Neural Barrier Certificates for Monotone Systems

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***Abstract*— Barrier certificates are real-valued functions used to formally verify the safety of dynamical systems. For systems with unknown dynamics, data-driven barrier certificates have been developed to guarantee safety using only a finite set of data. However, most existing methods rely on knowledge of Lipschitz bound of the system and require a fine discretization of the state set, leading to high sample complexity. In this paper, we propose a novel data-driven framework for learning barrier certificates for unknown monotone systems. Our approach is based on a suitable embedding of barrier certificates into a higher-dimensional space. By leveraging interval analysis, this embedding enables us to establish data-driven safety certificates for monotone systems. Unlike existing methods, our framework is independent of Lipschitz continuity and quantization parameters of the state set, allowing for arbitrary state-space discretization and thereby alleviating extensive sampling requirements. To efficiently construct barrier certificates, we introduce suitable neural network architectures and train them using an appropriately designed loss function. We illustrate our approach through two case studies, demonstrating that our method successfully finds separable embedded barrier certificates while substantially reducing sample complexity compared to conventional neural barrier certificate methods, all while maintaining formal correctness guarantees.**

I. Introduction

Autonomous systems are increasingly being deployed in real-world applications, including self-driving vehicles, robotics, and medical devices. A key concern in these systems is ensuring their safety, as even rare failures can result in life-threatening situations. While extensive simulations can provide valuable insights about safety of these systems, they do not offer any formal guarantees, as they cannot exhaustively explore every possible trajectory over time. Consequently, mathematical frameworks capable of ensuring system safety under all conditions are introduced in the literature. Existing mathematical frameworks for ensuring safety of autonomous systems include reachability analysis [1], abstraction-based methods [2], and barrier certificates [3].

The notion of barrier certificate has been used as an effective tool for safety verification and control synthesis of autonomous systems [4]. A barrier certificate is a real-valued function defined over the set of states that separates the safe and unsafe regions, providing sufficient condition for safe evolution of the system. Various versions of barrier certificates have been introduced and widely applied to ensure safety, including vector barriers [5], higher-order barrier functions [6], and stochastic barriers [7]. Despite their efficiency in verifying system safety, nearly all of these methods require a precise mathematical model to provide safety guarantees. Since a precise mathematical model is often unavailable in many applications, model-free approaches to barrier certificates have recently gained significant attentions.

Model-free approaches, including scenario-based and trajectory-based methods, construct barrier certificates using a finite set of data while still providing formal guarantees [8], [9]. Recently, neural networks have been used to learn barrier certificates [10] and control barrier functions [11], [12]. Unfortunately, most of these data-driven approaches suffer from sample complexity issues, meaning that the amount of data required to provide formal guarantees grows exponentially with the dimension of the system. Moreover, nearly all these methods require some knowledge of the systems' Lipschitz constants to construct barrier certificates correctly. This raises the question: *is it possible to relax the Lipschitz continuity requirements or decrease the amount of data needed for safety verification of system with specific structural properties, particularly those exhibiting monotonicity*?

Monotone systems are a class of dynamical systems whose trajectories preserve a partial order. They exhibit highly regular properties and are widely observed in real-world applications, including traffic networks [13] and biological systems [14]. It has been shown that the monotonicity of systems can reduce the sample complexity of their Lyapunov analysis [15]. However, the role of monotonicity in constructing barrier certificates is less studied the literature.

Contributions: In this paper, we present a novel data-driven framework for the safety verification of unknown monotone systems using a finite number of samples. By embedding barrier functions into a higher-dimensional space, we introduce a new formulation for system safety verification. A key advantage of this approach is its compatibility with interval analysis, enabling a data-driven method that leverages embedded barrier certificates to ensure the safety of monotone systems. We then train neural networks with suitably designed loss functions, to learn embedded barrier certificates. Our approach provides formal safety guarantees for monotone systems, does not use the knowledge of the system's Lipschitz bound, and can accommodate arbitrary state-space sampling. We demonstrate our framework on a two-dimensional system and showcase its efficiency and scalability in a large-scale traffic network. Our results indicate that neural embedded barrier certificates not only scale to high-dimensional systems but also outperform state-of-the-art algorithms in terms of sample complexity.

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II. Definitions and Preliminaries

A. Notation

For vector $x\in\mathbb{R}^n$, we denote its ith component by x_i. For vectors $x,y\in\mathbb{R}^n$, we denote $x\leq y$ if $x_i\leq y_i$, for every $i\in\{1,\dots,n\}$. We denote that ℓ_1-norm of vector x by $\|x\|_1=\sum_{i=1}^n |x_i|$. For sets A and $B\subseteq A$, we denote the set difference as $A\backslash B$. We represent a hyper rectangle by $[\underline{x},\overline{x}] = \{x\in\mathbb{R}^n \mid \underline{x}\leq x\leq\overline{x}\}$. For the Euclidean space $\mathbb{R}^{2n}$, we define the southeast order $\leq_{\mathrm{SE}}$ by $\left[\begin{smallmatrix} x \\ y\end{smallmatrix}\right] \leq_{\mathrm{SE}} \left[\begin{smallmatrix} \widehat{x} \\ \widehat{y}\end{smallmatrix}\right]$ if and only if $x\leq\widehat{x}$ and $\widehat{y}\leq y$. Given a set $\mathcal{X}$, we define $\mathcal{T}_{\mathcal{X}} \subseteq \mathcal{X}\times\mathcal{X}$ as the set $\mathcal{T}_{\mathcal{X}} = \{(x,y)\in\mathcal{X}\times\mathcal{X} \mid x\leq y \text{ or } y\leq x\}$. Consider the sets $\mathcal{X}\subseteq\mathbb{R}^n$ and $\mathcal{Y}\subseteq\mathbb{R}^m$ and let $\leq_{\mathcal{X}}$ and $\leq_{\mathcal{Y}}$ be partial orders on $\mathcal{X}$ and $\mathcal{Y}$, respectively. Then the map $f:\mathcal{X}\to\mathcal{Y}$ is monotone with respect to partial orders $\leq_{\mathcal{X}}$ and $\leq_{\mathcal{Y}}$ if, for every $x,y\in\mathcal{X}$ such that $x\leq_{\mathcal{X}} y$, we have $f(x)\leq_{\mathcal{Y}} f(y)$. When the partial orders $\leq_{\mathcal{X}}$ and $\leq_{\mathcal{Y}}$ are the standard partial orders on Euclidean spaces, we simply call f monotone. We define ReLU by $\mathrm{ReLU}(x)=\max(0,x)$.

B. Safety Verification using Barrier Certificate

We start by defining a discrete-time dynamical system.

Definition 2.1: A *discrete-time dynamical system* is a tuple $\mathfrak{S} := (\mathcal{X},\mathcal{X}_0,f)$, where $\mathcal{X}\subseteq\mathbb{R}^n$ denotes the set of states, $\mathcal{X}_0\subseteq\mathcal{X}$ is the set of initial states, and $f:\mathcal{X}\to\mathcal{X}$ is the state-transition map. A discrete-time system $\mathfrak{S} = (\mathcal{X},\mathcal{X}_0,f)$, initialized at $x_0\in\mathcal{X}_0$, evolves according to

$$x_{t+1} = f(x_t), \qquad \forall t\geq 0. \tag{1}$$

Given a discrete-time dynamical system $\mathfrak{S} = (\mathcal{X},\mathcal{X}_0,f)$ and a set of unsafe states $\mathcal{X}_u\subseteq\mathcal{X}$, we say that $\mathfrak{S}$ is *safe* if no trajectory of the system, originating from any state in $\mathcal{X}_0$, ever reaches $\mathcal{X}_u$. To verify the safety of $\mathfrak{S}$, we can employ the notion of *barrier certificates*, which provides sufficient conditions for ensuring safety.

Definition 2.2: Consider a discrete-time dynamical system $\mathfrak{S} = (\mathcal{X},\mathcal{X}_0,f)$. A function $B:\mathcal{X}\to\mathbb{R}$ is a *barrier certificate* for $\mathfrak{S}$ if it satisfies the following conditions:

$$\begin{aligned}
&B(x)\leq 0, && \forall x\in\mathcal{X}_0\\
&B(x)> 0, && \forall x\in\mathcal{X}_u, \text{ and}\\
&B(f(x))\leq 0, && \forall x \text{ s.t. } B(x)\leq 0.
\end{aligned} \tag{2}$$

The effectiveness of barrier certificates in verifying the safety of dynamical systems is shown in the following theorem [3].

Theorem 1 (Safety via barrier certificates): Consider a discrete-time dynamical system $\mathfrak{S}$. If a barrier certificate B exists for $\mathfrak{S}$, then the system is safe and $\Omega = \{x\in\mathcal{X} \mid B(x)\leq 0\}$ is a forward-invariant set for $\mathfrak{S}$.

When the state transition f is unknown, identifying a barrier certificate to prove the system's safety becomes challenging. Consequently, a common approach in the literature is to rely on scenario-based robust programming [16], [17].

C. Scenario-based barrier certificate

Scenario-based approaches fundamentally rely on evaluating the transition map f over a finite set of data points and account for various possible scenarios by incorporating uncertainties into the barrier certificate design. Prior to presenting the scenario-based framework for safety, we begin by introducing the following definition.

Definition 2.3 (Hyper-rectangular partition): A family of hyper-rectangles $\{[\underline{x}_i,\overline{x}_i]\}_{i\in\mathcal{P}}$, $\mathcal{P}=\{1,\dots,N\}$, is called a *hyper-rectangular partition* of compact set $\mathcal{X}$ if, for every $x\in\mathcal{X}$, there exists $i\in\mathcal{P}$ such that $x\in[\underline{x}_i,\overline{x}_i]$ and, for every $i,j\in\mathcal{P}$, we have $[\underline{x}_i,\overline{x}_i]\cap[\underline{x}_j,\overline{x}_j]=\emptyset$. The depth d of the hyper-rectangular partition $\{[\underline{x}_i,\overline{x}_i]\}_{i\in\mathcal{P}}$ is defined by $d=\max_{i\in\mathcal{P}}\left\{\frac{1}{\|\overline{x}_i-\underline{x}_i\|_\infty}\right\}$.

Given a partition $\{[\underline{x}_i,\overline{x}_i]\}_{i\in\mathcal{P}}$ and an initial state set $\mathcal{X}_0\subseteq\mathcal{X}$ and an unsafe set $\mathcal{X}_u\subseteq\mathcal{X}$, we define the indices $\mathcal{I}$ and $\mathcal{U}$ as the minimal subsets of $\mathcal{P}$ satisfying

$$\mathcal{X}_0\subseteq\bigcup_{i\in\mathcal{I}}[\underline{x}_i,\overline{x}_i], \qquad \mathcal{X}_u\subseteq\bigcup_{i\in\mathcal{U}}[\underline{x}_i,\overline{x}_i]. \tag{3}$$

The following theorem reformulates the barrier certificate conditions in a scenario-based program to ensure the safety of $\mathfrak{S}$.

Theorem 2: Consider a discrete-time dynamical system $\mathfrak{S} = (\mathcal{X},\mathcal{X}_0,f)$. Let $\{[\underline{x}_i,\overline{x}_i]\}_{i\in\mathcal{P}}$ be a hyper-rectangular partition of $\mathcal{X}$ with $\mathcal{I}$ and $\mathcal{U}$ defined as in (3) and let $\eta,\gamma>0$. Assume there exists $B:\mathcal{X}\to\mathbb{R}$ satisfying

$$B(\tfrac{\overline{x}_i+\underline{x}_i}{2})\leq-\eta \qquad \forall i\in\mathcal{I}, \tag{4}$$
$$B(\tfrac{\overline{x}_i+\underline{x}_i}{2})>\eta \qquad \forall i\in\mathcal{U}, \tag{5}$$
$$B(f(\tfrac{\overline{x}_i+\underline{x}_i}{2}))\leq-\gamma \qquad \forall i\in\mathcal{Z}_\eta, \tag{6}$$

where the index set $\mathcal{Z}_\eta\subseteq\mathcal{P}$ is defined as $B(\frac{\overline{x}_i+\underline{x}_i}{2})\leq\eta$, $\forall i\in\mathcal{Z}_\eta$. Let L_B and L_f denote the ℓ_∞-norm Lipschitz bound of the barrier function B and the transition map f, respectively. If for every $i\in\mathcal{P}$,

$$\|\overline{x}_i-\underline{x}_i\|_\infty\leq\tfrac{2\eta}{L_B}, \qquad \|\overline{x}_i-\underline{x}_i\|_\infty\leq\tfrac{2\gamma}{L_B L_f}, \tag{7}$$

Then B is a barrier certificate for $\mathfrak{S}$.

Proof: We show that if conditions (4)-(6) hold for hyper-rectangular partition $\{[\underline{x}_i,\overline{x}_i]\}_{i\in\mathcal{P}}$ of $\mathcal{X}$, then conditions (2) are satisfied. Note that for every $x\in\mathcal{X}_0$, there exists $i\in\mathcal{I}$ such that $x\in[\underline{x}_i,\overline{x}_i]$. Then

$$\begin{aligned}
B(x) &\leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) + B(x) - B(\tfrac{\overline{x}_i+\underline{x}_i}{2})\\
&\leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) + |B(x) - B(\tfrac{\overline{x}_i+\underline{x}_i}{2})|\\
&\leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) + L_B\|x-\tfrac{\underline{x}_i+\overline{x}_i}{2}\|_\infty\\
&\leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) + L_B\tfrac{\|\overline{x}_i-\underline{x}_i\|_\infty}{2} \leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2})+\eta\leq 0.
\end{aligned}$$

Similarly, one can show that, for every $x\in\mathcal{X}_u$, we have $B(x)>0$. Finally, consider any $x\in\mathcal{X}$ such that $B(x)\leq 0$. Then, there exists $i\in\mathcal{P}$ such that $x\in[\underline{x}_i,\overline{x}_i]$. This implies that

$$\begin{aligned}
B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) &= B(x) + B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) - B(x)\\
&\leq B(x) + |B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) - B(x)| \leq \tfrac{\|\overline{x}_i-\underline{x}_i\|_\infty}{2}L_B\leq\eta.
\end{aligned}$$

This implies that $i \in \mathcal{Z}$ and $B(f(\frac{\underline{x}_i+\overline{x}_i}{2})) \leq -\gamma$. Thus,

$$\begin{aligned} B(f(x)) &\leq B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2})) + B(f(x)) - B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2})) \\ &\leq B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2})) + |B(f(x)) - B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2}))| \\ &\leq B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2})) + \tfrac{\|\underline{x}_i-\overline{x}_i\|_\infty}{2} L_B L_f \\ &\leq B(f(\tfrac{\underline{x}_i+\overline{x}_i}{2})) + \gamma \leq 0. \end{aligned}$$

This completes the proof. ∎

The scenario-based approach in Theorem 2 has three key limitations: (i) it requires knowledge of the Lipschitz bound of the transition map f, or at least an upper bound on this value; (ii) it depends on specialized techniques for estimating the Lipschitz bound of the barrier function; and (iii) it is only applicable to partitioning schemes that satisfy the validity conditions (7), which may lead to high sample complexity.

III. Barrier Certificate for Monotone Systems

In this paper, we focus on a special class of dynamical systems known as monotone systems. For these systems, we propose a data-driven framework for learning barrier certificates using interval analysis. Our approach enables the construction of certificates through arbitrary partitioning of the state set, without prior knowledge of the Lipschitz constants of system's transition map and barrier certificates.

A. Problem Statement

We first introduce the class of monotone systems.

Definition 3.1 (Monotone systems): A discrete-time dynamical system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ is called monotone if the transition map f is monotone, i.e., for every $x, y \in \mathcal{X}$ such that $x \leq y$, we have $f(x) \leq f(y)$.

For differentiable transition map f and convex set $\mathcal{X}$, one can show that system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ is monotone if and only if $Df(x) \geq 0_{n\times n}$, for every $x \in \mathcal{X}$ [18].

We consider a monotone discrete-time dynamical system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ with unknown transition map f. We assume to have access to a simulator of f, allowing us to query its values at different points in the state set. Given this monotone discrete-time system $\mathfrak{S}$ and an unsafe set of states $\mathcal{X}_u \subseteq \mathcal{X}$, our objective is to provide guarantees for safety of $\mathfrak{S}$ using a finite number of samples.

B. Embedded Barrier Certificate

In this section, we embed barrier certificates into a higher-dimensional space and show that, for monotone systems, this embedding naturally leads to a novel data-driven formulation of barrier certificates, distinct from the scenario-based approach in (4)–(6). We call a function $H : \mathcal{T}_X \to \mathbb{R}$ an *embedded barrier certificate* for a discrete-time system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ if H is monotone with respect to southeast partial order $\leq_{\mathrm{SE}}$ and it satisfies

$$\begin{aligned} &H(x,x) \leq 0 && \forall x \in \mathcal{X}_0, \\ &H(x,x) > 0 && \forall x \in \mathcal{X}_u, \\ &H(f(x), f(x)) \leq 0 && \forall x \in \text{ s.t. } H(x,x) \leq 0. \end{aligned} \tag{8}$$

The following theorem establishes the equivalence between barrier certificates and embedded barrier certificates for ensuring the safety of $\mathfrak{S}$. It serves as a key ingredient in proving the main result of this paper (cf. Theorem 4).

Theorem 3 (Embedded Barrier certificates): Consider a discrete-time system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$. The following statements are equivalent:

1) there exists a barrier certificate $B : \mathcal{X} \to \mathbb{R}$ for $\mathfrak{S}$,
2) there exists an embedded barrier certificate $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$ for $\mathfrak{S}$.

Additionally, if $\mathcal{X}$ is compact and B is locally Lipschitz, then statement (1) is equivalent to the following statement:

3) there exists an embedded barrier certificate $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$ for $\mathfrak{S}$ such that H can be decomposed as $H(x,y) = B_1(x) - B_2(y)$, for all $(x,y) \in \mathcal{T}_{\mathcal{X}}$, for two monotone functions $B_1, B_2 : \mathcal{X} \to \mathbb{R}$.

Proof: We first show $2 \implies 1$. Let $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$ be an embedded barrier function for $\mathfrak{S}$. Then we can define $B : \mathcal{X} \to \mathbb{R}$ by $B(x) = H(x,x)$, for every $x \in \mathcal{X}$. Then, it is clear that conditions in (8) reduce to the ones in (2). Now we show that $1 \implies 2$. Suppose that there exists a barrier function $B : \mathcal{X} \to \mathbb{R}$ for $\mathfrak{S}$ which satisfies (2). We define $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$ as follows:

$$H(x,y) = \begin{cases} \min_{z\in[x,y]} B(z) & \text{if } \ x \leq y, \\ \max_{z\in[y,x]} B(z) & \text{if } \ y \leq x. \end{cases}$$

Using this definition, it is clear that $H(x,x) = B(x)$, for every $x \in \mathcal{X}$ and thus it satisfies conditions (8). So it suffices to show that H is monotone with respect to $\leq_{\mathrm{SE}}$. Let $\left[\begin{smallmatrix} x \\ y \end{smallmatrix}\right] \leq_{\mathrm{SE}} \left[\begin{smallmatrix} \widehat{x} \\ \widehat{y} \end{smallmatrix}\right]$. This implies that $x \leq \widehat{x}$ and $\widehat{y} \leq y$. We should consider two cases, (i) $x \leq y$, and (ii) $y \leq x$. If case (i) happens, then $H(x,y) = \min_{z\in[x,y]} B(z) \leq \min_{z\in[\widehat{x},\widehat{y}]} B(z) = H(\widehat{x},\widehat{y})$. If case (ii) happens, then $H(x,y) = \max_{z\in[y,x]} B(z) \leq \max_{z\in[\widehat{y},\widehat{x}]} B(z) = H(\widehat{x},\widehat{y})$. So in both cases, we have $H(x,y) \leq H(\widehat{x},\widehat{y})$. Finally, we show the equivalence $1 \iff 3$. First, note that the implication $3 \implies 1$ follows similarly to the proof of implication $2 \implies 1$. Therefore, we only need to show $1 \implies 3$. Since B is locally Lipschitz and $\mathcal{X}$ is compact, there exists $L \in \mathbb{R}_{\geq 0}$ such that $|B(y) - B(x)| \leq L\|y - x\|_1$, for every $x, y \in \mathcal{X}$. We define functions $B_1, B_2 : \mathcal{X} \to \mathbb{R}$ by $B_1(x) = L\mathbb{1}_n^\top x$ and $B_2(x) = L\mathbb{1}_n^\top x - B(x)$, for every $x \in \mathcal{X}$. We first show that B_1, B_2 are monotone. Let $x, y \in \mathcal{X}$ be such that $x \leq y$. Then $B_1(x) = L\mathbb{1}_n^\top x \leq \mathbb{1}_n^\top y = B_1(y)$. Moreover,

$$\begin{aligned} B_2(y) &= L\mathbb{1}_n^\top y - B(y) = L\mathbb{1}_n^\top x + L\mathbb{1}_n^\top (y-x) - B(y) \\ &\geq L\mathbb{1}_n^\top x + B(y) - B(x) - B(x) = B_2(x), \end{aligned}$$

where the inequality holds because $y - x \geq 0$ and $B(y) - B(x) \leq |B(y) - B(x)| \leq L\|y-x\|_1 = L\mathbb{1}_n^\top (y-x)$. Since B_1 and B_2 are both monotone functions, the function H defined by $H(x,y) = B_1(x) - B_2(y)$, for every $x, y \in \mathcal{T}_{\mathcal{X}}$ is monotone with respect to $\leq_{\mathrm{SE}}$. On the other hand, it is clear that $H(x,x) = B_1(x) - B_2(x) = B(x)$, for every $x \in \mathcal{X}$. Thus H satisfies conditions (8). This implies that H is an embedded barrier certificate for $\mathfrak{S}$. ∎

Theorem 3 states that switching from traditional barrier certificates to (separable) embedded barrier certificates does not introduce any additional conservatism for safety verification. For a discrete-time system $\mathfrak{S}$, the embedded barrier certificate H is closely related to the notion of inclusion function of the barrier function B in interval analysis [19]. In the next section, we demonstrate that a key advantage of embedded barrier certificates over traditional ones is their compatibility with interval analysis, which enables a novel data-driven formulation for safety verification.

C. Data-driven Embedded Barrier Certificate

In this section, we combine the notion of embedded barrier certificates with elements of interval analysis and propose a data-driven framework for ensuring the safety of unknown monotone systems using a finite number of samples.

Theorem 4 (Data-driven embedded barrier certificate): Consider a monotone discrete-time system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ with an unsafe set $\mathcal{X}_u \subseteq \mathcal{X}$ and suppose $\{[\underline{x}_i, \overline{x}_i]\}_{i\in\mathcal{P}}$ is a hyper-rectangular partition of $\mathcal{X}$ with indices $\mathcal{I}$ and $\mathcal{U}$ as defined in (3). If there exists a function $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$ which is monotone with respect to $\leq_{\mathrm{SE}}$ and satisfies

$$H(\overline{x}_i, \underline{x}_i) \leq 0 \qquad \forall i \in \mathcal{I}, \tag{9}$$

$$H(\underline{x}_i, \overline{x}_i) > 0 \qquad \forall i \in \mathcal{U}, \tag{10}$$

$$H(f(\overline{x}_i), f(\underline{x}_i)) \leq 0 \quad \forall i \in \mathcal{P} \text{ s.t. } H(\underline{x}_i, \overline{x}_i) \leq 0, \tag{11}$$

then $\mathfrak{S}$ is safe.

Proof: Since H is monotone with respect to $\leq_{\mathrm{SE}}$, we have $H(x, x) \leq H(\overline{x}_i, \underline{x}_i) \leq 0$. Similarly, we can show that $H(x, x) > 0$, for every $x \in \mathcal{X}_u$. Now, consider any $x \in \mathcal{X}$ such that $x \in [\underline{x}_i, \overline{x}_i]$ and $H(x, x) \leq 0$. Note that H is monotone with respect to $\leq_{\mathrm{SE}}$. Thus, one has $H(\underline{x}_i, \overline{x}_i) \leq H(x, x) \leq 0$. Since f is monotone, one gets $f(x) \leq f(\overline{x}_i)$ and $f(\underline{x}_i) \leq f(x)$. Using the monotonicity of H with respect to $\leq_{\mathrm{SE}}$, one can conclude that $H(f(x), f(x)) \leq H(f(\overline{x}_i), f(\underline{x}_i)) \leq 0$. This implies that H is an embedded barrier certificate for $\mathfrak{S}$. By Theorem 3, there exists of a barrier certificate $B : \mathcal{X} \to \mathbb{R}$ for $\mathfrak{S}$ and the safety of $\mathfrak{S}$ follows from Theorem 1. ∎

The data-driven approach proposed in Theorem 4 is fundamentally different from the scenario-based barrier certificate approach in Theorem 2, which guarantees safety by robustifying the original barrier certificate (2) and leveraging the Lipschitz bound of the transition map f. Indeed, the data-driven approach in Theorem 4 has two key advantages compared to the scenario-based approach in Theorem 2. First, it does not require prior knowledge of the Lipschitz bound of f. Second, it can be applied to arbitrary partitioning of the state set. However, a natural question arises: how does the conservatism of the data-driven approach in Theorem 4 compare to that of the scenario-based method in Theorem 2? The next theorem establishes that, for monotone systems, the data-driven approach in Theorem 4 is indeed less conservative than the scenario-based approach given in (4)–(6).

Theorem 5 (Accuracy of embedded barrier certificates): Consider a discrete-time monotone system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$, and let $\{[\underline{x}_i, \overline{x}_i]\}_{i\in\mathcal{P}}$ be a hyper-rectangular partition of $\mathcal{X}$ with indices $\mathcal{I}$ and $\mathcal{U}$ defined in (3). Suppose there exists a barrier certificate $B : \mathcal{X} \to \mathbb{R}$ for $\mathfrak{S}$ satisfying (4)-(6). Then, the function $H : \mathcal{T}_{\mathcal{X}} \to \mathbb{R}$, defined by

$$H(x, y) = \begin{cases} \min_{z\in[x,y]} B(z), & x \leq y, \\ \max_{z\in[y,x]} B(z), & y \leq x, \end{cases}$$

is an embedded barrier certificate for $\mathfrak{S}$.

Proof: We first show that condition (4) implies (9). Consider an index $i \in \mathcal{I}$ and let $z^* \in [\underline{x}_i, \overline{x}_i]$ be such that $\max_{z\in[\underline{x}_i,\overline{x}_i]} B(z) = B(z^*)$. Thus, we have $H(\overline{x}_i, \underline{x}_i) = B(z^*)$. As a result, one gets $B(z^*) - B(\frac{\overline{x}_i+\underline{x}_i}{2}) = \left|B(\frac{\overline{x}_i+\underline{x}_i}{2}) - B(z^*)\right| \leq L_B\|z^* - \frac{\overline{x}_i+\underline{x}_i}{2}\|_\infty \leq L_B\frac{\|\overline{x}_i-\underline{x}_i\|_\infty}{2} \leq \eta$, where the last inequality holds by the validity condition (7). This implies that $H(\overline{x}_i, \underline{x}_i) \leq B(\frac{\overline{x}_i+\underline{x}_i}{2}) + \eta$. This means that if $B(\frac{\underline{x}_i+\overline{x}_i}{2}) \leq -\eta$, then we have $H(\overline{x}_i, \underline{x}_i) \leq 0$. The fact that condition (5) implies condition (10) can be shown in a similar way. We finally need to show that condition (6) implies condition (11). Let $i \in \mathcal{P}$ be such that $H(\underline{x}_i, \overline{x}_i) \leq 0$ and $z^* \in [\underline{x}_i, \overline{x}_i]$ be such that $\min_{z\in[\underline{x}_i,\overline{x}_i]} B(z) = B(z^*)$. Using the definition of H, one has $B(z^*) = H(\underline{x}_i, \overline{x}_i) \leq 0$. Thus

$$\begin{aligned} B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) &\leq B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) - B(z^*) = \left|B(\tfrac{\overline{x}_i+\underline{x}_i}{2}) - B(z^*)\right| \\ &\leq L_B\|z^* - \tfrac{\overline{x}_i+\underline{x}_i}{2}\|_\infty \leq L_B\tfrac{\|\overline{x}_i-\underline{x}_i\|_\infty}{2} \leq \eta. \end{aligned}$$

Using condition (6), we conclude that $B(f(\frac{\overline{x}_i+\underline{x}_i}{2})) \leq -\eta$. As a result, for every $z \in [\underline{x}_i, \overline{x}_i]$,

$$\begin{aligned} B(f(z)) - B(f(\tfrac{\overline{x}_i+\underline{x}_i}{2})) &\leq \left|B(f(z)) - B(f(\tfrac{\overline{x}_i+\underline{x}_i}{2}))\right|_\infty \\ &\leq L_B L_f \left\|\tfrac{\overline{x}_i-\underline{x}_i}{2}\right\|_\infty \leq \eta, \end{aligned}$$

where the last inequality holds by the validity condition (7). This implies that $B(f(z)) \leq B(f(\frac{\overline{x}_i+\underline{x}_i}{2}))+\eta \leq 0$, for every $z \in [\underline{x}_i, \overline{x}_i]$. Therefore,

$$H(f(\overline{x}_i), f(\underline{x}_i)) = \min_{z\in[f(\underline{x}_i),f(\overline{x}_i)]} B(z) \leq B(f(\underline{x}_i)) \leq 0.$$

This completes the proof. ∎

IV. Neural Embedded Barrier Certificate

In this section, we employ feedforward neural networks to learn the data-driven embedded barrier certificates satisfying conditions (9)-(11). Consider a discrete-time monotone system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ with a hyper-rectangular partition $[\underline{x}_i, \overline{x}_i]_{i\in\mathcal{P}}$ of $\mathcal{X}$, where the indices $\mathcal{I}$ and $\mathcal{U}$ are defined in (3). Our objective is to learn an embedded barrier certificate for $\mathfrak{S}$ using an ℓ-layer fully connected feedforward neural network $N : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, defined as follows:

$$\begin{aligned} &\xi^{(k)} = \phi\left(W^{(k-1)}\xi^{(k-1)} + b^{(k-1)}\right), \quad k \in \{1, \dots, \ell\}, \\ &\xi^{(0)} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \qquad N(x_1, x_2) = W^{(\ell)}\xi^{(\ell)} + b^{(\ell)}, \end{aligned} \tag{12}$$

where $W^{(k-1)} \in \mathbb{R}^{n_k\times n_{k-1}}$ is the weight matrix of the kth layer (with n_k denoting the number of neurons in the kth layer), $b^{(k-1)} \in \mathbb{R}^{n_k}$ is the bias vector of the kth layer, $\xi^{(k)} \in \mathbb{R}^{n_k}$ is the hidden variables of the kth layer, and $\phi : \mathbb{R}^{n_k} \to \mathbb{R}^{n_k}$ is the diagonal activation function (identical across all hidden layers). Furthermore, this activation function satisfies $0 \leq \frac{\phi(x)-\phi(y)}{x-y} \leq 1$. We propose the following data-driven conditions for the neural network N:

$$\begin{aligned} & N(\overline{x}_i, -\underline{x}_i) \leq 0 && \forall i \in \mathcal{I}, \\ & N(\underline{x}_i, -\overline{x}_i) > 0 && \forall i \in \mathcal{U}, \\ & N(f(\overline{x}_i), -f(\underline{x}_i)) \leq 0 && \forall i \in \mathcal{Z}_{\mathcal{N}}, \\ & W^{(k-1)} \geq 0 && \forall k \in \{1, \ldots, \ell+1\}, \end{aligned} \tag{13}$$

where the index set $\mathcal{Z}_{\mathcal{N}} \subseteq \mathcal{P}$ is defined as

$$\mathcal{Z}_{\mathcal{N}} = \{ i \in \mathcal{P} \mid N(\underline{x}_i, -\overline{x}_i) \leq 0 \}. \tag{14}$$

One can show that a neural network N satisfying conditions (13) serves as an embedded barrier certificate for $\mathfrak{S}$.

Theorem 6 (Neural Embedded Barrier Certificates): Consider a monotone discrete-time system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ with an unsafe set $\mathcal{X}_u \subseteq \mathcal{X}$ and let $\{[\underline{x}_i, \overline{x}_i]\}_{i \in \mathcal{P}}$ be a hyper-rectangular partition of $\mathcal{X}$ with indices $\mathcal{I}$ and $\mathcal{U}$ defined in (3). If there exists a neural network $N : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ satisfying conditions (13), then $\mathfrak{S}$ is safe.

Proof: Let $(x, \widehat{x}), (y, \widehat{y}) \in \mathbb{R}^n \times \mathbb{R}^n$ be such that $x \leq \widehat{x}$ and $y \leq \widehat{y}$. Thus, $\xi^{(0)} = \left[\begin{smallmatrix} x \\ \widehat{x} \end{smallmatrix}\right] \leq \left[\begin{smallmatrix} y \\ \widehat{y} \end{smallmatrix}\right] = \eta^{(0)}$. Since $W^{(0)} \geq 0$, one gets that $W^{(0)}\xi^{(0)} + b^{(0)} \leq W^{(0)}\eta^{(0)} + b^{(0)}$. Now using the fact that the activation functions are diagonal and slope-restricted, one gets $\xi^{(1)} = \phi(W^{(0)}\xi^{(0)} + b^{(0)}) \leq \phi(W^{(0)}\eta^{(0)} + b^{(0)}) = \eta^{(1)}$. One can repeat this argument to show that $\xi^{(i)} \leq \eta^{(i)}$, for every $i \in \{0, \ldots, \ell\}$ and thus $N(x, \widehat{x}) \leq N(y, \widehat{y})$. This means that N is monotone with respect to standard partial order on $\mathbb{R}^n \times \mathbb{R}^n$. Moreover, $N(\overline{x}, \underline{x})$ is monotone with respect to the standard partial order on $\mathbb{R}^n \times \mathbb{R}^n$ if and only if $N(\overline{x}, -\underline{x})$ is monotone with respect to the southeast order $\leq_{\mathrm{SE}}$. Therefore, using Theorem 4, the neural network $N : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ satisfying conditions (13) is an embedded barrier certificate for $\mathfrak{S}$. ■

To train a neural network that satisfies conditions (13), we define three ReLU loss functions:

$$\begin{aligned} \mathcal{L}_1 &= \sum_{i \in \mathcal{S}} \mathrm{ReLU}(N(\overline{x}_i, -\underline{x}_i)), \\ \mathcal{L}_2 &= \sum_{i \in \mathcal{U}} \mathrm{ReLU}(\epsilon - N(\underline{x}_i, -\overline{x}_i)), \\ \mathcal{L}_3 &= \sum_{i \in \mathcal{Z}_N} \mathrm{ReLU}(N(f(\overline{x}_i), -f(\underline{x}_i))). \end{aligned} \tag{15}$$

Here, a small constant $\epsilon > 0$ is chosen to ensure that $N(\underline{x}_i, -\overline{x}_i)$ is always positive, for every $i \in \mathcal{U}$. We then train the neural network using the composite loss function $\mathcal{L}_{\text{total}} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3$, and terminate the training once $\mathcal{L}_{\text{total}}$ exactly reaches zero. When the loss function becomes zero, we can ensure that conditions in (13) are satisfied. Algorithm 1 provides an overview of our proposed method.

Algorithm 1 Neural Embedded Barrier Certificate

Input: Monotone system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$, an unsafe set $\mathcal{X}_u \subseteq \mathcal{X}$, partitioning depth d, an architecture for neural network N, maximum iterations number $n_{\max}$, and maximum partitioning depth $d_{\max}$.
Output: Neural barrier certificate N and final loss $\mathcal{L}_{\text{total}}$.

```
L_total ← 1
for d ≤ d_max and L_total ≠ 0 do
    Construct a hyper-rectangular partition with depth d.
    Initialize neural network N with L_total as in (15).
    i ← 0
    while L_total ≠ 0 and i ≤ n_max do
        Train N for one epoch with the loss function L_total.
        i ← i + 1
    end while
    d ← 2d
end for
Return N and L_total.
```

When the state set $\mathcal{X}$ is compact, part 3 of Theorem 3 can be used as an alternative approach to construct separable embedded barrier certificates for monotone systems. Consequently, the neural barrier certificates in (13) can be reformulated to search for two feedforward neural networks $N_1, N_2 : \mathbb{R}^n \to \mathbb{R}$ satisfying the following conditions:

$$\begin{aligned} & N_1(\overline{x}_i) - N_2(\underline{x}_i) \leq 0 && \forall i \in \mathcal{I}, \\ & N_1(\underline{x}_i) - N_2(\overline{x}_i) > 0 && \forall i \in \mathcal{U}, \\ & N_1(f(\overline{x}_i)) - N_2(f(\underline{x}_i)) \leq 0 && \forall i \in \mathcal{Z}_{N_1,N_2}, \\ & W_1^{(k-1)} \geq 0, \quad W_2^{(k-1)} \geq 0 && \forall k \in \{1, \ldots, \ell+1\}, \end{aligned} \tag{16}$$

where the index set $\mathcal{Z}_{N_1,N_2} \subseteq \mathcal{P}$ is defined as $i \in \mathcal{P}$ for which $N_1(\underline{x}_i) - N_2(\overline{x}_i) \leq 0$. Using part 3 of Theorem 3 and Theorem 4, one can show that if there exist two neural networks $N_1 : \mathbb{R}^n \to \mathbb{R}$ and $N_2 : \mathbb{R}^n \to \mathbb{R}$ satisfying conditions (16), then $\mathfrak{S}$ is safe.

V. Numerical Experiments

Here, we use numerical experiments to show the efficacy of our approach for safety verification. All experiments were conducted on an Nvidia RTX 4090 GPU.

A. 2-D linear system

As an illustrative example, we consider a two-dimensional monotone discrete-time system $\mathfrak{S} = (\mathcal{X}, \mathcal{X}_0, f)$ where $\mathcal{X} = [-2, 2] \times [-2, 2]$, $\mathcal{X}_0 = [-2, -1] \times [1, 2]$. The transition function f is defined as follows:

$$\begin{aligned} f_1(x) &= (1 - 2h)x_1 + hx_2 - h, \\ f_2(x) &= hx_1 + (1 - 2h)x_2 + h, \end{aligned}$$

where $x = [x_1, x_2]^\top$ and $h = 0.1$. Since the Jacobian $Df(x) = \left[\begin{smallmatrix} (1-2h) & h \\ h & (1-2h) \end{smallmatrix}\right]$ has nonnegative entries and the system is monotone on $\mathcal{X}$. We study neural barrier certificates for two different scenarios. First, we consider the unsafe set $\mathcal{X}_u = [1, 2] \times [-1, 1]$ and we train a neural network satisfying conditions (13). Second, we consider the unsafe set $\mathcal{X}_u = [1, 2] \times [-1, 1] \cup [0, 2] \times [-2, -1]$ and train two neural networks satisfying conditions (16). The architecture for all the neural networks are considered as $\tanh(2{\times}40{\times}60{\times}60{\times}60{\times}60{\times}1)$. In both cases, we use Algorithm 1 with a partitioning depth of $d = 1$. Our method converges in 1.57s within 76 epochs for the first and converges in 12.4s within 545 epochs for the second scenario. Figure 1 illustrates the trained barriers for these two settings.

B. Traffic networks model

As the second example, we consider a Daganzo cell transmission model, with demand and supply constraints on a line digraph for traffic networks, as in Figure 2. The traffic network is described by a monotone discrete-time system $\mathfrak{S}{=}(\mathcal{X}, \mathcal{X}_0, f)$, with the transition map f [20, Lemma 4.28]

$$\begin{aligned} f_1(q) &= q_1 + h(F_{0\to1} - F_{1\to2}(q)),\\ f_i(q) &= q_i + h(F_{i-1\to i}(q) - F_{i\to i+1}(q)), \;\; i{\in}\{2,\dots,n{-}1\},\\ f_n(q) &= q_n + h(F_{n-1\to n}(q) - F_{n\to0}(q)), \end{aligned} \tag{17}$$

where $h = 0.1$ and $q = \begin{bmatrix} q_1 & \dots & q_n \end{bmatrix}^\top$ with $q_i \geq 0$ being the density of vehicles at the road segment i. The function $F_{i\to j}$ is the flow from road segment i to j defined by:

$$F_{i\to j}(q){=}\min\{\varphi_i(q_i), \sigma_j(q_j)\}, \;\; F_{n\to0}(q) = \varphi_n(q_n), \tag{18}$$

where $\varphi_i(q_i)$ represents the increasing outflow demand of the road segment i and $\sigma_j(q_j)$ denotes the decreasing inflow supply of the road segment j. For every road segment $i \neq 2$, we define $\varphi_i(q_i) = 15(1{-}e^{-0.038q_i})$, $\sigma_i(q_i) = \mathrm{ReLU}(15(1-(\frac{q_i}{100})^4))$. For the road segment 2, we define $\varphi_2(q_2) = 10(1{-}e^{-0.138q_2})$, $\sigma_2(q_2) = \mathrm{ReLU}(10(1{-}(\frac{q_2}{50})^4))$. We consider $\mathcal{X} = [0, 50]^n$, the initial set $\mathcal{X}_0 = [0, 5] \times [0, 18] \times [0, 5]^{n-2}$, and the on-ramp input by $F_{0\to1} = 9$. Since road segment 2 has the smallest flow capacity, the system is unsafe whenever the vehicle density in this road segment is in the interval $[30, 50]$.

We train two neural networks satisfying (16) to guarantee the safety of this traffic system for various dimensions n. All neural network architectures are $\tanh(n{\times}40{\times}40{\times}40{\times}40{\times}40{\times}1)$. To reduce sample complexity, we consider a point outside the initial set $\mathcal{X}_0$ and partition $\mathcal{X}\backslash\mathcal{X}_u$ by projecting this point onto all axes, treating the remaining part of the state set as an additional partition. This partitioning scheme results in $4(n+1)$ samples for the traffic system $\mathfrak{S}$. Table I compare our proposed method with the state-of-the-art neural barrier methods in the literature. The results show that, compared to state-of-the-art algorithms, our method scales to high-dimensional systems, requires significantly fewer samples, and exhibits a reasonably small convergence time.

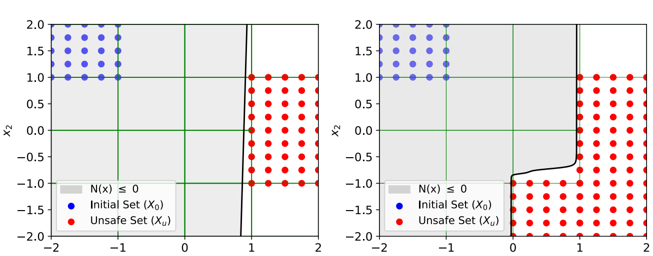

Fig. 1: **Left**: Invariant set ($N(x) \leq 0$) for the first scenario of the 2-D example. **Right**: Invariant set ($N_1(x) - N_2(x) \leq 0$) for the second scenario of the 2-D example. Green lines are hyper rectangular partitioning with depth $d = 1$.

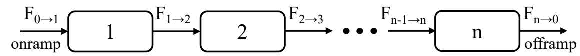

Fig. 2: A line digraph representing an n-dim traffic network.

Dimensions n	Method	3	6	8	12	20
# of samples	Ours	16	28	36	52	84
	[21]	500	500	500	500	500
	[22]	125	15626	390625	49M	95T
Convergence time (s)	Ours	16.3	36.9	110	150	350
	[21]	2	240	N.A.	N.A.	N.A.
	[22]	1.2	1.9	3.4	N.A.	N.A.

TABLE I: Neural barrier certificates for traffic networks.

VI. Conclusion

In this paper, we developed a suitable embedding of barrier functions that is compatible with interval analysis. Leveraging this embedding, we proposed a framework for learning neural barrier certificates for unknown monotone discrete-time systems without requiring prior knowledge of the Lipschitz bound of their dynamics. Our numerical experiments demonstrated that, compared to state-of-the-art methods, our framework is scalable to large systems and does not suffer from exponential sample complexity.

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