, transfer learning has been successfully applied in designing control logic for dynamical systems (Christiano et al., 2016; Salvato et al., 2021; Nagabandi et al., 2018), albeit without guarantees. However, for safety-critical dynamical systems, control design must provide correctness guarantees, motivating our work. We present a transfer learning approach for stochastic control systems that provides probabilistic guarantees on behavior transfer.

Controller Synthesis and Transfer Learning. This work focuses on controller synthesis for continuous-space stochastic control systems described by difference equations. Examples of such systems include autonomous vehicles, implantable medical devices, and power grids. The safety-critical nature of these systems demands formal guarantees—such as safety, liveness, and more expressive logic-based requirements—on the behavior of the resulting control. While deploying the classic control-theoretic approaches may not necessarily require a mathematical model of the system, and use search and symbolic exploration to synthesize controllers, many of these approaches (Tabuada, 2009) still depend on a mathematical model to provide formal guarantees of correctness. These symbolic approaches typically face the curse-of-dimensionality where the systems with high dimensions become exceedingly cumbersome and time-consuming to design. To overcome these challenges, machine learning based approaches (Zhao et al., 2020; Abate et al., 2022), among others, have been proposed to synthesize control for high-dimensional and complex systems. By making reasonable assumptions (such as Lipschitz continuity) regarding the system, these approaches are able to provide guarantees about their performance. More recently, transfer learning has shown promise (Christiano et al., 2016; Fu et al., 2016; Bousmalis et al., 2018) in transferring controllers from a *source domain* (a *low-fidelity* model or a simulation environment) to a *target domain* (*high-fidelity* model or real system). Some of these approaches (Nadali et al., 2023, 2024a) also aim to transfer *proof certificates* in addition to transferring control.

Specification-Agnostic Control Transfer. Current approaches (Nadali et al., 2023, 2024a) enable the transfer of control policies and proof certificates when a formal specification is available. However, in typical transfer learning scenarios, control is often inherited from a legacy system deemed desirable for various implicit reasons that are difficult to formalize. As a result, extracting a complete and precise specification becomes challenging. We posit that if structured, unambiguous interfaces—referred to as *semantic anchors* (Velasquez, 2023)—are available to relate observations between the source and target environments, then behaviorally equivalent transfer can be achieved by ensuring the probabilistic closeness of these observations as the system evolves over time. To this end, we introduce *Stochastic Neural Simulation Functions*, which enables the probabilistic transfer of any controller designed for a *source* system to a *target* system, independent of the specification.

Stochastic Neural Simulation Functions. For discrete-time stochastic systems with continuous state spaces, finite abstractions were first introduced in Abate et al. (2008) for the formal synthesis of this class of systems. This method was later refined (Esmaeil Zadeh Soudjani and Abate, 2013)

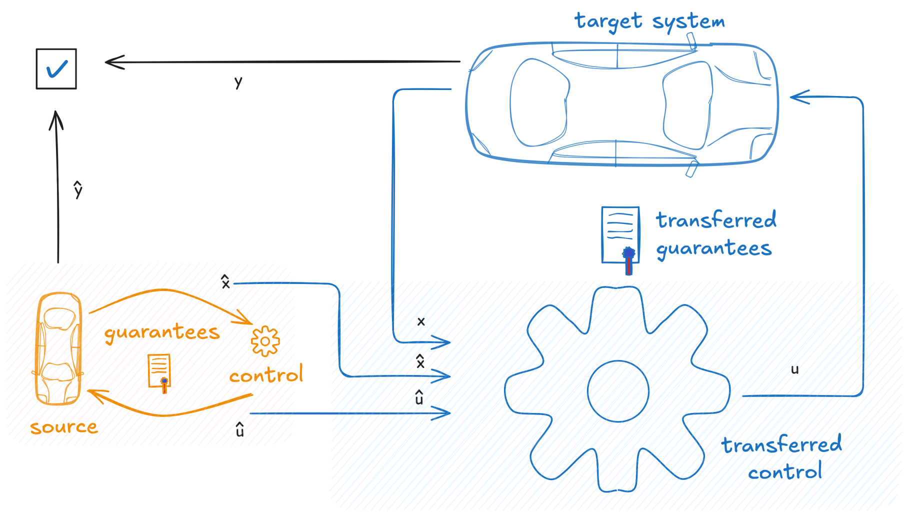

Figure 1: Behavior transfer framework: The existence of a relation and an interface function between source and target implies the closeness of their behaviors.

and implemented into FAUST (Soudjani et al., 2015). The extension of these techniques to infinite-horizon properties is proposed in Tkachev and Abate (2011), while formal abstraction-based policy synthesis is explored in Tkachev et al. (2013). A novel notion of approximate similarity relation is introduced in (Haesaert and Soudjani, 2020a), accounting for deviations in both stochastic evolution and system outputs. Finally, Lavaei et al. (2019) proposed a method to find an abstraction of networks of stochastic systems.

Our Approach: a Behavior Transfer Framework. In this work, we assume access to a simulation environment (digital twin or black-box model) of the source system $\hat{\mathfrak{S}}$. In our proposed behavior transfer approach, as depicted in Figure 1, given a source system $\hat{\mathfrak{S}}$ and a target system $\mathfrak{S}$, we design an interface function $\mathcal{K}$ that can transfer an arbitrary controller from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$. It does so by finding a stochastic -approximate- simulation function V between the states of the source and target systems; such that for any pair of related states, and any input in the source environment, there exists an input in the target environment that keeps the next states related according to V. Moreover, it also guarantees that any pair of states, related via V, have similar observations probabilistically. The existence of such simulation functions implies that any behavior on the source system, due to any chosen controller, can be mimicked in the target system.

In this work, we train two neural networks to approximate the simulation function V and the interface function $\mathcal{K}$. Under reasonable assumptions, we provide validity conditions that, when satisfied, guarantee the probabilistic lower bound of the outputs of two systems, equipped with their corresponding controllers, thereby eliminating post-facto verification.

Our proposed approach differs from previous work in three key aspects. First, it is model-free, meaning it does not require explicit mathematical equations governing the systems. Second, it provides probabilistic guarantees over an infinite-time horizon. Lastly, we learn an interface function that serves as a controller for the target system—that is, we synthesize a feedback controller rather than focusing solely on verification.

Contribution. This work investigates infinite-horizon output closeness between two given systems. We propose sufficient data-driven criteria, dubbed *Stochastic Neural Simulation Relation*, to ensure probabilistic transfer of controllers designed for source systems, along with their correctness proofs (if existing), to target systems; owing to the explicit computation of the output error bounds related to both systems, this work provides an approach to lift guarantees that is effectively property-independent. In particular, we introduce a training framework that parameterizes the simulation function and its associated interface function as neural networks. Furthermore, by proposing validity conditions to ensure the correctness of these functions, we provide probabilistic guarantees for behavioral transfer from a source to a target system, eliminating the need for post-facto verification.

To the best of our knowledge, this is the first probabilistically correct result that aims to find a stochastic simulation function and its interface function in a data-driven manner between two given systems, for infinite horizon. In general, existing works are primarily focused on constructing a source (abstract) system given a target (concrete) system (Abate et al., 2022, 2024; Devonport et al., 2021; Hashimoto et al., 2022; Kazemi et al., 2024), deterministic systems (Nadali et al., 2024b), or a fixed specification (Schön et al., 2024). In contrast, our approach does not construct any abstraction. Instead, it establishes a probabilistically correct transfer of controllers designed for a given abstract (source) system to a concrete (target) system. Methods that aim to find a simulation function between two given systems typically make restrictive assumptions about the models of both the source and target systems. For example, the results in Zhong et al. (2024) assume linear systems, while Smith et al. (2019) considers only polynomial systems. Furthermore, both methods require access to the mathematical models of the systems. In contrast, our approach makes no assumptions about the specific models of the systems, requiring only access to a black-box representation and the Lipschitz continuity of the dynamics.

Related Work. Transfer learning aims at using previously acquired knowledge in one domain in a different domain. Traditional studies in transfer learning focused on utilizing the acquired weights of a neural network from a particular source domain to accelerate training in a related target domain (Bozinovski, 2020; Torrey and Shavlik, 2010). Transfer learning for control is concerned with transferring a controller from simulation to a real-world system which is based on adapting a controller (Fu et al., 2016; Christiano et al., 2016; Bousmalis et al., 2018; Salvato et al., 2021; Nagabandi et al., 2018), or robust control methods that are not affected by the mismatch between the simulator and the real world (Mordatch et al., 2015; Zhou and Doyle, 1998; Berberich et al., 2020). Though these results have shown great promise, they either lack theoretical guarantees or require a model of the system. Another approach is to leverage simulation relations (Girard and Pappas, 2011), which is mainly concerned with controlling a complex target system through a simpler source system. Girard and Pappas (2011, 2009) introduced a sound hierarchical control scheme based on the notion of an *approximate simulation function (relation)*, bringing together control and automata theory under a unified framework. This relation has had a profound impact on synthesizing controllers against logical properties (da Silva et al., 2019; Fainekos et al., 2007; Zhong et al., 2023) across a variety of systems, such as piecewise affine (Song et al., 2022), control affine (Smith et al., 2019, 2020), and descriptor systems (Haesaert and Soudjani, 2020b). Additionally, it has been applied in various robotics applications, such as legged (Kurtz et al., 2020) and humanoid (Kurtz et al., 2019) robots. Moreover, Abate et al. (2024) proposed bisimulation learning to find a finite abstract system. The results in Nadali et al. (2024b) have recently proposed the notion of neural simulation relations for non-stochastic systems. This present work extends that work to handle stochastic systems.

2. Problem Formulation

We denote the set of reals and non-negative reals by $\mathbb{R}$ and $\mathbb{R}_{\geq 0}$, respectively. Given sets A and B, $A \setminus B$ and $A \times B$ represent the set difference and Cartesian product between A and B, respectively, and $|A|$ represents the cardinality of a set A. Moreover, we consider n-dimensional Euclidean space $\mathbb{R}^n$ equipped with the infinity norm, defined as $\|x - y\| := \max_{1\leq i\leq n} |x_i - y_i|$ for $x=(x_1, x_2, \ldots, x_n), y=(y_1, y_2, \ldots, y_n) \in \mathbb{R}^n$. Furthermore, we denote the mean squared loss as $MSE(x, y) := \frac{1}{2n}\sum_{i=1}^{n}(x_i - y_i)^2$, where $x, y \in \mathbb{R}^n$. A function $\gamma : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is said to be class κ function if it is continuous, strictly increasing, and $\gamma(0) = 0$. A class κ function is said to be a class κ_∞ function if $\gamma(r) = \infty$ as $r \to \infty$.

Definition 1 (Discrete-Time Stochastic Control System) *A discrete-time stochastic control system (dtSCS) is a tuple $\mathfrak{S}:=(\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$, where $\mathcal{X}\subseteq\mathbb{R}^n$ represents the state set, $\mathcal{X}_0\subseteq\mathcal{X}$ is the initial state set, $U\subseteq\mathbb{R}^m$ is the set of inputs, and $\mathcal{Y}\subseteq\mathbb{R}^l$ is the set of outputs, V_m is the uncertainty set, and w denotes a sequence of independent and identically distributed (i.i.d.) random variables on the set V_m as $w := \{w(k) : \Omega \to V_m, k \in \mathbb{N}\}$. Furthermore, $f:\mathcal{X}\times U \times V_m \to \mathcal{X}$ is the measurable state transition function, and $h : \mathcal{X}\to\mathcal{Y}$ is the output function. The evolution of the system is described by:*

$$x(t + 1) = f(x(t), u(t), w(t)) \textit{ and } y(t) = h(x(t)), \quad \textit{for all } t \in \mathbb{N}.$$

A state sequence is denoted by $\langle x_0, x_1, \ldots\rangle$, where $x_0\in\mathcal{X}_0$, and $x(t + 1)=f(x(t), u(t), w(t))$, $u(t) \in U$, $w(t) \in V_m$. We assume that sets $\mathcal{X}$, U, and $\mathcal{Y}$ are compact, and maps f and h are unknown but can be simulated via a black-box model. Since the codomain of the map f is $\mathcal{X}$, this implicitly implies that the state set $\mathcal{X}$ is forward invariant, which might seem conservative when dealing with unbounded noise, especially when $\mathcal{X}$ is compact. Following the convention introduced in Kushner (1967); Xue (2024); Anand et al. (2022), to ensure the forward invariance of $\mathcal{X}$, we adopt the standard assumption of stopping the stochastic process. Moreover, we assume that f and h are Lipschitz continuous, as stated in the following assumption.

Assumption 2 (Lipschitz Continuity) *Consider a discrete-time stochastic control system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$. The map f is Lipschitz continuous in the sense that there exists constants $\mathcal{L}_u, \mathcal{L}_x \in \mathbb{R}_{\geq 0}$ such that for all x,$x'\in\mathcal{X}$, and $u, u'\in U$, one has:*

$$\|f(x, u, w) - f(x', u', w)\| \leq \mathcal{L}_x\|x - x'\| + \mathcal{L}_u\|u - u'\|. \tag{1}$$

Furthermore, the map h is Lipschitz continuous in the sense that there exists a constant $\mathcal{L}_h \in \mathbb{R}_{\geq 0}$ such that for all $x, x' \in \mathcal{X}$, one has $\|h(x) - h(x')\| \leq \mathcal{L}_h\|x - x'\|$.

Without loss of generality, we assume that Lipschitz constants of functions f and h are known. If the Lipschitz constants are unknown, one can leverage sampling methods (Calliess et al., 2020) to estimate those constants.

Definition 3 (Stochastic Behavior Transfer) *Consider two discrete-time stochastic control systems $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$ and $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$, representing the target and the source system, respectively. A* stochastic behavior transfer *from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ exists if, for any state sequence $\hat{x}(t)$, $\forall t \in \mathbb{N}$, in the source system equipped with its controller, there exists a controller and* *a state sequence $x(t)$, $\forall t \in \mathbb{N}$, in the target system, such that the following holds with confidence $1-\beta$, where $\beta \in (0,1)$:*

$$\mathbb{P}[\max_{t\in\mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \le \epsilon | x(0), \hat{x}(0)] \ge 1-\gamma,$$

for some $\epsilon, \gamma \in \mathbb{R}_{>0}$.

Intuitively, if a *stochastic behavior transfer* exists from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$, any control policy designed for $\hat{\mathfrak{S}}$ can be adapted to $\mathfrak{S}$ while ensuring that their outputs remain bounded with probability $1-\gamma$ and confidence of $1-\beta$. To automate the transfer of control policies, we pose the following *stochastic behavior transfer* problem.

Problem 4 (Stochastic Behavior Transfer) *Consider two discrete-time stochastic control systems $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_M, w)$ and $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_M, \hat{w})$, representing the target and source systems, respectively. Determine whether a behavior transfer from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ exists.*

Our solution to the behavior transfer problem (Problem 4) utilizes the following notion.

Definition 5 (Stochastic Approximate Simulation Function) *Consider two discrete-time stochastic control systems $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_M, w)$ and $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$, representing the target system and the source system, respectively. A function $V := \mathcal{X} \times \hat{\mathcal{X}} \to \mathbb{R}_{\ge 0}$ is a stochastic approximate simulation function from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ if the following conditions hold for an $\alpha \in \kappa_\infty$:*

$$(i)\ \alpha(\|h(x) - \hat{h}(\hat{x})\|) \le V(x, \hat{x}),\ \forall x \in \mathcal{X}, \hat{x} \in \hat{\mathcal{X}}, \tag{2}$$

$$(ii) \forall x{\in}\mathcal{X}, \forall \hat{x}{\in}\hat{\mathcal{X}}, \forall \hat{u}{\in}\hat{U},\ \exists u{\in}U \text{ s.t. } \mathbb{E}\big[V(f(x,u,w), \hat{f}(\hat{x},\hat{u},\hat{w})) | x, \hat{x}, u, \hat{u}\big] {\le} V(x, \hat{x}). \tag{3}$$

Note that condition (3) tacitly implies the existence of an interface function $\mathcal{K} : \mathcal{X} \times \hat{\mathcal{X}} \times \hat{U} \to U$, as illustrated in Figure 1, which acts as a transferred controller for $\mathfrak{S}$. To demonstrate the merit of the stochastic approximate simulation relation, in comparing the output trajectories of two dtSCSs in a probabilistic setting, we rely on the following proposition; which shows that one can solve Problem 4 by searching for a *stochastic approximate simulation function* from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ (if existing).

Proposition 6 (Stochastic Simulation Relations and Transfer) *Consider two discrete-time stochastic control systems $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$ and $\hat{\mathfrak{S}} {=} (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$, representing the target and the source systems, respectively. If there exists a stochastic approximate simulation function from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ as in Definition 5, then there exists a stochastic behavior transfer from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$.*

The proof can be found in appendix A.1. From this proposition, Problem 4 reduces to the search for a stochastic approximate simulation function V from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$, along with its associated interface function $\mathcal{K}$. To circumvent the need for mathematical models of $\hat{\mathfrak{S}}$ and $\mathfrak{S}$ and to enable the discovery of V through their black-box representations, we learn the function V and the interface function $\mathcal{K}$ as neural networks (Goodfellow et al., 2016).

Definition 7 *A neural network with $k{\in}\mathbb{N}$ layers is a function $F{:}\mathbb{R}^{n_i}{\to}\mathbb{R}^{n_o}$, which computes an output $y_k{\in}\mathbb{R}^{n_o}$ for any input $y_0{\in}\mathbb{R}^{n_i}$ such that $y_j{=}\sigma(W_j y_{j-1}{+}b_j)$, with $j{\in}\{1,\ldots,k\}$, where W_j and b_j are weight matrix and bias vectors, respectively, and σ is the activation function. Additionally, y_{j-1} and y_j are referred to as the input and output of the j-th layer, respectively.*

In this paper, we consider neural networks with ReLU activation function, defined as $\sigma(x) := \max(0, x)$. Such networks describe Lipschitz continuous functions, with Lipschitz constant $\mathcal{L}_F \in \mathbb{R}_{\geq 0}$, in the sense that for all $x'_1, x'_2 \in \mathbb{R}^{n_i}$, one has:

$$\|F(x'_1) - F(x'_2)\| \leq \mathcal{L}_F \|x'_1 - x'_2\|. \tag{4}$$

We obtain an upper bound for Lipschitz constant of a neural network with ReLU activations using spectral norm (Combettes and Pesquet, 2020). Leveraging Proposition 6, we propose a data-driven approach to learn a neural-network-based stochastic approximate simulation relation from a source system $\hat{\mathfrak{S}}$ to a target system $\mathfrak{S}$, thereby addressing Problem 4.

3. Stochastic Neural Simulation Functions

This section explores the training of neural networks to construct a neural simulation function (cf. Definition 8), addressing Problem 4. To this end, we first introduce the construction of the dataset for training these networks. We consider the training set $\mathcal{T} := \mathcal{X} \times \hat{\mathcal{X}}$. Then, to construct the data sets with finitely many points, we cover $\mathcal{T}$ by finitely many disjoint hypercubes $\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_M$, by picking a discretization $\mathfrak{e} > 0$, such that:

$$\|\mathfrak{t} - \mathfrak{t}_i\| \leq \frac{\mathfrak{e}}{2}, \text{ for all } \mathfrak{t} \in \mathcal{T}_i, \tag{5}$$

where $\mathfrak{t}_i$ is the center of hypercube $\mathcal{T}_i$, $i \in \{1, \ldots, M\}$. Accordingly, we pick the centers of these hypercubes as sample points, and denote the set of all sample points by $\mathcal{T}_d := \{\mathfrak{t}_1, \ldots, \mathfrak{t}_M\}$. We discretize $\hat{U}$ in the same manner with discretization parameter $\hat{\mathfrak{e}}$, resulting in data sets $\hat{U}_d$. Having these data sets, we can now introduce the notion of *stochastic neural simulation function*.

Definition 8 (Stochastic Neural Simulation Functions) *Consider two discrete-time stochastic control systems $\mathfrak{S}=(\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$ and $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$, representing the target and the source system, respectively, and neural networks $V : \mathcal{X} \times \hat{\mathcal{X}} \rightarrow \mathbb{R}_{\geq 0}$ and $\mathcal{K} : \mathcal{X} \times \hat{\mathcal{X}} \times \hat{U} \rightarrow U$. A function V is called a* stochastic neural simulation function *from $\hat{\mathfrak{S}}$ to $\mathfrak{S}$ with the associated interface function $\mathcal{K}$, if for all $(x, \hat{x}) \in \mathcal{T}_d$ we have:*

a) $$\alpha(\|h(x) - \hat{h}(\hat{x})\|) \leq V(x, \hat{x}) - \eta, \tag{6}$$

b) $$\forall \hat{u} \in \hat{U}_d, \ \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w_k), \hat{f}(\hat{x}, \hat{u}, w_j)) \leq V(x, \hat{x}) - \eta - \delta, \tag{7}$$

where $\eta, \delta \in \mathbb{R}_{>0}$ are some user-defined robustness parameters, and α is a class κ_∞ function.

Due to the stochastic nature of systems, we replaced the expectation with empirical mean, and added δ as a robustness parameter to mitigate the error we incur by replacing the expectation with empirical mean. In order to obtain a neural simulation function V, and its associated interface function $\mathcal{K}$, satisfying (6)-(7), we train the network V with loss l:

$$l := MSE(V(x, \hat{x}), \lambda \alpha(\|h(x) - \hat{h}(\hat{x})\|)), \forall (x, \hat{x}) \in \mathcal{T}_d \ \text{ s.t. } V(x, \hat{x}) < \alpha(\|h(x) - \hat{h}(\hat{x})\|) + \eta, \tag{8}$$

Algorithm 1 Learning Stochastic Neural Simulation Functions

Input: Sets $\mathcal{X}, U, \hat{\mathcal{X}}, \hat{U}$ for target and source systems, respectively, as in Definition 1; discretization parameters $\mathfrak{e}, \hat{\mathfrak{e}}$ for sets $\mathcal{X}, \hat{\mathcal{X}}, \hat{U}$ as in (5); $\mathcal{L}_x$, $\mathcal{L}_u$, $\mathcal{L}_h$, $\mathcal{L}_{\hat{x}}$, $\mathcal{L}_{\hat{u}}$, $\mathcal{L}_{\hat{h}}$ as introduced in Assumption 2; number of simulations for source $\hat{N}$ and target N systems respectively; upper-bound of variance of simulation function M as in Assumption 9, the architecture of the networks V and $\mathcal{K}$ as in Definition 7; a class κ_∞ function α, and a confidence $1-\beta$, where $\beta \in (0,1)$.
Output: Neural networks V (for the simulation relation as in Definition 8) and $\mathcal{K}$.

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1: Construct data sets $\mathcal{T}_d$, and $\hat{U}_d$ according to (5).
2: Initialize networks $V$ and $\mathcal{K}$ (Goodfellow et al., 2016).
3: $\mathcal{L}_V \leftarrow$ Upper bound of Lipschitz constant of $V$ (Combettes and Pesquet, 2020).
4: $\mathcal{L}_K \leftarrow$ Upper bound of Lipschitz constant of $\mathcal{K}$ (Combettes and Pesquet, 2020).
5: while Conditions (6)-(7) and (10)-(12) are not satisfied do
       Construct losses $l$ and $l_k$ according to (8) and (9), respectively
       Train $V$ with loss $l$.
       Train $\mathcal{K}$ via loss $l_k$
       $\mathcal{L}_V \leftarrow$ Upper bound of Lipschitz constant of $V$ (Combettes and Pesquet, 2020).
       $\mathcal{L}_K \leftarrow$ Upper bound of Lipschitz constant of $\mathcal{K}$ (Combettes and Pesquet, 2020).
   end
6: Return $V, \mathcal{K}$
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where $\lambda > 1$. Additionally, we train the network $\mathcal{K}$ employing the following loss

$$l_k := MSE(h_1(f(x, \mathcal{K}(x, \hat{x}, \hat{u}))), \hat{h}_1(\hat{f}(\hat{x}, \hat{u}))),\ \forall (x, \hat{x}) \in \mathcal{T}_d,\ \forall \hat{u} \in \hat{U}_d, \tag{9}$$

where $h_1 := \sum_{i=1}^{N} h(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w_i)))$, and $\hat{h}_1 := \sum_{i=1}^{\hat{N}} \hat{h}(\hat{f}(\hat{x}, \hat{u}, \hat{w}_i))$, are empirical means of outputs of target and source systems, respectively. By leveraging l_k, the network $\mathcal{K}$ is trained to produce an input for the target system such that the outputs of the target and source systems remain close at the next time step, regardless of the input provided to the source system. Note that a stochastic neural simulation function, as in Definition 8, is not necessarily a valid stochastic approximate simulation function as in Definition 5. Since neural networks are trained on finitely many data points, out-of-sample guarantees are required to prove correctness. To tackle this issue, we propose the following validity conditions to show that a stochastic neural simulation function satisfies condition (2)-(3) (cf. Theorem 10).

Assumption 9 *Consider two discrete-time stochastic control systems $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$ (a.k.a. source system) and $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$ (a.k.a. target system), and two fully connected neural networks $V : \mathcal{X} \times \hat{\mathcal{X}} \to \mathbb{R}_{\geq 0}$ and $\mathcal{K} : \mathcal{X} \times \hat{\mathcal{X}} \times \hat{U} \to U$, with ReLU activations, satisfying (6)-(7). We assume the following validity conditions:*

$$\alpha\big((\mathcal{L}_h + \mathcal{L}_{\hat{h}})\frac{\mathfrak{e}}{2}\big) + \mathcal{L}_V \frac{\mathfrak{e}}{2} - \eta \leq 0, \tag{10}$$

$$N \times \hat{N} \geq \frac{M}{\delta^2 \beta}, \tag{11}$$

$$\mathcal{L}_V\big(\max\big[(\mathcal{L}_x + \mathcal{L}_u\mathcal{L}_K)\frac{\mathfrak{e}}{2}, \mathcal{L}_{\hat{x}}\frac{\mathfrak{e}}{2} + \mathcal{L}_{\hat{u}}\frac{\hat{\mathfrak{e}}}{2}\big] + 1\big) - \eta \leq 0, \tag{12}$$

where $\eta, \delta \in \mathbb{R}_{>0}$ are user-defined parameters as in Definition 8, $\mathcal{T}_d, \hat{U}_d$ are constructed according to (5) with discretization parameter $\mathfrak{e}$. Additionally, $\mathcal{L}_V, \mathcal{L}_h, \mathcal{L}_{\hat{h}}, \mathcal{L}_K$ are Lipschitz constants of $V, h, \hat{h}$, and $\mathcal{K}$, respectively (cf. Assumption 2 and equation (4)), and $\mathcal{L}_x, \mathcal{L}_u$ (resp. $\mathcal{L}_{\hat{x}}, \mathcal{L}_{\hat{u}}$) are Lipschitz constants of the target system (resp. the source system), as in Definition 2, and $M \geq$ Var$(V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w), \hat{f}(\hat{x}, \hat{u}, \hat{w})))$, for all $x \in \mathcal{X}, \hat{x} \in \hat{\mathcal{X}}, \hat{u} \in \hat{U}$, is an upper bound for the variance of V, and $\beta \in (0, 1)$.

The intuition behind Assumption 9 is to leverage Lipschitz continuity to enable formal guarantees beyond the training data. Since neural networks are trained on finite samples, it is essential to establish out-of-sample correctness. Lipschitz continuity allows these guarantees to extend from training points to their surrounding neighborhoods. Assumption 4 formalizes this idea by ensuring that if a training sample satisfies the stochastic simulation relation, then all points within an $\mathfrak{e}$-neighborhood around it also satisfy the same conditions. This provides a theoretical foundation for generalizing correctness across the entire state space. Based on Definition 8 and Assumption 9, Algorithm 1 outlines the data-driven construction of a stochastic neural simulation relation with formal guarantees.

4. Formal Guarantee for Stochastic Neural Simulation Functions

In this section, we propose the main result of our paper. This result shows that a stochastic neural simulation function acquired by using Algorithm 1, conditioned on its termination, is in fact a stochastic approximate simulation function, *i.e.* it satisfies conditions (2)-(3) and therefore can be deployed to solve Problem 4.

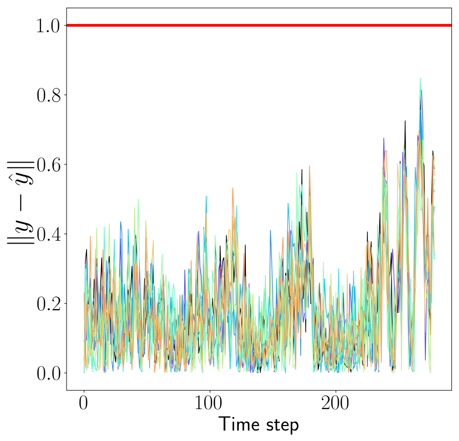
Theorem 10 *Consider two discrete-time stochastic control systems, $\hat{\mathfrak{S}} = (\hat{\mathcal{X}}, \hat{\mathcal{X}}_0, \mathcal{Y}, \hat{U}, \hat{f}, \hat{h}, \hat{V}_m, \hat{w})$ (a.k.a. the source system), with its Lipschitz constants $\mathcal{L}_{\hat{x}}, \mathcal{L}_{\hat{u}}$, and $\mathcal{L}_{\hat{h}}$, and $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, \mathcal{Y}, U, f, h, V_m, w)$ (a.k.a. the target system), with its Lipschitz constants $\mathcal{L}_x, \mathcal{L}_u$, and $\mathcal{L}_h$. If there exist neural networks V with a Lipschitz constant $\mathcal{L}_V$ and $\mathcal{K}$ with a Lipschitz constant $\mathcal{L}_K$ that satisfy conditions (6) to (12) with κ_∞ function α, then for any closed-loop trajectory of the source system, starting from $\hat{x}_0$, there exists a closed-loop trajectory of the target system equipped with controller $\mathcal{K}$ and starting from x_0 such that with confidence $1 - \beta$, $\beta \in (0, 1)$, the following inequality holds:*

$$\mathbb{P}\big[\max_{t\in\mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \leq \alpha(\epsilon) | x_0, \hat{x}_0\big] \geq 1 - \frac{V(x_0, \hat{x}_0)}{\alpha(\epsilon)}, \textit{ for any } \epsilon \geq 0.$$

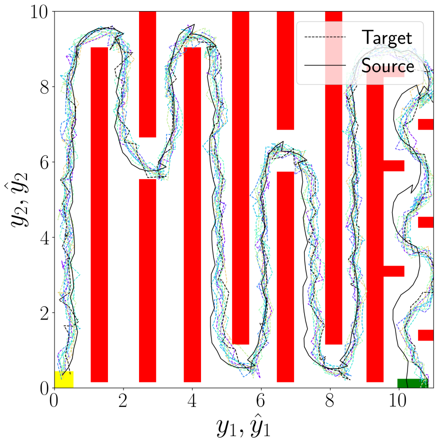
A proof is provided in the appendix A.2. Theorem 10 provides probabilistic closeness of output behaviors of two systems in infinite horizon with confidence $1 - \beta$.

5. Experimental Results

In this paper, the effectiveness of the proposed method is demonstrated through four case studies. We refer the reader to appendix B for the details of all experimental results. In particular, we have done a vehicle control transfer from a 3-dimensional model to a 5-dimensional model. The error between outputs of source and target systems over a state sequence of 300 steps is depicted in Figure 2, for 10 different realizations. We leveraged the tool `SCOTS` (Rungger and Zamani, 2016) to design a



(a) Error between outputs.



(b) Trajectories for both systems.

Figure 2: Vehicle control transfer from 3D to 5D. (a) The error between the outputs, and (b) the trajectories for both systems, for 10 different realizations.

controller for the source system (without the noise), ensuring it reaches the goal (depicted by the green rectangle) while avoiding obstacles (depicted by red rectangles) from the initial set of states (depicted by the yellow rectangle). In this case study, for $\alpha(\epsilon) = 1$, with 99% confidence, we get: $\mathbb{P}\big[\max_{t\in\mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \leq 1 | x_0, \hat{x}_0\big] \geq 0.9287$. We conducted these experiments with 10000 different realizations, and in only 52 cases did the difference between the outputs exceed 1, which aligns with the theoretical results.

6. Conclusion

This paper presents a data-driven approach for behavior transfer between a source and target stochastic control systems, offering probabilistic guarantees. We employ neural networks to encode and search for a stochastic simulation function and its corresponding interface function, collectively termed stochastic neural simulation functions. The existence of these functions ensures that the output error between the two systems remains within a bounded range, facilitating probabilistic behavior transfer. To guarantee correctness, we propose validity conditions for the neural networks representing the stochastic simulation and interface functions, eliminating the need for post-facto verification. Experimental results from four case studies demonstrate the effectiveness of the proposed control transfer approach. A promising future direction is to reduce sample complexity by leveraging structural properties of both the source and target systems, such as monotonicity (Angeli and Sontag, 2003) and mixed-monotonicity (Coogan and Arcak, 2015).

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Appendix A. Omitted Proofs

A.1. Proof of Proposition 6

Proof Condition (3) implies that process $V(x(t),\hat{x}(t))$ is a nonnegative supermartingle. Therefore, one obtains:

$$\mathbb{P}\big[\max_{t\in\mathbb{N}}\|h(x(t)){-}\hat{h}(\hat{x}(t))\|{\ge}\epsilon|x(0),\hat{x}(0)\big] = \mathbb{P}\big[\max_{t\in\mathbb{N}}\alpha(\|h(x(t)){-}\hat{h}(\hat{x}(t))\|){\ge}\alpha(\epsilon)|x(0),\hat{x}(0)\big]$$

$$\le\mathbb{P}\big[\max_{t\in\mathbb{N}}V(x(t),\hat{x}(t))\ge\alpha(\epsilon)|x(0),\hat{x}(0)\big] \tag{13}$$

$$\le\frac{V(x(0),\hat{x}(0))}{\alpha(\epsilon)}, \tag{14}$$

where (14) follows from the nonnegative supermartingle property ((Kushner, 1967), Theorem 12, p. 71), and (13) is obtained by using inequality (2). Therefore:

$$\mathbb{P}\big[\max_{t\in\mathbb{N}}\|h(x(t))-\hat{h}(\hat{x}(t))\|\le\epsilon|x(0),\hat{x}(0)\big]\ge 1-\frac{V(x(0),\hat{x}(0))}{\alpha(\epsilon)}. \tag{15}$$

The proof is now complete. ■

A.2. Proof of Theorem 10

Proof For all $x\in\mathcal{X}$, all $\hat{x}\in\hat{\mathcal{X}}$, all $\hat{u}\in\hat{U}$, consider the following:

$$\frac{1}{N\times\hat{N}}\sum_{(k,j)=(1,1)}^{(N,\hat{N})}V(f(\bar{X}_k),\hat{f}(\hat{X}_j))-V(x,\hat{x}),$$

where $\bar{X}_k:=(x,\mathcal{K}(x,\hat{x},\hat{u}),w_k)$ and $\hat{X}_j:=(\hat{x},\hat{u},\hat{w}_j)$. According to (5), there exists $(x_i,\hat{x}_i)\in\mathcal{T}_d$ and $\hat{u}_i\in\hat{U}_d$ such that $\|(x_i,\hat{x}_i)-(x,\hat{x})\|\le\frac{\epsilon}{2}$, and $\|\hat{u}-\hat{u}_i\|\le\frac{\epsilon}{2}$, respectively. Then:

$$\frac{1}{N\times\hat{N}}\sum_{(k,j)=(1,1)}^{(N,\hat{N})}V(f(\bar{X}_k),\hat{f}(\hat{X}_j))-V(x,\hat{x})=\frac{1}{N\times\hat{N}}\sum_{(k,j)=(1,1)}^{(N,\hat{N})}V(f(\bar{X}_k),\hat{f}(\hat{X}_j))-V(x,\hat{x})$$

$$-\frac{1}{N\times\hat{N}}\sum_{(k,j)=(1,1)}^{(N,\hat{N})}V(f(\bar{X}_{k,i}),\hat{f}(\hat{X}_{j,i}))+\frac{1}{N\times\hat{N}}\sum_{(k,j)=(1,1)}^{(N,\hat{N})}V(f(\bar{X}_{k,i}),\hat{f}(\hat{X}_{j,i})),$$

where $\bar{X}_{k,i} := (x_i, \mathcal{K}(x_i, \hat{x}_i, \hat{u}_i), w_k)$ and $\hat{X}_{j,i} := (\hat{x}_i, \hat{u}_i, \hat{w}_j)$. Employing Lipschitz continuity of V as in (4), one gets:

$$\begin{aligned}
&\frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j)) - V(x, \hat{x}) \\
&\quad - \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) \\
\leq& \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} \mathcal{L}_V \| (f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - (f(\bar{X}_k), \hat{f}(\hat{X}_j)) \| \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}) \\
\leq& \mathcal{L}_V \| (f(\bar{X}_i), \hat{f}(\hat{X}_i)) - (f(\bar{X}), \hat{f}(\hat{X})) \| \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}) \\
\leq& \mathcal{L}_V \| \max \big[\| f(\bar{X}_i) - f(\bar{X}) \|, \| \hat{f}(\hat{X}_i) - \hat{f}(\hat{X})) \| \big] \| \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}) \\
\leq& \mathcal{L}_V \| \max \big[(\| \mathcal{L}_x \| x - x_i \| + \mathcal{L}_u \mathcal{L}_K \| x - x_i \| \|), (\| \mathcal{L}_{\hat{x}} \| \hat{x} - \hat{x}_i \| + \mathcal{L}_{\hat{u}} \| \hat{u} - \hat{u}_i \| \|) \big] \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}) \qquad (16) \\
\leq& \mathcal{L}_V \frac{\mathfrak{e}}{2} \big(\max \big[(\mathcal{L}_x + \mathcal{L}_u \mathcal{L}_K) \frac{\mathfrak{e}}{2}, \mathcal{L}_{\hat{x}} \frac{\mathfrak{e}}{2} + \mathcal{L}_{\hat{u}} \frac{\hat{\mathfrak{e}}}{2} \big] \big) \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}), \\
\leq& \mathcal{L}_V \frac{\mathfrak{e}}{2} \big(\max \big[(\mathcal{L}_x + \mathcal{L}_u \mathcal{L}_K) \frac{\mathfrak{e}}{2}, \mathcal{L}_{\hat{x}} \frac{\mathfrak{e}}{2} + \mathcal{L}_{\hat{u}} \frac{\hat{\mathfrak{e}}}{2} \big] \big) \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) - V(x, \hat{x}) + V(x_i, \hat{x}_i) - V(x_i, \hat{x}_i), \\
\leq& \mathcal{L}_V \frac{\mathfrak{e}}{2} \big(\max \big[(\mathcal{L}_x + \mathcal{L}_u \mathcal{L}_K) \frac{\mathfrak{e}}{2}, \mathcal{L}_{\hat{x}} \frac{\mathfrak{e}}{2} + \mathcal{L}_{\hat{u}} \frac{\hat{\mathfrak{e}}}{2} \big] \big) \\
&\quad + \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_{k,i}), \hat{f}(\hat{X}_{j,i})) + \mathcal{L}_V \frac{\mathfrak{e}}{2} - V(x_i, \hat{x}_i) \qquad (17)
\end{aligned}$$

where (16) follows from Lipschitz continuity of source and target systems as defined in (1), and (17) follows from Lipschitz continuity of V, respectively. Substituting (7), one gets:

$$\frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j)) - V(x, \hat{x}) \tag{18}$$

$$\leq \mathcal{L}_V \frac{\mathfrak{e}}{2}\big(\max \big[(\mathcal{L}_x + \mathcal{L}_u \mathcal{L}_K)\frac{\mathfrak{e}}{2}, \mathcal{L}_{\hat{x}}\frac{\mathfrak{e}}{2} + \mathcal{L}_{\hat{u}}\frac{\hat{\mathfrak{e}}}{2}\big]\big) + \mathcal{L}_V\frac{\mathfrak{e}}{2} - \eta - \delta \overset{(12)}{\rightarrow}$$

$$\leq - \delta, \quad \text{for all } x \in \mathcal{X}, \text{ all } \hat{x} \in \hat{\mathcal{X}}, \text{ all } \hat{u} \in \hat{U}. \tag{19}$$

One could use similar argument to show condition (6) along with validity condition (10) implies condition (2), however, it is omitted here for brevity.

As mentioned previously, to train neural networks V and $\mathcal{K}$, we have replaced the expectation with average mean. To capture the error introduced by this, we have added another robustness parameter δ in Definition 8. We utilize Chebyshev's inequality (Hernández, 2001) to quantify such an error with the associated confidence. The difference between empirical mean in (7) and the expected value in (3) can be quantified by invoking the Chebyshev's inequality as:

$$\mathbb{P}_w\bigg(|\mathbb{E}[V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w), \hat{f}(\hat{x}, \hat{u}), \hat{w})|x, \hat{x}]$$

$$- \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j))| \leq \delta \bigg) \geq 1 - \frac{M}{\delta^2 N \times \hat{N}}, \tag{20}$$

for all $x \in \mathcal{X}, \hat{x} \in \hat{\mathcal{X}}, \hat{u} \in \hat{U}$, where M is an upper-bound for variance of function V, in which we have $\beta \geq \frac{M}{\delta^2 N \times \hat{N}}$. This implies $N \times \hat{N} \geq \frac{M}{\delta^2 \beta}$, which is satisfied according to (11). Finally, consider the following:

$$\mathbb{E}[V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w), \hat{f}(\hat{x}, \hat{u}), \hat{w})|x, \hat{x}] - V(x, \hat{x}) =$$

$$\mathbb{E}[V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w), \hat{f}(\hat{x}, \hat{u}), \hat{w})|x, \hat{x}] - V(x, \hat{x})$$

$$+ \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j)) - \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j))$$

$$\leq \mathbb{E}[V(f(x, \mathcal{K}(x, \hat{x}, \hat{u}), w), \hat{f}(\hat{x}, \hat{u}), \hat{w})|x, \hat{x}] - \frac{1}{N \times \hat{N}} \sum_{(k,j)=(1,1)}^{(N,\hat{N})} V(f(\bar{X}_k), \hat{f}(\hat{X}_j)) - \delta, \tag{21}$$

for all $x \in \mathcal{X}$, all $\hat{x} \in \hat{\mathcal{X}}$, all $\hat{u} \in \hat{U}$, where (21) is followed by (19). According to (20), with probability $1 - \beta$, the difference between absolute value of expectation and average mean in (21) is less than δ, thus, with confidence $1 - \beta$, neural network V along with its corresponding interface function $\mathcal{K}$ satisfies condition (3), and they form a stochastic approximate simulation function as defined in Definition 5. ∎

Appendix B. Experiments

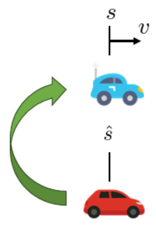
In this section, the effectiveness of the proposed method is demonstrated through four case studies. All experiments are conducted on an Nvidia RTX 4090 GPU. Both networks are parameterized with 5 hidden layers, each containing 200 neurons, and employ ReLU activation. For all experiments, the networks are trained using Algorithm 1 with $\beta = 0.01$. Although mathematical models of all systems are reported for simulation purposes, they were not used to encode neural simulation relation conditions.

B.1. Transfer of Vehicle Control

In these case studies, we aim to transfer a controller designed for a lower-dimensional vehicle model to higher-dimensional ones. The first case study examines the transfer of a simple proportional controller from a one-dimensional vehicle model (position) to a two-dimensional model (position and velocity). The second case study extends this approach by transferring control from a three-dimensional model (with formal guarantees) to a five-dimensional one.

From 1d to 2d. The source system is a one dimensional model:

$$\hat{s}(t+1) = \hat{s}(t) + \tau \hat{u}(t) + \hat{w}(t), \;\; \hat{y}(t) = \hat{s}(t), \quad t \in \mathbb{N},$$



where $\hat{s}(t)$ is position and $\hat{u}(t)$ is velocity at time step t. The target system is a 2 dimensional car model:

$$x(t+1) = \begin{bmatrix} 1 & \tau \\ 0 & 1 \end{bmatrix} x(t) + \begin{bmatrix} 0.5\tau^2 \\ \tau \end{bmatrix} u(t) + w(t), \;\; y(t) = \begin{bmatrix} 1 & 0 \end{bmatrix} x(t), \quad t \in \mathbb{N},$$

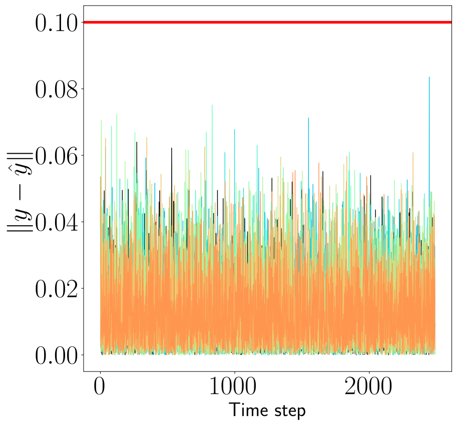
where $\tau = 0.1$ is the sampling time, and $x(t) := [s(t); v(t)]$ is the state vector, in which $s(t)$ and $v(t)$ are position and velocity of the vehicle at time step t, respectively, and $u(t)$ is the acceleration of the vehicle as the control input. Furthermore, we consider $\mathcal{X} = \mathcal{X}_0 = [0, 4] \times [-0.3, 0.3]$, $U = [-0.5, 0.5]$, $\hat{U} = [-0.2, 0.2]$, and $\hat{\mathcal{X}} = \hat{\mathcal{X}}_0 = [0, 4]$ represent the state, initial state and input set of the target system, input and state, and initial state set of the source system, respectively. The corresponding Lipschitz constants are $\mathcal{L}_x = 1.1, \mathcal{L}_u = 0.1, \mathcal{L}_h = 1, \mathcal{L}_{\hat{x}} = 1, \mathcal{L}_{\hat{u}} = 0.1,$ and $\mathcal{L}_{\hat{h}} = 1$. Our method converged in 4 minutes with the following parameters: η=0.001, δ=0.048, $\hat{\mathfrak{e}} = \mathfrak{e}$=0.01, $\mathcal{L}_V$=0.5, $N = \hat{N} = 100, M = 0.01, \alpha(x) = \log(1 + x),$ and $\mathcal{L}_K$=6.75×10^{-5}. In this case study, for $\alpha(\epsilon) = 0.1$, with 99% confidence, we get:

$$\mathbb{P}\big[\max_{t \in \mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \leq 0.1 | x_0, \hat{x}_0\big] \geq 0.9467,$$

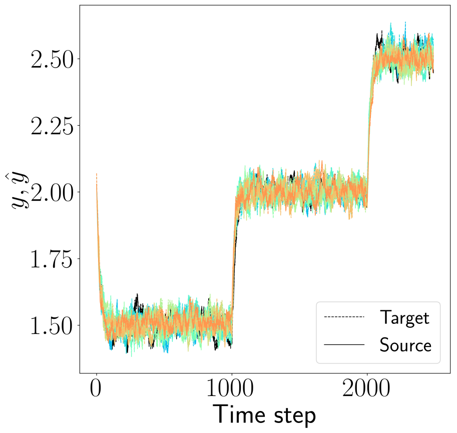
for $\|h(x(0)) - \hat{h}(\hat{x}(0))\| \leq 0.01$

The error between outputs of source and target systems over an state sequence of 2500 steps is depicted in Figure 3, for 10 different realizations. Source system is controlled by a simple proportional controller, and the setpoint was changed with every 1000 steps. We conducted these experiments with 10000 different realizations, and in only three cases did the difference between the outputs exceed 0.1, which aligns with the theoretical results.

From 3d to 5d. For our next case study, we borrowed the source vehicle model from (Ajeleye et al., 2023), and the target system from (Althoff et al., 2017). Here the target system is complex



(a) Error between the outputs.



(b) Trajectories for both systems.

Figure 3: Vehicle control transfer from 1D to 2D. (a) The error between the outputs, and (b) the trajectories for both systems, for 10 different realizations.

five-dimensional model, while the source system is the unicycle model. The target system is a 5 dimensional car:

$$x(t+1) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ \delta(t) \\ v(t) \\ \psi(t) \end{bmatrix} + \tau \begin{bmatrix} v(t)\sin(\psi(t)) \\ v(t)\cos(\psi(t)) \\ u_1(t) \\ u_2(t) \\ v(t)\tan(\delta(t)) \end{bmatrix}, y(t) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} x(t),$$

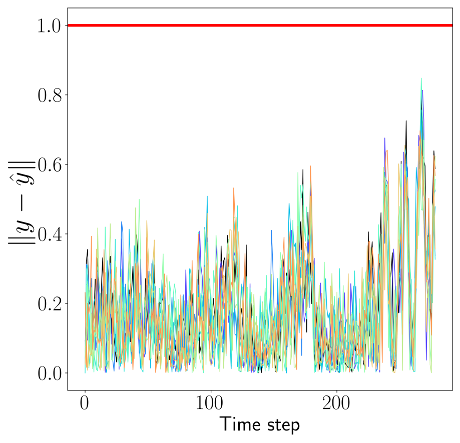
where $\tau = 0.25$ is the sampling time, and $x(t) := [x_1(t); x_2(t); \delta(t); v(t); \psi(t)]$ is the state vector, in which $x_1(t), x_2(t), \delta(t), v(t), \psi(t)$ are horizontal position, vertical position, steering angle, velocity, and heading angle at time step k, respectively. $u_1(t), u_2(t) \in [-1, 1]$ are acceleration and steering of the vehicle as control inputs, at time step t, respectively. The source system is a popular (Zhang et al., 2023; Zhao et al., 2020; Ajeleye et al., 2023) three dimensional unicycle model, given as:

$$\hat{x}(t+1) = \begin{bmatrix} \hat{x}_1(t) \\ \hat{x}_2(t) \\ \hat{x}_3(t) \end{bmatrix} + \tau \begin{bmatrix} \hat{u}_1(t)\cos(q(t)+\hat{x}_3(t))/\cos(q(t)) \\ \hat{u}_1(t)\sin(q(t)+\hat{x}_3(t))/\cos(q(t)) \\ \hat{u}_1(t)\tan(\hat{u}_2(t)) \end{bmatrix}, \hat{y}(t) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \hat{x}(t),$$

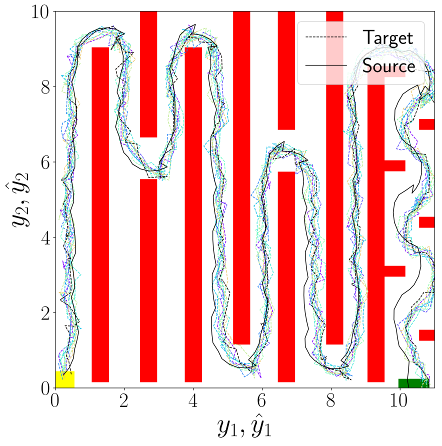
where $\hat{x} := [\hat{x}_1, \hat{x}_2, \hat{x}_3]$ is the state vector, in which $\hat{x}_1, \hat{x}_2, \hat{x}_3$ are horizontal position, vertical position, and steering angle, respectively, and $q(t) := \tan^{-1}(\tan \hat{u}_2(t)/2)$. Furthermore, $u_1, u_2 \in [-1, 1]$ are inputs to the system.

We consider $\hat{\mathcal{X}} = [0, 10] \times [0, 10] \times [-\pi, \pi]$, $\hat{\mathcal{X}}_0 = [0, 1] \times [0, 1] \times [0, 0.2]$, $\hat{U} = [-0.9, 0.9]^2$, which represent the state, initial state and input set of the source system, respectively. Moreover, $\mathcal{X} = \hat{\mathcal{X}} \times [-1, 1]^2$, $\mathcal{X}_0 = \hat{\mathcal{X}}_0 \times [-1, 1]^2$, $U = [-1, 1]^2$, represent the state, initial state and input set of the target system.

The corresponding Lipschitz constants are $\mathcal{L}_x = 1.1, \mathcal{L}_u = 0.1, \mathcal{L}_h = 1, \mathcal{L}_{\hat{x}} = 1.1, \mathcal{L}_{\hat{u}} = 0.1,$ and $\mathcal{L}_{\hat{h}} = 1$. The training converged in 120 minutes with following parameters: η=0.03, $\delta =$



(a) Error between the outputs.



(b) Trajectories for both systems.

Figure 4: Vehicle control transfer from 3D to 5D. (a) The error between the outputs, and (b) the trajectories for both systems, for 10 different realizations.

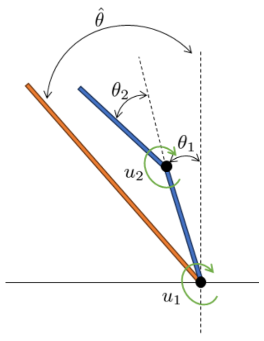
$0.02, \mathfrak{e}{=}0.002, \mathcal{L}_V{=}4, N = \hat{N} = 200, M = 0.1, \alpha(x) = \log(x+1),$ and $\mathcal{L}_K{=}4.1$. In this case study, for $\alpha(\epsilon) = 1$, with 99% confidence, we get:

$$\mathbb{P}\big[\max_{t\in\mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \leq 1 | x_0, \hat{x}_0\big] \geq 0.9287,$$

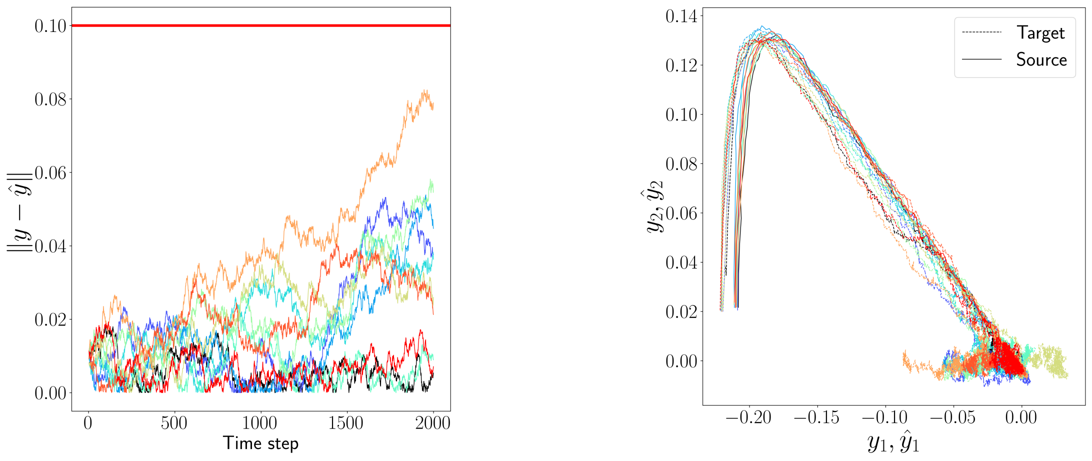
for $\|h(x(0)) - \hat{h}(\hat{x}(0))\| \leq 0.1$.

The error between outputs of source and target systems over an state sequence of 300 steps is depicted in Figure 4, for 10 different realizations. We leveraged the tool `SCOTS` (Rungger and Zamani, 2016) to design a controller for the source system, ensuring it reaches the goal (depicted by the green rectangle) while avoiding obstacles (depicted by red rectangles) from the initial set of states (depicted by the yellow rectangle). Note that applying `SCOTS` to the target system is infeasible due to its high dimensionality. We conducted these experiments with 10000 different realizations, and in only 52 cases did the difference between the outputs exceed 1, which aligns with the theoretical results.

B.2. Pendulum Control: From Single-Jointed to Double-Jointed



For our third case study, we transfer control from a single-jointed inverted pendulum to a double-jointed one as shown in the inset. This system serves as a classic benchmark in control theory due to its combination of inherent instability and nonlinearity, making it an ideal platform for assessing control transfer methods. Practical applications of the double inverted pendulum include bipedal locomotion in robotics, self-balancing vehicles, and crane load stabilization—all of which demand precise control of unstable, high-dimensional systems. The target system has the following model:



(a) Error between the outputs. (b) Trajectories for both systems.

Figure 5: Single-jointed pendulum control transfer to double-jointed pendulum. (a) The error between the outputs, and (b) the trajectories for both systems, for 10 different realizations.

$$\begin{bmatrix}\theta_1(t{+}1)\\ \omega_1(t{+}1)\\ \theta_2(t{+}1)\\ \omega_2(t{+}1)\end{bmatrix} = \begin{bmatrix}\theta_1(t){+}\tau\omega_1(t)\\ \omega_1(t){+}\tau(g\sin(\theta_1(t)){-}\sin(\theta_1(t){-}\theta_2(t))\omega_1^2(t))\\ \theta_2(t){+}\tau\omega_2(t)\\ \omega_2(t){+}\tau(g\sin(\theta_2(t)){+}\sin(\theta_1(t){-}\theta_2(t))\omega_2^2(t))\end{bmatrix} + \tau\begin{bmatrix}0 & 0\\ 30 & 0\\ 0 & 0\\ 0 & 39\end{bmatrix}U(t),$$

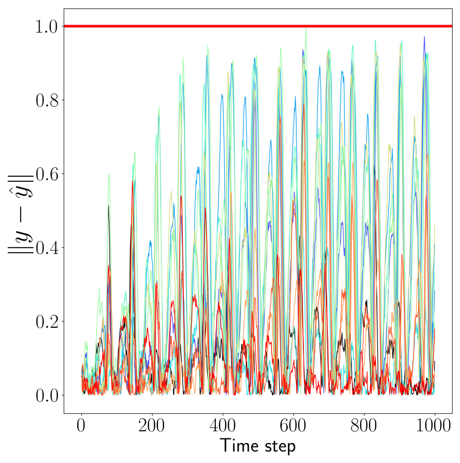
where $[\theta_1(t);\omega_1(t);\theta_2(t);\omega_2(t)] \in [-0.5, 0.5]^4$, and $y(t) = [\theta_1(t), \omega_1(t)]$ is the output. Here, θ_1 and θ_2 represent the angular position of the first and the second joint, respectively, and ω_1 and ω_2 are the angular velocity, respectively, and $U{\in}[-1, 1]^2$ are the inputs applied to the first and second joint, respectively. The initial set of states are $\mathcal{X}_0 = \mathcal{X}, \hat{\mathcal{X}}_0 = \hat{\mathcal{X}}$ for the target and the source systems, respectively. This is a simplified version of double inverted pendulum, where we assumed the second derivative of both angles are zero, to be able to discretize this system. The source system is an inverted pendulum with the following model:

$$\begin{bmatrix}\hat{\theta}(t+1)\\ \hat{\omega}(t+1)\end{bmatrix} = \begin{bmatrix}\hat{\theta}(t) + \tau\hat{\omega}(t)\\ \hat{\omega}(t) + \tau g\sin(\hat{\theta}(t))\end{bmatrix} + \tau\begin{bmatrix}0\\ 9.1\end{bmatrix}\hat{u}(t), \quad \hat{y}(t) = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\hat{x}(t),$$

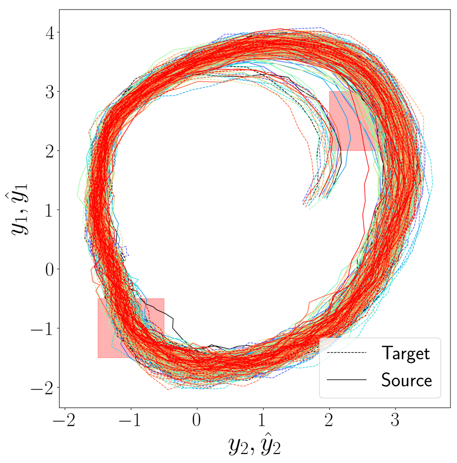
where $[\hat{\theta}(t);\hat{\omega}(t)]{\in}[-0.5, 0.5]^2$ represent the angular position and velocity, respectively, and $\tau{=}0.01$ is the sampling time, and $\hat{U} = [-1, 1]$ is the input set. Furthermore, for both systems, $g = 9.8$ is the gravitational acceleration. The Lipschitz constants are $\mathcal{L}_x{=}1.098, \mathcal{L}_u = 0.39, \mathcal{L}_h{=}1, \mathcal{L}_{\hat{x}}{=}1.098, \mathcal{L}_{\hat{u}}{=}0.091$, and $\mathcal{L}_{\hat{h}} = 1$.

The training converged in 150 minutes with following parameters: $\eta{=}0.01, \delta = 0.01, \hat{\mathfrak{e}} = 0.1, \mathfrak{e} = 0.001, \mathcal{L}_V = 1.2, N = \hat{N} = 100, M = 0.005, \alpha(x) = \log(x + 1)$, and $\mathcal{L}_K{=}5.9$. In this case study, for $\alpha(\epsilon) = 0.1$, with 99% confidence, we get:

$$\mathbb{P}\big[\max_{t\in\mathbb{N}} \|h(x(t)) - \hat{h}(\hat{x}(t))\| \le 0.1 | x_0, \hat{x}_0\big] \ge 0.8567,$$



(a) Error between the outputs.



(b) Trajectories for both systems.

Figure 6: Marine vessel control transfer from 3D to 6D. (a) The error between the outputs, and (b) the trajectories for both systems, for 10 different realizations.

for $\|h(x(0)) - \hat{h}(\hat{x}(0))\| \leq 0.01$.

The error between outputs of source and target systems over an state sequence of 2000 steps is depicted in Figure 3, for 10 different realizations. Source system is controlled by a simple proportional controller, and the setpoint was changed with every 1000 steps. We conducted these experiments with 10000 different realizations, and in only 867 cases did the difference between the outputs exceed 0.1, which aligns with the theoretical results. The source system is controlled by a formally correct neural control barrier certificate borrowed from (Nadali et al., 2025), which keeps the pendulum in the upright position.

B.3. Marine Vessel

Our final case study is the marine vessel system from (Meyer et al., 2020). The target system is a complex six-dimensional vessel, while the source system includes only its kinematic components. The target system has the following model:

$$\eta(t+1) = \eta(t) + \tau(R(\psi(t))\nu(t)),$$
$$\nu(t+1) = \nu(t) + \tau M^{-1}\big(U(t) - C(\nu)\nu(t) - D\nu(t)\big),$$

where $\eta := [x, y, \psi]$ are the South-North and West-East positions and heading of the ship, and $\nu := [u; v; r]$ are the surge and sway velocities, and yaw rate of the ship. $R(\psi)$ is a rotation matrix, and $U \in \mathbb{R}^3$ is the control input affecting the three acceleration states of the ship. Moreover, M, D, C represent the inertia matrix including hydrodynamic added mass, damping matrix, and Coriolis matrix:

$$M = \begin{bmatrix} 87.4 & 0 & 0 \\ 0 & 98.3 & 2.48 \\ 0 & 2.48 & 22.2 \end{bmatrix}, C = u \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 98.3 \\ 0 & 0 & 2.48 \end{bmatrix}, D = \begin{bmatrix} 6.58 & 0 & 0 \\ 0 & 37.7 & 2.66 \\ 0 & 2.66 & 19.3 \end{bmatrix}.$$

The source system is only the kinematics part of the target system:

$$\hat{\eta}(t+1) = \hat{\eta}(t) + \tau R(\hat{\psi}(t))\hat{U}(t).$$

The output of both systems are South-North and West-East positions of both systems, respectively.

Due to the high dimensionality of the target and source systems, formal guarantees are infeasible as the sample complexity is prohibitively high. However, we present this case study to showcase the success of our training and provide empirical evidence of its correctness. Figure 6 illustrates the output sequences of both systems, over 10 realizations. We utilized the tool `SCOTS` to design a controller for the source system, ensuring infinite visits to both pink rectangles. Note that, applying `SCOTS` directly to the target system is infeasible due to its high dimensionality. This demonstrates the utility of our approach in enabling control transfer when traditional methods are impractical.