Infinite Time Horizon Safety of Bayesian Neural Networks

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Abstract

Bayesian neural networks (BNNs) place distributions over the weights of a neural network to model uncertainty in the data and the network’s prediction. We consider the problem of verifying safety when running a Bayesian neural network policy in a feedback loop with infinite time horizon systems. Compared to the existing sampling-based approaches, which are inapplicable to the infinite time horizon setting, we train a separate deterministic neural network that serves as an infinite time horizon safety certificate. In particular, we show that the certificate network guarantees the safety of the system over a subset of the BNN weight posterior’s support. Our method first computes a safe weight set and then alters the BNN’s weight posterior to reject samples outside this set. Moreover, we show how to extend our approach to a safe-exploration reinforcement learning setting, in order to avoid unsafe trajectories during the training of the policy. We evaluate our approach on a series of reinforcement learning benchmarks, including non-Lyapunovian safety specifications.

1 Introduction

The success of deep neural networks (DNNs) across different domains has created the desire to apply them in safety-critical applications such as autonomous vehicles [28, 30] and healthcare systems [41]. The fundamental challenge for the deployment of DNNs in these domains is certifying their safety [9]. Thus, formal safety verification of DNNs in isolation and closed control loops [26, 23, 17, 43, 13] has become an active research topic.

Bayesian neural networks (BNNs) are a family of neural networks that place distributions over their weights [36]. This allows learning uncertainty in the data and the network’s prediction, while preserving the strong modelling capabilities of DNNs [32]. In particular, BNNs can learn arbitrary data distributions from much simpler (e.g. Gaussian) weight distributions. This makes BNNs very appealing for robotic and medical applications [33] where uncertainty is a central component of data.

Despite the large body of literature on verifying safety of DNNs, the formal safety verification of BNNs has received less attention. Notably, [8, 45] have proposed sampling-based techniques for obtaining probabilistic guarantees about BNNs. Although these approaches provide some insight
into BNN safety, they suffer from two key limitations. First, sampling provides only bounds on the probability of the BNN’s safety which is insufficient for systems with critical safety implications. For instance, having an autonomous vehicle with a 99.9% safety guarantee is still insufficient for deployment if millions of vehicles are deployed. Second, samples can only simulate the system for a finite time, making it impossible to reason about the system’s safety over an unbounded time horizon.

In this work, we study the safety verification problem for BNN policies in safety-critical systems over the infinite time horizon. Formally, we consider discrete-time closed-loop systems defined by a dynamical system and a BNN policy. Given a set of initial states and a set of unsafe (or bad) states, the goal of the safety verification problem is to verify that no system execution starting in an initial state can reach an unsafe state. Unlike existing literature which considers probability of safety, we verify sure safety, i.e. safety of every system execution of the system. In particular, we present a method for computing safe weight sets for which every system execution is safe as long as the BNN samples its weights from this set.

Our approach to restrict the support of the weight distribution is necessary as BNNs with Gaussian weight priors typically produce output posteriors with unbounded support. Consequently, there is a low but non-zero probability for the output variable to lie in an unsafe region, see Figure 1. This implies that BNNs are usually unsafe by default. We therefore consider the more general problem of computing safe weight sets. Verifying that a weight set is safe allows re-calibrating the BNN policy by rejecting unsafe weight samples in order to guarantee safety.

As most BNNs employ uni-modal weight priors, e.g. Gaussians, we naturally adopt weight sets in the form of products of intervals centered at the means of the BNN’s weight distributions. To verify safety of a weight set, we search for a safety certificate in the form of a safe positive invariant (also known as safe inductive invariant). A safe positive invariant is a set of system states that contains all initial states, is closed under the system dynamics and does not contain any unsafe state. The key advantage of using safe positive invariants is that their existence implies the infinite time horizon safety. We parametrize safe positive invariant candidates by (deterministic) neural networks that classify system states for determining set inclusion. Moreover, we phrase the search for an invariant as a learning problem. A separated verifier module then checks if a candidate is indeed a safe positive invariant by checking the required properties via constraint solving. In case the verifier finds a counterexample demonstrating that the candidate violates the safe positive invariant condition, we re-train the candidate on the found counterexample. We repeat this procedure until the verifier concludes that the candidate is a safe positive invariant ensuring that the system is safe.

The safe weight set obtained by our method can be used for safe exploration reinforcement learning. In particular, generating rollouts during learning by sampling from the safe weight set allows an exploration of the environment while ensuring safety. Moreover, projecting the (mean) weights onto the safe weight set after each gradient update further ensures that the improved policy stays safe.

Contributions Our contributions can be summarized as follows:

1. We define a safety verification problem for BNN policies which overcomes the unbounded posterior issue by computing and verifying safe weight sets. The problem generalizes the sure safety verification of BNNs and solving it allows re-calibrating BNN policies via rejection sampling to guarantee safety.
2. We introduce a method for computing safe weight sets in BNN policies in the form of products of intervals around the BNN weights’ means. To verify safety of a weight set, our novel algorithm learns a safe positive invariant in the form of a deterministic neural network.
3. We evaluate our methodology on a series of benchmark applications, including non-linear systems and non-Lyapunovian safety specifications.
2 Related work

Verification of feed-forward NN Verification of robustness and safety properties in feed-forward DNNs has received much attention but remains an active research topic [26, 23, 17, 40, 7, 43]. As the majority of verification techniques were designed for deterministic NNs, they cannot be readily applied to BNNs. The safety verification of feed-forward BNNs has been considered in [8] by using samples to obtain statistical guarantees on the safety probability. The work of [45] also presents a sampling-based approach, however it provides certified lower bounds on the safety probability.

The literature discussed above considers NNs in isolation, which can provide input-output guarantees on a NN but are unable to reason holistically about the safety of the system that the NN is applied in. Verification methods that concern the safety of NNs interlinked with a system require different approaches than standalone NN verification, which we will discuss in the rest of this section.

Finite time horizon safety of BNN policies The work in [34] extends the method of [8] to verifying safety in closed-loop systems with BNN policies. However, similar to the standalone setting of [8], their method obtains only statistical guarantees on the safety probability and for the system’s execution over a finite time horizon.

Safe RL Safe reinforcement learning has been primarily studied in the form of constrained Markov decision processes (CMDPs) [2, 18]. Compared to standard MDPs, an agent acting in a CMDP must satisfy an expected auxiliary cost term aggregated over an episode. The CMDP framework has been the base of several RL algorithms [44], notably the Constrained Policy Optimization (CPO) [1]. Despite these algorithms providing a decent performance, the key limitation of CMDPs is that the constraint is satisfied in expectation, which makes violations unlikely but nonetheless possible. Consequently, the CMDP framework is unsuited for systems where constraint violations are critical.

Lyapunov-based stability Safety in the context of “stability”, i.e. always returning to a ground state, can be proved by Lyapunov functions [4]. Lyapunov functions have originally been considered to study stability of dynamical systems [29]. Intuitively, a Lyapunov function assigns a non-negative value to each state, and is required to decrease with respect to the system’s dynamics at any state outside of the stable set. A Lyapunov-based method is proposed in [11] to ensure safety in CMDPs during training. Recently, the work of [9] presented a method for learning a policy as well as a neural network Lyapunov function which guarantees the stability of the policy. Similarly to our work, their learning procedure is counterexample-based. However, unlike [9], our work considers BNN policies and safety definitions that do not require returning to a set of ground states.

Barrier functions for dynamical systems Barrier functions can be used to prove infinite time horizon safety in dynamical systems [38, 39]. Recent works have considered learning neural network barrier functions [47], and a counterexample-based learning procedure is presented in [37].

Finite time horizon safety of NN policies Safety verification of continuous-time closed-loop systems with deterministic NN policies has been considered in [24, 19], which reduces safety verification to the reachability analysis in hybrid systems [10]. The work of [13] presents a method which computes a polynomial approximation of the NN policy to allow an efficient approximation of the reachable state set. Both works consider finite time horizon systems.

Our safety certificate most closely resembles inductive invariants for safety analysis in programs [14] and positive invariants for dynamical systems [5].

3 Preliminaries and problem statement

We consider a discrete-time dynamical system

\[ x_{t+1} = f(x_t, u_t), \quad x_0 \in \mathcal{X}_0. \]

The dynamics are defined by the function \( f : \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X} \) where \( \mathcal{X} \subseteq \mathbb{R}^m \) is the state space and \( \mathcal{U} \subseteq \mathbb{R}^n \) is the control action space, \( \mathcal{X}_0 \subseteq \mathcal{X} \) is the set of initial states and \( t \in \mathbb{N} \) denotes a discretized time. At each time step \( t \), the action is defined by the (possibly probabilistic) positional policy \( \pi : \mathcal{X} \rightarrow D(\mathcal{U}) \), which maps the current state \( x_t \) to a distribution \( \pi(x_t) \in D(\mathcal{U}) \) over the set of actions. We use \( D(\mathcal{U}) \) to denote the set of all probability distributions over \( \mathcal{U} \). The next action is then sampled according to \( u_t \sim \pi(x_t) \), and together with the current state \( x_t \) of the system gives rise to the next state \( x_{t+1} \) of the system according to the dynamics \( f \). Thus, the dynamics \( f \) together
with the policy $\pi$ form a closed-loop system (or a feedback loop system). The aim of the policy is to maximize the expected cumulative reward (possibly discounted) from each starting state. Given a set of initial states $X_0$ of the system, we say that a sequence of state-action pairs $(x_t, u_t)_{t=0}^\infty$ is a trajectory if $x_0 \in X_0$ and we have $u_t \in \text{supp}(\pi(x_t))$ and $x_{t+1} = f(x_t, u_t)$ for each $t \in \mathbb{N}_{\geq 0}$.

A neural network (NN) is a function $\pi : \mathbb{R}^m \rightarrow \mathbb{R}^n$ that consists of several sequentially composed layers $\pi = l_1 \circ \cdots \circ l_L$. Formally, a NN policy maps each system state to a Dirac-delta distribution which picks a single action with probability 1. Each layer $l_i$ is parametrized by learned weight values of the appropriate dimensions and an activation function $a$,

$$l_i(x) = a(W_i x + b_i), \quad W_i \in \mathbb{R}^{n_i \times m_i}, \quad b_i \in \mathbb{R}^{n_i}.$$ 

In this work, we consider ReLU activation functions $a(x) = \text{ReLU}(x) = \max\{x, 0\}$, although other piecewise linear activation such as the leaky-ReLU $[25]$ and PReLU $[21]$ are applicable as well.

In Bayesian neural networks (BNNs), weights are random variables and their values are sampled, each according to some distribution. Then each vector of sampled weights gives rise to a (deterministic) neural network. Given a training set $D$, in order to train the BNN we assume a prior distribution $p(w, b)$ over the weights. The learning then amounts to computing the posterior distribution $p(w, b | D)$ via the application of the Bayes rule. As analytical inference of the posterior is in general infeasible due to non-linearity introduced by the BNN architecture $[32]$, practical training algorithms rely on approximate inference, e.g. Hamiltonian Monte Carlo $[50]$, variational inference $[6]$ or dropout $[15]$.

When the policy in a dynamical system is a BNN, the policy maps each system state $x_t$ to a probability distribution $\pi(x_t)$ over the action space. Informally, this distribution is defined as follows. First, BNN weights $w, b$ are sampled according to the posterior BNN weight distribution, and the sampled weights give rise to a deterministic NN policy $\pi_{w,b}$. The action of the system is then defined as $u_t = \pi_{w,b}(x_t)$. Formal definition of the distribution $\pi(x_t)$ is straightforward and proceeds by considering the product measure of distributions of all weights.

**Problem statement** We now define the two safety problems that we consider in this work. The first problem considers feed-forward BNNs, and the second problem considers closed-loop systems with BNN policies. While our solution to the first problem will be a subprocedure in our solution to the second problem, the reason why we state it as a separate problem is that we believe that our solution to the first problem is also of independent interest for the safety analysis of feed-forward BNNs.

Let $\pi$ be a BNN. Suppose that the vector $(w, b)$ of BNN weights in $\pi$ has dimension $p + q$, where $p$ is the dimension of $w$ and $q$ is the dimension of $b$. For each $1 \leq i \leq p$, let $\mu_i$ denote the mean of the random variable $w_i$. Similarly, for each $1 \leq i \leq q$, let $\mu_{p+i}$ denote the mean of the random variable $b_i$. Then, for each $\epsilon \in [0, \infty]$, we define the set $W_\pi^\epsilon$ of weight vectors via

$$W_\pi^\epsilon = \prod_{i=1}^{p+q} [\mu_i - \epsilon, \mu_i + \epsilon] \subseteq \mathbb{R}^{p+q}.$$

We now proceed to defining our safety problem for feed-forward BNNs. Suppose that we are given a feed-forward BNN $\pi$, a set $X_0 \subseteq \mathbb{R}^m$ of input points and a set $X_u \subseteq \mathbb{R}^n$ of unsafe (or bad) output points. For a concrete vector $(w, b)$ of weight values, let $\pi_{w,b}$ to be the (deterministic) NN defined by these weight values. We say that $\pi_{w,b}$ is safe if for each $x \in X_0$ we have $\pi_{w,b}(x) \not\in X_u$, i.e. if evaluating $\pi_{w,b}$ on all input points does not lead to an unsafe output.

**Problem 1** (Feed-forward BNNs). Let $\pi$ be a feed-forward BNN, $X_0 \subseteq \mathbb{R}^m$ a set of input points and $X_u \subseteq \mathbb{R}^n$ a set of unsafe output points. Let $\epsilon \in [0, \infty]$. Determine whether each deterministic NN in $\{\pi_{w,b} \mid (w, b) \in W_\pi^\epsilon\}$ is safe.

Next, we define our safety problem for closed-loop systems with BNN policies. Consider a closed-loop system defined by a dynamics function $f$, a BNN policy $\pi$ and an initial set of states $X_0$. Let $X_u \subseteq \mathcal{X}$ be a set of unsafe (or bad) states. We say that a trajectory $(x_t, u_t)_{t=0}^\infty$ is safe if $x_t \not\in X_u$ for all $t \in \mathbb{N}_0$, hence if it does not reach any unsafe states. Note that this definition implies infinite time horizon safety of the trajectory. Given $\epsilon \in [0, \infty]$, define the set $\text{Traj}_t^{l,m}$ to be the set of all system trajectories in which each sampled weight vector belongs to $W_\pi^\epsilon$. 


We use Section 4.1 considering Problem 1 and Section 4.2 considering Problem 2. Both problems
consider safety verification with respect to a given value of \( \epsilon \in [0, \infty) \), so in Section 4.3 we present
our method for computing the value of \( \epsilon \) for which our solutions to Problem 1 and Problem 2 may be
used to verify safety. We then show in Section 4.4 how our new methodology can be adapted to the
safe exploration RL setting.

4 Main results

In this section we present our method for solving the safety problems defined in the previous section,
with Section 4.1 considering Problem 1 and Section 4.2 considering Problem 2. Both problems
consider safety verification with respect to a given value of \( \epsilon \in [0, \infty) \), so in Section 4.3 we present
our method for computing the value of \( \epsilon \) for which our solutions to Problem 1 and Problem 2 may be
used to verify safety. We then show in Section 4.4 how our new methodology can be adapted to the
safe exploration RL setting.

4.1 Safe weight sets for feed-forward BNNs

Consider a feed-forward BNN \( \pi \), a set \( \mathcal{X}_0 \subseteq \mathbb{R}^m \) of inputs and a set \( \mathcal{X}_u \subseteq \mathbb{R}^n \) of unsafe output of
the BNN. Fix \( \epsilon \in [0, \infty) \). To solve Problem 1 we show that the decision problem of whether each
deterministic NN in \( \{ \pi_{w,b} \mid (w, b) \in W^\epsilon \} \) is safe can be encoded as a system of constraints and
reduced to constraint solving.

Suppose that \( \pi = l_1 \circ \cdots \circ l_k \) consists of \( k \) layers, with each \( l_i(x) = \text{ReLU}(W_i x + b_i) \). Denote by
\( M_i \) the matrix of the same dimension as \( W_i \), with each entry equal to the mean of the corresponding
random variable weight in \( W_i \). Similarly, define the vector \( m_i \) of means of random variables in \( b_i \).

The real variables of our system of constraints are as follows, each of appropriate dimension:

- \( x_0 \) encodes the BNN inputs, \( x_i \) encodes the BNN outputs;
- \( x_i^{\text{out}} \) encode vectors of output values of each neuron in the hidden layers;
- \( x_i^{\text{neg}}, x_i^{\text{pos}} \) are dummy variable vectors of the same dimension as \( x_0 \) and which will
be used to distinguish between positive and negative NN inputs in \( x_0 \), respectively.

We use 1 to denote the vector/matrix whose all entries are equal to 1, of appropriate dimensions
defined by the formula in which it appears. Our system of constraints is as follows:

\[
\begin{align*}
    x_0 & \in \mathcal{X}_0, \quad x_i \in \mathcal{X}_u & \quad \text{(Input-output conditions)} \\
    x_i^{\text{out}} &= \text{ReLU}(x_i^{\text{in}}), \quad \text{for each } 1 \leq i \leq l - 1 & \quad \text{(ReLU encoding)} \\
    (M_i - \epsilon \cdot 1) x_i^{\text{out}} + (m_i - \epsilon \cdot 1) & \leq x_i^{\text{in}}, \quad \text{for each } 1 \leq i \leq l - 1 & \quad \text{(BNN hidden layers)} \\
    x_{i+1}^{\text{in}} & \leq (M_i + \epsilon \cdot 1) x_i^{\text{out}} + (m_i + \epsilon \cdot 1), \quad \text{for each } 1 \leq i \leq l - 1 \\
    x_{0,\text{pos}} & = \text{ReLU}(x_0), \quad x_{0,\text{neg}} = -\text{ReLU}(-x_0) & \quad \text{(BNN input layer)} \\
    (M_0 - \epsilon \cdot 1) x_{0,\text{pos}} + (M_0 + \epsilon \cdot 1) x_{0,\text{neg}} + (m_0 - \epsilon \cdot 1) \leq x_1^{\text{in}} \\
    x_1^{\text{in}} & \leq (M_0 + \epsilon \cdot 1) x_{0,\text{pos}} + (M_0 - \epsilon \cdot 1) x_{0,\text{neg}} + (m_0 + \epsilon \cdot 1)
\end{align*}
\]

Denote by \( \Phi(\pi, x_0, \mathcal{X}_u, \epsilon) \) the system of constraints defined above. The proof of Theorem 1 shows
that it encodes that \( x_0 \in \mathcal{X}_0 \) is an input point for which the corresponding output point of \( \pi \) is
unsafe, i.e. \( x_l = \pi(x_0) \in \mathcal{X}_u \). The first equation encodes the input and output conditions.

The second equation encodes the ReLU input-output relation for each hidden layer neuron. The remaining
equations encode the relation between neuron values in successive layers of the BNN as well as that
the sampled BNN weight vector is in \( W^\epsilon \). For hidden layers, we know that the output value of each
neuron is nonnegative, i.e. \( x_i^{\text{out}} \geq 0 \) for the \( i \)-th hidden layer where \( 1 \leq i \leq l - 1 \), and so

\[
(M_i - \epsilon \cdot 1) x_i^{\text{out}} \leq (M_i + \epsilon \cdot 1) x_i^{\text{out}}.
\]
Hence, the BNN weight relation with neurons in the successive layer as well as the fact that the sampled weights are in $W^{\pi}_\epsilon$ is encoded as in equations 3-4 above. For the input layer, however, we do not know the signs of the input neuron values $x_0$ and so we introduce dummy variables $x_{0,\text{pos}} = \text{ReLU}(x_0)$ and $x_{0,\text{neg}} = -\text{ReLU}(-x_0)$ in equation 5. This allows encoding the BNN weight relations between the input layer and the first hidden layer as well as the fact that the sampled weight vector is in $W^{\pi}_\epsilon$, as in equations 6-7. Theorem 1 shows that Problem 1 is equivalent to solving the system of constraints $\Phi(\pi, X_0, X_u, \epsilon)$. Its proof can be found in the Supplementary Material.

**Theorem 1.** Let $\epsilon \in [0, \infty]$. Then each deterministic NN in $\{\pi_{w,b} \mid (w, b) \in W^{\pi}_\epsilon\}$ is safe if and only if the system of constraints $\Phi(\pi, X_0, X_u, \epsilon)$ is not satisfiable.

**Solving the constraints** Observe that $\epsilon$, $M$, and $m_i$, $1 \leq i \leq l-1$, are constant values that are known at the time of constraint encoding. Thus, in $\Phi(\pi, X_0, X_u, \epsilon)$, only the ReLU constraints and possibly the input-output conditions are not linear. Depending on the form of $X_0$ and $X_u$ and on how we encode the ReLU constraints, we may solve the system $\Phi(\pi, X_0, X_u, \epsilon)$ in several ways:

1. **MILP.** It is shown in [31][12][43] that the ReLU relation between two real variables can be encoded via mixed-integer linear constraints (MILP) by introducing 0/1-integer variables to encode whether a given neuron is active or inactive. Hence, if $X_0$ and $X_u$ are given by linear constraints, we may solve $\Phi(\pi, X_0, X_u, \epsilon)$ by a MILP solver. The ReLU encoding requires that each neuron value is bounded, which is ensured if $X_0$ is a bounded set and if $\epsilon < \infty$.

2. **Reluplex.** In order to allow unbounded $X_0$ and $\epsilon = \infty$, we may use algorithms based on the Reluplex calculus [26][27] to solve $\Phi(\pi, X_0, X_u, \epsilon)$. Reluplex is an extension of the standard simplex algorithm for solving systems of linear constraints, designed to allow ReLU constraints as well. While Reluplex does not impose the boundedness condition, it is in general less scalable than MILP-solving.

3. **NRA-SMT.** Alternatively, if $X_0$ or $X_u$ are given by non-linear constraints we may solve them by using an NRA-SMT-solver (non-linear real arithmetic satisfiability modulo theory), e.g. dReal [16]. To use an NRA-SMT-solver, we can replace the integer 0/1-variables of the MILP constraints, we may solve $\Phi(\pi, X_0, X_u, \epsilon)$ by a MILP solver. The ReLU encoding requires that each neuron value is bounded, which is ensured if $X_0$ is a bounded set and if $\epsilon < \infty$.

**Safety via rejection sampling** As discussed in Section 1 once the safety of NNs in $\{\pi_{w,b} \mid (w, b) \in W^{\pi}_\epsilon\}$ has been verified, we can “re-calibrate” the BNN to reject sampled weights which are not in $W^{\pi}_\epsilon$. Hence, rejection sampling gives rise to a safe BNN.

### 4.2 Safe weight sets for closed-loop systems with BNN Policies

Now consider a closed-loop system with a dynamics function $f : X \times U \rightarrow X$ with $X \subseteq \mathbb{R}^m$ and $U \subseteq \mathbb{R}^n$, a BNN policy $\pi$, an initial state set $X_0 \subseteq X$ and an unsafe state set $X_u \subseteq X$. Fix $\epsilon \in [0, \infty]$. In order to solve Problem 2 and verify safety of each trajectory contained in $\text{Traj}_f^{\epsilon,\pi}$, our method searches for a positive invariant-like safety certificate that we define below.

**Positive invariants for safety** A positive invariant in a dynamical system is a set of states which contains all initial states and which is closed under the system dynamics. These conditions ensure that states of all system trajectories are contained in the positive invariant. Hence, a positive invariant which does not contain any unsafe states can be used to certify safety of every trajectory over infinite time horizon. In this work, however, we are not trying to prove safety of every trajectory, but only of those trajectories contained in $\text{Traj}_f^{\epsilon,\pi}$. To that end, we define $W^{\pi}_\epsilon$-safe positive invariants. Intuitively, a $W^{\pi}_\epsilon$-safe positive invariant is required to contain all initial states, to be closed under the dynamics $f$ and the BNN policy $\pi$ when the sampled weight vector is in $W^{\pi}_\epsilon$, and not to contain any unsafe state.

**Definition 1** ($W^{\pi}_\epsilon$-safe positive invariants). A set $\text{Inv} \subseteq X$ is said to be a $W^{\pi}_\epsilon$-positive invariant if $X_0 \subseteq \text{Inv}$, for each $x \in \text{Inv}$ and $(w, b) \in W^{\pi}_\epsilon$ we have that $f(x, \pi_{w,b}(x)) \in \text{Inv}$, and $\text{Inv} \cap X_u = \emptyset$.

Theorem 2 shows that $W^{\pi}_\epsilon$-safe positive invariants can be used to verify safety of all trajectories in $\text{Traj}_f^{\epsilon,\pi}$ in Problem 2. The proof is straightforward and is deferred to the Supplementary Material.

**Theorem 2.** If there exists a $W^{\pi}_\epsilon$-safe positive invariant, then each trajectory in $\text{Traj}_f^{\epsilon,\pi}$ is safe.
Algorithm 1 Learning algorithm for $W_\varepsilon^+$-safe positive invariants

**Input** Dynamics function $f$, BNN policy $\pi$, Initial state set $X_0$, Unsafe state set $X_u$, $\epsilon \in [0, \infty)$

$\tilde{X}_0, \tilde{X}_u \leftarrow$ random samples of $X_0, X_u$

$D_{\text{spec}} \leftarrow \tilde{X}_0 \times \{0\} \cup \tilde{X}_u \times \{1\}$, $D_{\text{ce}} \leftarrow \emptyset$

Optional (bootstrapping): $S_{\text{bootstrap}} \leftarrow$ sample finite trajectories with initial state sampled from $\mathcal{X}$

$D_{\text{spec}} \leftarrow D_{\text{spec}} \cup \{(x,0)| \exists s \in S_{\text{bootstrap}} \text{ that starts in } x \in \mathcal{X} \text{ and reaches } X_u\}$

$D_{\text{spec}} \leftarrow D_{\text{spec}} \cup \{(x,1)| \exists s \in S_{\text{bootstrap}} \text{ that starts in } x \in \mathcal{X} \text{ and does not reach } X_u\}$

Pre-train neural network $g^{\text{inv}}$ on datasets $D_{\text{spec}}$ and $D_{\text{ce}}$ with loss function $\mathcal{L}$

**while** timeout not reached **do**

**if** $\exists (x,x', u, w, b)$ s.t. $g^{\text{inv}}(x) \geq 0$, $g^{\text{inv}}(x') < 0$, $(w, b) \in W_\varepsilon^+$, $u = \pi_{w,b}(x)$, $x' = f(x, u)$

then $D_{\text{ce}} \leftarrow D_{\text{ce}} \cup \{(x, x')\}$

**else if** $\exists (x)$ s.t. $x \in X_0$, $g^{\text{inv}}(x) < 0$

then $D_{\text{spec}} \leftarrow D_{\text{spec}} \cup \{(x, 1)\}$

**else if** $\exists (x)$ s.t. $x \in X_u$, $g^{\text{inv}}(x) \geq 0$

then $D_{\text{spec}} \leftarrow D_{\text{spec}} \cup \{(x, 0)\}$

**else**

Return Safe

**end if**

Train neural network $g^{\text{inv}}$ on datasets $D_{\text{spec}}$ and $D_{\text{ce}}$ with loss function $\mathcal{L}$

**end while**

Return Unsafe

**Learning positive invariants** We now present a learning algorithm for a $W_\varepsilon^+$-safe positive invariant. It learns a neural network $g^{\text{inv}}: \mathbb{R}^m \rightarrow \mathbb{R}$, where the positive invariant is then defined as the set $\text{Inv} = \{x \in \mathcal{X} | g^{\text{inv}}(x) \geq 0\}$. The pseudocode is given in Algorithm 1.

The algorithm first samples $\tilde{X}_0$ from $X_0$ and $\tilde{X}_u$ from $X_u$ and initializes the specification set $D_{\text{spec}}$ to $\tilde{X}_0 \times \{0\} \cup \tilde{X}_u \times \{1\}$ and the counterexample set $D_{\text{ce}}$ to an empty set. Optionally, the algorithm also bootstraps the positive invariant network by initializing $D_{\text{spec}}$ with random samples from the state space $\mathcal{X}$ labeled with Monte-Carlo estimates of reaching the unsafe states. The rest of the algorithm consists of two modules which are composed into a loop: the learner and the verifier. In each loop iteration, the learner first learns a $W_\varepsilon^+$-safe positive invariant candidate which takes the form of a neural network $g^{\text{inv}}$. This is done by minimizing the loss function $\mathcal{L}$ that depends on $D_{\text{spec}}$ and $D_{\text{ce}}$:

$$\mathcal{L}(g^{\text{inv}}) = \frac{1}{|D_{\text{spec}}|} \sum_{(x,y) \in D_{\text{spec}}} \mathcal{L}_{\text{cls}}(g^{\text{inv}}(x), y) + \lambda \frac{1}{|D_{\text{ce}}|} \sum_{(x,x') \in D_{\text{ce}}} \mathcal{L}_{\text{ce}}(g^{\text{inv}}(x), g^{\text{inv}}(x'))$$

where $\lambda$ is a tuning parameter and $\mathcal{L}_{\text{cls}}$ a binary classification loss function, e.g. the 0/1-loss $\mathcal{L}_{\text{cls}}(z, y) = 1[|z| \geq 0] \neq y$ or the logistic loss $\mathcal{L}_{\text{log}}(z, y) = z - y \cdot \log(1 + \exp(-z))$ as its differentiable alternative. The term $\mathcal{L}_{\text{ce}}$ is the counterexample loss which we define via

$$\mathcal{L}_{\text{ce}}(z, z') = 1[z > 0] \mathcal{I}[z' < 0] \mathcal{L}_{\text{cls}}(z, 0) \mathcal{L}_{\text{cls}}(z', 1).$$

Intuitively, the first sum in eq. (1) forces $g^{\text{inv}}$ to be nonnegative at initial states and negative at unsafe states contained in $D_{\text{spec}}$, and the second term forces each counterexample in $D_{\text{ce}}$ not to destroy the closedness of $\text{Inv}$ under the system dynamics.

Once $g^{\text{inv}}$ is learned, the verifier checks whether $\text{Inv}$ is indeed a $W_\varepsilon^+$-safe positive invariant. To do this, the verifier needs to check the three defining properties of $W_\varepsilon^+$-safe positive invariants:

1. **Closedness of $\text{Inv}$ under system dynamics.** The verifier checks if there exist states $x \in \text{Inv}$, $x' \notin \text{Inv}$ and a BNN weight vector $(w, b) \in W_\varepsilon^+$ such that $f(x, \pi_{w,b}(x)) = x'$. To do this, it introduces real variables $x, x', y, y' \in \mathbb{R}^m$, $u \in \mathbb{R}^n$ and $y, y' \in \mathbb{R}$, and solves:

   maximize $y - y'$ subject to
   
   $y \geq 0, y' < 0, y = g^{\text{inv}}(x), y' = g^{\text{inv}}(x')$
   
   $x' = f(x, u)$
   
   $u$ is an output of $\pi$ on input $x$ and weights $(w, b) \in W_\varepsilon^+$
We perform an experimental evaluation of our proposed method for learning positive invariant neural networks. We disable different core components of Algorithm 1 and measure their effects on the obtained results when optimizing the policy using Deep Q-learning or policy gradient methods, i.e., performing projected gradient descent.

If the verifier in Algorithm 1 shows that constraints in three checks are unsatisfiable, then the computed \( L(x) \) is a \( W_{\epsilon}^\pi \)-safe positive invariant and \( \pi \) is indeed a \( W_{\epsilon}^\pi \)-safe positive invariant. Hence, Algorithm 1 is correct.

Safety via rejection sampling: As discussed in Section 1, once the safety of all trajectories in \( \text{Traj}_{x}^{f,\pi} \) has been verified, we can “re-calibrate” the BNN policy to reject sampled weights which are not in \( W_{\epsilon}^\pi \). Hence, rejection sampling gives rise to a safe BNN policy.

4.3 Computation of safe weight sets and the value of \( \epsilon \)

Problems 1 and 2 assume a given value of \( \epsilon \) for which safety needs to be verified. In order to compute the largest value of \( \epsilon \) for which our approach can verify safety, we start with a small value of \( \epsilon \) and iteratively increase it until we reach a value that cannot be certified or until the timeout is reached, in order to compute a large safe weight set as possible. In each iteration, our Algorithm 1 does not start from scratch but is initialized with the \( g^{\text{inv}} \) and \( D_{\text{spec}} \) from the previous successful iteration, i.e., attempting to enlarge the current safe weight set. Our iterative process significantly speeds up the search process compared to naively restarting our algorithm in every iteration.

4.4 Safe exploration reinforcement learning

Given a safe but non-optimal initial policy \( \pi_0 \), safe exploration reinforcement learning (SERL) concerns the problem of improving the expected return of \( \pi_0 \) while ensuring safety when collecting samples of the environment. Our method from Section 4.2 for computing safe weight sets can be adapted to this setting with minimal effort. In particular, the safety bound \( \epsilon \) for the intervals centered at the weight means can be used in combination with the rejection sampling to generate safe but randomized rollouts on the environment. Moreover, \( \epsilon \) provides bounds on the gradient updates when optimizing the policy using Deep Q-learning or policy gradient methods, i.e., performing projected gradient descent. We sketch an algorithm for SERL in the Supplementary Material.

5 Experiments

We perform an experimental evaluation of our proposed method for learning positive invariant neural networks that prove infinite time horizon safety. Our evaluation consists of an ablation study where we disable different core components of Algorithm 1 and measure their effects on the obtained results.
safety bounds and the algorithm’s runtime. First, we run the algorithm without any re-training on the counterexamples. In the second step, we run Algorithm 1 by initializing $D_{\text{spec}}$ with samples from $X_0$ and $X_u$ only. Finally, we bootstrap the positive invariant network by initializing $D_{\text{spec}}$ with random samples from the state space labeled with Monte-Carlo estimates of reaching the unsafe states. We consider environments with a piecewise linear dynamic function, initial and unsafe state sets so that the verification steps of our algorithm can be reduced to MILP-solving using Gurobi [20]. Details on our evaluation are in the Supplementary Material. Code is publicly available.\footnote{https://github.com/mlech26l/bayesian_nn_safety}

We conduct our evaluation on three benchmark environments that differ in terms of complexity and safety specifications. We train two BNN policies for each benchmark-ablation pair, one with Bayesian weights from the second layer on (with $\mathcal{N}(0, 0.1)$ prior) and one with Bayesian weights in all layers (with $\mathcal{N}(0, 0.05)$ prior). Recall, in our BNN encoding in Section 4.1, we showed that encoding of the BNN input layer requires additional constraints and extra care, since we do not know the signs of input neuron values. Hence, we consider two BNN policies in our evaluation in order to study how the encoding of the input layer affects the safe weight set computation.

Our first benchmark represents an unstable linear dynamical system of the form $x_{t+1} = Ax_t + Bu_t$. A BNN policy stabilizes the system towards the point $(0, 0)$. Consequently, the set of unsafe states is defined as $\{x \in \mathbb{R}^2 \mid |x|_\infty \geq 1.2\}$, and the initial states as $\{x \in \mathbb{R}^2 \mid |x|_\infty \leq 0.6\}$.

Our second benchmark is the inverted pendulum task, which is a classical non-linear control problem. The two state variables $a$ and $b$ represent the angle and angular velocity of a pendulum that must be controlled in an upward direction. The actions produced by the policy correspond to a torque applied to the anchor point. Our benchmark concerns a variant of the original problem where the non-linearity in $f$ is expressed by piecewise linear functions. The resulting system, even with a trained policy, is highly unstable, as shown in Figure 2. The set of initial states corresponds to pendulum states in an almost upright position and with small angular velocity. The set of unsafe states represents the pendulum falling down. Figure 2 visualizes the system and the learned invariant’s decision boundary for the inverted pendulum task.

While the previous two benchmarks concern stability specifications, we evaluate our method on a non-Lyapunovian safety specification in our third benchmark. In particular, our third benchmark is a collision avoidance task, where the system does not stabilize to the same set of terminal states in every execution. The system is described by three variables. The first variable specifies the agent’s own vertical location, while the other two variables specify an intruder’s vertical and horizontal position. The objective is to avoid colliding with the intruder who is moving toward the agent by lateral movement commands as the policy’s actions. The initial states represent far-away intruders, and crashes with the intruder define the unsafe states.

Table 1 shows the results of our evaluation. Our results demonstrate that re-training with the counterexamples is the key component that determines our algorithm’s success. In all cases, except for the linear dynamical system, the initial guess of the invariant candidate violates the invariant
Table 1: Results of our benchmark evaluation. The epsilon values are multiples of the weight’s standard deviation $\sigma$. We evaluated several epsilon values, and the table shows the largest that could be proven safe. A dash “-” indicates an unsuccessful invariant search. Runtime in seconds.

| Environment        | No re-training Verified | $\text{Init } D_{\text{spec}}$ with $\lambda_0$ and $\lambda_u$ Verified | Bootstrapping $D_{\text{spec}}$ Verified | Verified Runtime | Runtime |
|--------------------|-------------------------|------------------------------------------------------------------------|----------------------------------------|------------------|---------|
| Unstable LDS       | -                       | 1.5$\sigma$                                                            | 2$\sigma$                              | -                | 569     |
| Unstable LDS (all) | 0.2$\sigma$             | 0.5$\sigma$                                                            | 0.5$\sigma$                           | 6                | 760     |
| Pendulum           | -                       | 2$\sigma$                                                              | 2$\sigma$                              | -                | 220     |
| Pendulum (all)     | -                       | 0.2$\sigma$                                                            | 1729                                   | -                | 96      |
| Collision avoid.   | -                       | -                                                                      | -                                      | -                | 154     |
| Collision avoid. (all) | -                | -                                                                      | -                                      | -                | 225     |

condition. Moreover, bootstrapping $D_{\text{spec}}$ with random points labeled by empirical estimates of reaching the unsafe states improves the search process significantly.

6 Conclusion

In this work we formulated the safety verification problem for BNN policies in infinite time horizon systems, that asks to compute safe BNN weight sets for which every system execution is safe as long as the BNN samples its weights from this set. Solving this problem allows re-calibrating the BNN policy to reject unsafe weight samples in order to guarantee system safety. We then introduced a methodology for computing safe weight sets in BNN policies in the form of products of intervals around the BNN weight’s means, and a method for verifying their safety by learning a positive invariant-like safety certificate. We believe that our results present an important first step in guaranteeing safety of BNNs for deployment in safety-critical scenarios. While adopting products of intervals around the BNN’s weight means is a natural choice given that BNN priors are typically unimodal distributions, this is still a somewhat restrictive shape for safe weight sets. Thus, an interesting direction of future work would be to study more general forms of safe weight sets that could be used for re-calibration of BNN posteriors and their safety verification. Another interesting problem would be to design an approach for refuting a weight set as unsafe which would complement our method, or to consider closed-loop systems with stochastic environment dynamics.

Any verification method for neural networks, even more so for neural networks in feedback loops, suffers from scalability limitations due to the underlying complexity class [26,24]. Promising research directions on improving the scalability of our approach by potentially speeding up the constraint solving step are gradient based optimization techniques [22] and to incorporate the constraint solving step already in the training procedure [46].

Since the aim of AI safety is to ensure that systems do not behave in undesirable ways and that safety violating events are avoided, we are not aware of any potential negative societal impacts.

Acknowledgments

This research was supported in part by the Austrian Science Fund (FWF) under grant Z211-N23 (Wittgenstein Award), ERC CoG 863818 (FoRM-SMArt), and the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Grant Agreement No. 665385.

References

[1] Joshua Achiam, David Held, Aviv Tamar, and Pieter Abbeel. Constrained policy optimization. In International Conference on Machine Learning, pages 22–31. PMLR, 2017.

[2] Eitan Altman. Constrained Markov decision processes, volume 7. CRC Press, 1999.

[3] Dario Amodei, Chris Olah, Jacob Steinhardt, Paul Christiano, John Schulman, and Dan Mané. Concrete problems in ai safety. arXiv preprint arXiv:1606.06565, 2016.
[4] Felix Berkenkamp, Matteo Turchetta, Angela P. Schoellig, and Andreas Krause. Safe model-based reinforcement learning with stability guarantees. In Isabelle Guyon, Ulrike von Luxburg, Samy Bengio, Hanna M. Wallach, Rob Fergus, S. V. N. Vishwanathan, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, pages 908–918, 2017. URL https://proceedings.neurips.cc/paper/2017/hash/766ebcd59621e305170616ba3d3dac32-Abstract.html

[5] Franco Blanchini and Stefano Miani. *Set-theoretic methods in control*. Springer, 2008.

[6] Charles Blundell, Julien Cornebise, Koray Kavukcuoglu, and Daan Wierstra. Weight uncertainty in neural network. In *International Conference on Machine Learning*, pages 1613–1622. PMLR, 2015.

[7] Rudy Bunel, Ilker Turkaslan, Philip H. S. Torr, Pushmeet Kohli, and Pawan Kumar Mudigonda. A unified view of piecewise linear neural network verification. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolò Cesa-Bianchi, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 4795–4804, 2018. URL https://proceedings.neurips.cc/paper/2018/hash/be53d253d6bc3258a8160556dda3e9b2-Abstract.html

[8] Luca Cardelli, Marta Kwiatkowska, Luca Laurenti, Nicola Paoletti, Andrea Patane, and Matthew Wicker. Statistical guarantees for the robustness of bayesian neural networks. In Sarit Kraus, editor, *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pages 5693–5700. ijcai.org, 2019. doi: 10.24963/ijcai.2019/789. URL https://doi.org/10.24963/ijcai.2019/789

[9] Ya-Chien Chang, Nima Roohi, and Sicun Gao. Neural lyapunov control. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d’Alché-Buc, Emily B. Fox, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada*, pages 3240–3249, 2019. URL https://proceedings.neurips.cc/paper/2019/hash/2647c1dba23bc0e0f9cd175339e120d2-Abstract.html

[10] Xin Chen, Erika Ábrahám, and Sriram Sankaranarayanan. Flow*: An analyzer for non-linear hybrid systems. In Natasha Sharygina and Helmut Veith, editors, *Computer Aided Verification - 25th International Conference, CAV 2013, Saint Petersburg, Russia, July 13-19, 2013. Proceedings*, volume 8044 of *Lecture Notes in Computer Science*, pages 258–263. Springer, 2013. doi: 10.1007/978-3-642-39799-8_18. URL https://doi.org/10.1007/978-3-642-39799-8_18

[11] Yinlam Chow, Ofir Nachum, Edgar A. Duñez-Guzmán, and Mohammad Ghavamzadeh. A lyapunov-based approach to safe reinforcement learning. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolò Cesa-Bianchi, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 8103–8112, 2018. URL https://proceedings.neurips.cc/paper/2018/hash/4fe5149039b52765bde64beb9f674940-Abstract.html

[12] Souradeep Dutta, Susmit Jha, Sriram Sankaranarayanan, and Ashish Tiwari. Output range analysis for deep feedforward neural networks. In *NASA Formal Methods Symposium*, pages 121–138. Springer, 2018.

[13] Souradeep Dutta, Xin Chen, and Sriram Sankaranarayanan. Reachability analysis for neural feedback systems using regressive polynomial rule inference. In Necmiye Ozay and Pavithra Prabhakar, editors, *Proceedings of the 22nd ACM International Conference on Hybrid Systems: Computation and Control, HSCC 2019, Montreal, QC, Canada, April 16-18, 2019*, pages 157–168. ACM, 2019. doi: 10.1145/3302504.3311807. URL https://doi.org/10.1145/3302504.3311807
[14] Robert W. Floyd. Assigning meanings to programs. *Proceedings of Symposium on Applied Mathematics*, 19:19–32, 1967. URL [http://laser.cs.umass.edu/courses/cs521-621Spr06/papers/Floyd.pdf](http://laser.cs.umass.edu/courses/cs521-621Spr06/papers/Floyd.pdf)

[15] Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In Maria-Florina Balcan and Kilian Q. Weinberger, editors, *Proceedings of the 33nd International Conference on Machine Learning, ICML 2016, New York City, NY, USA, June 19-24, 2016*, volume 48 of *JMLR Workshop and Conference Proceedings*, pages 1050–1059. JMLR.org, 2016. URL [http://proceedings.mlr.press/v48/gal16.html](http://proceedings.mlr.press/v48/gal16.html)

[16] Sicun Gao, Jeremy Avigad, and Edmund M Clarke. $\delta$-complete decision procedures for satisfiability over the reals. In *International Joint Conference on Automated Reasoning*, pages 286–300. Springer, 2012.

[17] Timon Gehr, Matthew Mirman, Dana Drachslr-Cohen, Petar Tsankov, Swarat Chaudhuri, and Martin T. Vechev. AI2: safety and robustness certification of neural networks with abstract interpretation. In *2018 IEEE Symposium on Security and Privacy, SP 2018, Proceedings, 21-23 May 2018, San Francisco, California, USA*, pages 3–18. IEEE Computer Society, 2018. doi: 10.1109/SP.2018.00058. URL [https://doi.org/10.1109/SP.2018.00058](https://doi.org/10.1109/SP.2018.00058)

[18] Peter Geibel. Reinforcement learning for mdps with constraints. In Johannes Fünkranz, Tobias Scheffer, and Myra Spiliopoulou, editors, *Machine Learning: ECML 2006, 17th European Conference on Machine Learning, Berlin, Germany, September 18-22, 2006, Proceedings*, volume 4212 of *Lecture Notes in Computer Science*, pages 646–653. Springer, 2006. doi: 10.1007/11871842_63. URL [https://doi.org/10.1007/11871842_63](https://doi.org/10.1007/11871842_63)

[19] Sophie Gruenbacher, Jacek Cyranka, Mathias Lechner, Md Ariful Islam, Scott A Smolka, and Radu Grosu. Lagrangian reachtubes: The next generation. In *2020 59th IEEE Conference on Decision and Control (CDC)*, pages 1556–1563. IEEE, 2020.

[20] LLC Gurobi Optimization. Gurobi optimizer reference manual, 2021. URL [http://www.gurobi.com](http://www.gurobi.com)

[21] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In *2015 IEEE International Conference on Computer Vision, ICCV 2015, Santiago, Chile, December 7-13, 2015*, pages 1026–1034. IEEE Computer Society, 2015. doi: 10.1109/ICCV.2015.123. URL [https://doi.org/10.1109/ICCV.2015.123](https://doi.org/10.1109/ICCV.2015.123)

[22] Patrick Henriksen and Alessio R. Lomuscio. Efficient neural network verification via adaptive refinement and adversarial search. In *ECAI*, volume 325 of *Frontiers in Artificial Intelligence and Applications*, pages 2513–2520. IOS Press, 2020.

[23] Thomas A. Henzinger, Mathias Lechner, and Dorde Zikelic. Scalable verification of quantized neural networks. In *AAAI*, pages 3787–3795. AAAI Press, 2021.

[24] Radoslav Ivanov, James Weimer, Rajeev Alur, George J. Pappas, and Insup Lee. Verisig: verifying safety properties of hybrid systems with neural network controllers. In Necmiye Ozay and Pavithra Prabhakar, editors, *Proceedings of the 22nd ACM International Conference on Hybrid Systems: Computation and Control, HSCC 2019, Montreal, QC, Canada, April 16-18, 2019*, pages 169–178. ACM, 2019. doi: 10.1145/3302504.3311806. URL [https://doi.org/10.1145/3302504.3311806](https://doi.org/10.1145/3302504.3311806)

[25] Kevin Jarrett, Koray Kavukcuoglu, Marc’Aurelio Ranzato, and Yann LeCun. What is the best multi-stage architecture for object recognition? In *IEEE 12th International Conference on Computer Vision, ICCV 2009, Kyoto, Japan, September 27 - October 4, 2009*, pages 2146–2153. IEEE Computer Society, 2009. doi: 10.1109/ICCV.2009.5459469. URL [https://doi.org/10.1109/ICCV.2009.5459469](https://doi.org/10.1109/ICCV.2009.5459469)

[26] Guy Katz, Clark W. Barrett, David L. Dill, Kyle Julian, and Mykel J. Kochenderfer. Reluplex: An efficient SMT solver for verifying deep neural networks. In Rupak Majumdar and Viktor Kuncak, editors, *Computer Aided Verification - 29th International Conference, CAV 2017*, pages 306–323. Springer, 2017.
[27] Guy Katz, Derek A. Huang, Duligur Ibeling, Kyle Julian, Christopher Lazarus, Rachel Lim, Parth Shah, Shantanu Thakoor, Haoze Wu, Aleksandar Zeljic, David L. Dill, Mykel J. Kochenderfer, and Clark W. Barrett. The marabou framework for verification and analysis of deep neural networks. In Isil Dillig and Serdar Tasiran, editors, *Computer Aided Verification - 31st International Conference, CAV 2019, New York City, NY, USA, July 15-18, 2019, Proceedings, Part I*, volume 11561 of *Lecture Notes in Computer Science*, pages 443–452. Springer, 2019. doi: 10.1007/978-3-030-25540-4_26. URL https://doi.org/10.1007/978-3-030-25540-4_26.

[28] Alex Kendall, Jeffrey Hawke, David Janz, Przemyslaw Mazur, Daniele Reda, John-Mark Allen, Vinh-Dieu Lam, Alex Bewley, and Amar Shah. Learning to drive in a day. In *2019 International Conference on Robotics and Automation (ICRA)*, pages 8248–8254. IEEE, 2019.

[29] Hassan K Khalil and Jessy W Grizzle. *Nonlinear systems*, volume 3. Prentice hall Upper Saddle River, NJ, 2002.

[30] Mathias Lechner, Ramin Hasani, Alexander Amini, Thomas A Henzinger, Daniela Rus, and Radu Grosu. Neural circuit policies enabling auditable autonomy. *Nature Machine Intelligence*, 2(10):642–652, 2020.

[31] Alessio Lomuscio and Lalit Maganti. An approach to reachability analysis for feed-forward relu neural networks. *arXiv preprint arXiv:1706.07351*, 2017.

[32] David J. C. MacKay. A practical bayesian framework for backpropagation networks. *Neural Comput.*, 4(3):448–472, 1992. doi: 10.1162/neco.1992.4.3.448. URL https://doi.org/10.1162/neco.1992.4.3.448.

[33] Rowan McAllister, Yarin Gal, Alex Kendall, Mark Van Der Wilk, Amar Shah, Roberto Cipolla, and Adrian Weller. Concrete problems for autonomous vehicle safety: Advantages of bayesian deep learning. International Joint Conferences on Artificial Intelligence, Inc., 2017.

[34] Rhiannon Michelmore, Matthew Wicker, Luca Laurenti, Luca Cardelli, Yarin Gal, and Marta Kwiatkowska. Uncertainty quantification with statistical guarantees in end-to-end autonomous driving control. In *2020 IEEE International Conference on Robotics and Automation, ICRA 2020, Paris, France, May 31 - August 31, 2020*, pages 7344–7350. IEEE, 2020. doi: 10.1109/ICRA40945.2020.9196844. URL https://doi.org/10.1109/ICRA40945.2020.9196844.

[35] Yashwanth Kumar Nakka, Angi Liu, Guanya Shi, Anima Anandkumar, Yisong Yue, and Soon-Jo Chung. Chance-constrained trajectory optimization for safe exploration and learning of nonlinear systems. *IEEE Robotics and Automation Letters*, 6(2):389–396, 2020.

[36] Radford M Neal. *Bayesian learning for neural networks*, volume 118. Springer Science & Business Media, 2012.

[37] Andrea Peruffo, Daniele Ahmed, and Alessandro Abate. Automated and formal synthesis of neural barrier certificates for dynamical models. In Jan Friso Groote and Kim Gulstrand Larsen, editors, *Tools and Algorithms for the Construction and Analysis of Systems - 27th International Conference, TACAS 2021, Held as Part of the European Joint Conferences on Theory and Practice of Software, ETAPS 2021, Luxembourg City, Luxembourg, March 27 - April 1, 2021, Proceedings, Part I*, volume 12651 of *Lecture Notes in Computer Science*, pages 370–388. Springer, 2021. doi: 10.1007/978-3-030-72016-2_20. URL https://doi.org/10.1007/978-3-030-72016-2_20.

[38] Stephen Prajna and Ali Jadbabaie. Safety verification of hybrid systems using barrier certificates. In Rajeev Alur and George J. Pappas, editors, *Hybrid Systems: Computation and Control, 7th International Workshop, HSCC 2004, Philadelphia, PA, USA, March 25-27, 2004. Proceedings*, volume 2993 of *Lecture Notes in Computer Science*, pages 477–492. Springer, 2004. doi: 10.1007/978-3-540-24743-2_32. URL https://doi.org/10.1007/978-3-540-24743-2_32.
[39] Stephen Prajna, Ali Jadbabaie, and George J. Pappas. A framework for worst-case and stochastic safety verification using barrier certificates. *IEEE Trans. Autom. Control.*, 52(8):1415–1428, 2007. doi: 10.1109/TAC.2007.902736. URL https://doi.org/10.1109/TAC.2007.902736

[40] Wenjie Ruan, Xiaowei Huang, and Marta Kwiatkowska. Reachability analysis of deep neural networks with provable guarantees. In Jérôme Lang, editor, *Proceedings of the Twenty-Seventh International Joint Conference on Artificial Intelligence, IJCAI 2018, July 13-19, 2018, Stockholm, Sweden*, pages 2651–2659. ijcai.org, 2018. doi: 10.24963/ijcai.2018/368. URL https://doi.org/10.24963/ijcai.2018/368

[41] Dinggang Shen, Guorong Wu, and Heung-Ill Suk. Deep learning in medical image analysis. *Annual review of biomedical engineering*, 19:221–248, 2017.

[42] Christopher A Strong, Haoze Wu, Aleksandar Zeljić, Kyle D Julian, Guy Katz, Clark Barrett, and Mykel J Kochenderfer. Global optimization of objective functions represented by relu networks. *arXiv preprint arXiv:2010.03258*, 2020.

[43] Vincent Tjeng, Kai Y. Xiao, and Russ Tedrake. Evaluating robustness of neural networks with mixed integer programming. In *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. OpenReview.net, 2019. URL https://openreview.net/forum?id=HyGIdiRqtM

[44] Eiji Uchibe and Kenji Doya. Constrained reinforcement learning from intrinsic and extrinsic rewards. In *2007 IEEE 6th International Conference on Development and Learning*, pages 163–168. IEEE, 2007.

[45] Matthew Wicker, Luca Laurenti, Andrea Patane, and Marta Kwiatkowska. Probabilistic safety for bayesian neural networks. In Ryan P. Adams and Vibhav Gogate, editors, *Proceedings of the Thirty-Sixth Conference on Uncertainty in Artificial Intelligence, UAI 2020, virtual online, August 3-6, 2020*, volume 124 of *Proceedings of Machine Learning Research*, pages 1198–1207. AUAI Press, 2020. URL http://proceedings.mlr.press/v124/wicker20a.html

[46] Huan Zhang, Hongge Chen, Chaowei Xiao, Sven Gowal, Robert Stanforth, Bo Li, Duane S. Boning, and Cho-Jui Hsieh. Towards stable and efficient training of verifiably robust neural networks. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net, 2020. URL https://openreview.net/forum?id=SkxukfFwB

[47] Hengjun Zhao, Xia Zeng, Taolue Chen, and Zhiming Liu. Synthesizing barrier certificates using neural networks. In Aaron D. Ames, Sanjit A. Seshia, and Jyotirmoy Deshmukh, editors, *HSCC ’20: 23rd ACM International Conference on Hybrid Systems: Computation and Control, Sydney, New South Wales, Australia, April 21-24, 2020*, pages 25:1–25:11. ACM, 2020. doi: 10.1145/3365365.3382222. URL https://doi.org/10.1145/3365365.3382222
A Proofs

Theorem 1. Let \( \epsilon \in [0, \infty) \). Then each deterministic NN in \( \{ \pi_{w,b} \mid (w,b) \in W_\pi^\epsilon \} \) is safe if and only if the system of constraints \( \Phi(\pi, \lambda_0, \lambda_0, \epsilon) \) is not satisfiable.

Proof. We prove the equivalent claim that there exists a weight vector \((w,b) \in W_\pi^\epsilon\) for which \(\pi_{w,b}\) is unsafe if and only if \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\) is satisfiable.

First, suppose that there exists a weight vector \((w,b) \in W_\pi^\epsilon\) for which \(\pi_{w,b}\) is unsafe and we want to show that \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\) is satisfiable. This direction of the proof is straightforward since values of the network’s neurons on the unsafe input give rise to a solution of \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\). Indeed, by assumption there exists a vector of input neuron values \(x_0 \in \lambda_0\) for which the corresponding vector of output neuron values \(x_l = \pi_{w,b}(x_0)\) is unsafe, i.e., \(x_i \in \lambda_i\). By defining \(x_i^{\text{in}}, x_i^{\text{out}}\) to be the vectors of the corresponding input and output neuron values for the \(i\)-th hidden layer for each \(1 \leq i \leq l - 1\) and by setting \(x_{0,\text{pos}} = \text{ReLU}(x_0)\) and \(x_{0,\text{neg}} = -\text{ReLU}(-x_0)\), we easily see that these variable values satisfy the Input-output conditions, the ReLU encoding conditions and the BNN input and hidden layer conditions, therefore we get a solution to the system of constraints \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\).

We now proceed to the more involved direction of this proof and show that any solution to the system of constraints \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\) gives rise to weights \((w,b) \in W_\pi^\epsilon\) for which \(\pi_{w,b}\) is unsafe. Let \(x_0, x_l, x_{0,\text{pos}}, x_{0,\text{neg}}\) and \(x_i^{\text{in}}, x_i^{\text{out}}\) for \(1 \leq i \leq l - 1\), be real vectors that satisfy the system of constraints \(\Phi(\pi, \lambda_0, \lambda_0, \epsilon)\). Fix \(1 \leq i \leq l - 1\). From the BNN hidden layers constraint for layer \(i\), we have

\[
(M_i - \epsilon \cdot 1)x_i^{\text{out}} + (m_i - \epsilon \cdot 1) \leq x_i^{\text{in}} \leq (M_i + \epsilon \cdot 1)x_i^{\text{out}} + (m_i + \epsilon \cdot 1). \tag{3}
\]

We show that there exist values \(W_i, b_i^*\) of BNN weights between layers \(i\) and \(i + 1\) such that each weight value is at most \(\epsilon\) apart from its mean, and such that \(x_{i+1}^{\text{in}} = W_i^* x_i^{\text{out}} + b_i^*\). Indeed, to formally show this, we define \(W_i^* [i]\) to be the set of all weight vectors between layers \(i\) and \(i + 1\) such that each weight value is distant from its mean by at most \(\epsilon\) (hence, \(W_i^* [i]\) is a projection of \(W_i^* \) onto dimensions that correspond to the weights between layers \(i\) and \(i + 1\)). We then consider a continuous function \(h_i : W_i^* [i] \to \mathbb{R}\) defined via

\[
h_i(W_i, b_i) = W_i x_i^{\text{out}} + b_i.
\]

Since \(W_i^* [i] \subseteq \mathbb{R}^{m_i \times n_i} \times \mathbb{R}^{n_i}\) is a product of intervals and therefore a connected set w.r.t. the Euclidean metric and since \(h_i\) is continuous, the image of \(W_i^* [i]\) under \(h_i\) is also connected in \(\mathbb{R}\). But note that

\[
h_i(M_i - \epsilon \cdot 1, m_i - \epsilon \cdot 1) = (M_i - \epsilon \cdot 1)x_i^{\text{out}} + (m_i - \epsilon \cdot 1)
\]

and

\[
h_i(M_i + \epsilon \cdot 1, m_i + \epsilon \cdot 1) = (M_i + \epsilon \cdot 1)x_i^{\text{out}} + (m_i + \epsilon \cdot 1),
\]

with \((M_i - \epsilon \cdot 1, m_i - \epsilon \cdot 1), (M_i + \epsilon \cdot 1, m_i + \epsilon \cdot 1) \in W_i^* [i]\). Thus, for the two points to be connected, the image set must also contain \(x_{i+1}^{\text{in}}\) which lies in between by eq. (3). Thus, there exists \((W_i^*, b_i^*) \in W_i^* [i]\) with \(x_{i+1}^{\text{in}} = W_i^* x_i^{\text{out}} + b_i^*\), as desired.

For the input and the first hidden layer, from the BNN input layer constraint we know that

\[
(M_0 - \epsilon \cdot 1)x_{0,\text{pos}} + (M_0 + \epsilon \cdot 1)x_{0,\text{neg}} + (m_0 - \epsilon \cdot 1) \leq x_1^{\text{in}} \leq (M_0 + \epsilon \cdot 1)x_{0,\text{pos}} + (M_0 - \epsilon \cdot 1)x_{0,\text{neg}} + (m_0 + \epsilon \cdot 1).
\]

Again, define \(W_0^* [0]\) to be the set of all weight vectors between the input and the first hidden layer such that each weight value is distant from its mean by at most \(\epsilon\). Consider a continuous function \(h_0 : W_0^* [0] \to \mathbb{R}\) defined via

\[
h_0(W_0, b_0) = W_0 x_0 + b_0.
\]

Let \(M_{\text{sign}}(x_0)\) be a matrix of the same dimension as \(M_0\), with each column consisting of 1’s if the corresponding component of \(x_0\) is nonnegative, and of -1’s if it is negative. Then note that

\[
h_0(M_0 - \epsilon \cdot M_{\text{sign}}(x_0), m_0 - \epsilon \cdot 1) = (M_0 - \epsilon \cdot 1)x_{0,\text{pos}} + (M_0 + \epsilon \cdot 1)x_{0,\text{neg}} + (m_0 - \epsilon \cdot 1)
\]

and

\[
h_0(M_0 + \epsilon \cdot M_{\text{sign}}(x_0), m_0 + \epsilon \cdot 1) = (M_0 + \epsilon \cdot 1)x_{0,\text{pos}} + (M_0 - \epsilon \cdot 1)x_{0,\text{neg}} + (m_0 + \epsilon \cdot 1).
\]
Since \((M_0 - \epsilon \cdot M\text{sign}(x_0))\), \((M_0 + \epsilon \cdot M\text{sign}(x_0))\), \((M_0 + \epsilon \cdot 1)\) \(\in W^*\), analogous image connectedness argument as the one above shows that there exist values \(W_0\), \(b_0\) of BNN weights such that \((W_0, b_0) \in W^*\), and such that \(x_0 = W_0 x_0 + b_0\).

But now, collecting \(W_i, b_i^*\) and \(W_i, b_i^*\) for \(1 \leq i \leq l - 1\) gives rise to a BNN weight vector \((W^*, b^*)\) which is contained in \(W^*\). Furthermore, combining what we showed above with the constraints in \(\Phi(\pi, x_0, X_u, \epsilon)\), we get that:

- \(x_i \in X_u\), from the Input-output condition in \(\Phi(\pi, X_0, X_u, \epsilon)\);
- \(x_{i+1} = \text{ReLU}(x_i)\) for each \(1 \leq i \leq l - 1\), from the ReLU-encoding;
- \(x_0 = W_0 x_0 + b_0^*\) and \(x_i = W_i x_i + b_i^*\) for each \(1 \leq i \leq l - 1\), as shown above.

Hence, \(x_i \in X_u\) is the vector of neuron output values of \(\pi_{w,b}\) on the input neuron values \(x_0 \in X_0\), so as \((W^*, b^*) \in W^*\) we conclude that there exists a deterministic NN in \(\{\pi_{w,b} | (w, b) \in W^*\}\) which is not safe. This concludes the proof.

**Theorem 2.** If there exists a \(W^*\)-safe positive invariant, then each trajectory in \(\text{Traj}^{f,\pi}_e\) is safe.

**Proof.** Let \(\text{Inv}\) be a \(W^*\)-safe positive invariant. Given a trajectory \((x_t, u_t)_{t=0}^{\infty}\) in \(\text{Traj}^{f,\pi}_e\), we need to show that \(x_t \notin X_u\) for each \(t \in \mathbb{N}_{\geq 0}\). Since \(\text{Inv} \cap X_u = \emptyset\), it suffices to show that \(x_t \notin \text{Inv}\) for each \(t \in \mathbb{N}_{\geq 0}\). We prove this by induction on \(t\).

The base case \(x_0 \in \text{Inv}\) follows since \(x_0 \in X_0 \subseteq \text{Inv}\). As an inductive hypothesis, suppose now that \(x_t \notin \text{Inv}\) for some \(t \in \mathbb{N}_{\geq 0}\). We need to show that \(x_{t+1} \notin \text{Inv}\).

Since the trajectory is in \(\text{Traj}^{f,\pi}_e\), we know that the BNN weight vector \((w_t, b_t)\) sampled at the time-step \(t\) belongs to \(W^*\), i.e. \((w_t, b_t) \in W^*\). Thus, since \(x_t \notin \text{Inv}\) by the induction hypothesis and since \(\text{Inv}\) is closed under the system dynamics when the sampled weight vector is in \(W^*\), it follows that \(x_{t+1} = f(x_t, u_t) = f(x_t, \pi_{w_t,b_t}(x_t)) \in \text{Inv}\). This concludes the proof by induction.

**Theorem 3.** The loss function \(L\) is nonnegative for any neural network \(g\), i.e. \(L(g) \geq 0\). Moreover, if \(\text{Inv}\) is a \(W^*\)-safe positive invariant and \(L_{\text{cls}}\) the 0/1-loss, then \(L(g_{\text{Inv}}) = 0\). Hence, neural networks \(g_{\text{Inv}}\) for which \(\text{Inv}\) is a \(W^*\)-safe positive invariant are global minimizers of the loss function \(L\) when \(L_{\text{cls}}\) is the 0/1-loss.

**Proof.** Recall, the loss function \(L\) for a neural network \(g\) is defined via

\[
L(g) = \frac{1}{|D_{\text{spec}}|} \sum_{(x, y) \in D_{\text{spec}}} L_{\text{cls}}(g(x), y) + \lambda \frac{1}{|D_{\text{ce}}|} \sum_{(x, x') \in D_{\text{ce}}} L_{\text{ce}}(g(x), g(x')) ,
\]

where \(\lambda\) is a tuning parameter and \(L_{\text{cls}}\) a binary classification loss function, e.g. the 0/1-loss

\[
L_{\text{cls}}(z, y) = \mathbb{1}[z \geq 0] \neq y
\]

or the logistic loss

\[
L_{\log}(z, y) = z - z \cdot y + \log(1 + \exp(-z))
\]

as its differentiable alternative. The term \(L_{\text{ce}}\) is the counterexample loss which we define via

\[
L_{\text{ce}}(z, z') = \mathbb{1}[z > 0] \mathbb{1}[z' < 0] L_{\text{cls}}(z, 0) L_{\text{cls}}(z', 1).
\]

The fact that \(L(g) \geq 0\) for each neural network \(g\) follows immediately from the fact that summands in the first sum in eq. (4) are loss functions which are nonnegative, and summands in the second sum are products of indicator and nonnegative loss functions and therefore also nonnegative.

We now show that, if \(L_{\text{cls}}\) is the 0/1-loss, \(L(g_{\text{Inv}}) = 0\) whenever \(\text{Inv}\) is a \(W^*\)-safe positive invariant, which implies the global minimization claim in the theorem. This follows from the following two items:

- For each \((x, y) \in D_{\text{spec}}\), we have \(L_{\text{cls}}(g_{\text{Inv}}(x), y) = 0\). Indeed, for \((x, y)\) to be added to \(D_{\text{spec}}\) in Algorithm 1, we must have that either \(x \in X_0\) and \(y = 1\), or that \(x \notin X_0\) and \(y = 0\). Thus, since \(\text{Inv}\) is assumed to be a \(W^*\)-safe positive invariant, \(g_{\text{Inv}}\) correctly classifies \((x, y)\) and the corresponding loss is 0.
- For each \((x, x') \in D_{\text{ce}}\) we have \(L_{\text{ce}}(g_{\text{Inv}}(x), g_{\text{Inv}}(x')) = 0\). Indeed, since

\[
L_{\text{ce}}(g_{\text{Inv}}(x), g_{\text{Inv}}(x')) = \mathbb{1}[g_{\text{Inv}}(x) > 0] \mathbb{1}[g_{\text{Inv}}(x') < 0] L_{\text{cls}}(g_{\text{Inv}}(x), 0) L_{\text{cls}}(g_{\text{Inv}}(x'), 1),
\]

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Algorithm 2 Safe Exploration Reinforcement Learning

**Input** Initial policy $\pi_0$, learning rate $\alpha$, number of iterations $N$

for $i \in 1, \ldots, N$ do

$\epsilon \leftarrow$ find safe $\epsilon$ for $\pi_{i-1}$

collect rollouts of $\pi_{i-1}$ with rejection sampling $\epsilon$

compute $\nabla \mu_{i-1}$ for parameters $\mu_{i-1}$ of $\pi_{i-1}$ using DQN/policy gradient

$\mu_i \leftarrow \mu_{i-1} - \alpha \nabla \mu_{i-1}$ (gradient descent)

project $\mu_i$ back to interval $[\mu_{i-1} - \epsilon, \mu_{i-1} + \epsilon]$

end for

Return $\pi_N$

for the loss to be non-zero we must have that $g^{\text{inv}}(x) \geq 0$ and $g^{\text{inv}}(x) < 0$. But this is impossible since Inv is assumed to be a $W^\pi_\epsilon$-safe positive invariant and $(x, x')$ was added by Algorithm 1 as a counterexample to $\mathcal{D}_c$, meaning that $x'$ can be reached from $x$ by following the dynamics function and sampling a BNN weight vector in $W^\pi_\epsilon$. Therefore, by the closedness property of $W^\pi_\epsilon$-safe positive invariants when the sampled weight vector is in $W^\pi_\epsilon$, we cannot have both $g^{\text{inv}}(x) \geq 0$ and $g^{\text{inv}}(x) < 0$. Hence, the loss must be 0.

\[\Box\]

**Theorem 4.** If the verifier in Algorithm 1 shows that constraints in three checks are unsatisfiable, then the computed Inv is indeed a $W^\pi_\epsilon$-safe positive invariant. Hence, Algorithm 1 is correct.

**Proof.** The fact that the first check in Algorithm 1 correctly checks whether there exist $x, x' \in \mathcal{X}_0$ and a weight vector $(w, b) \in W^\pi_\epsilon$ such that $x' = f(x, \pi_{w,b}(x))$ with $g^{\text{inv}}(x) \geq 0$ and $g^{\text{inv}}(x') < 0$ follows by the correctness of our encoding in Section 4.1, which was proved in Theorem 1. The fact that checks 2 and 3 correctly check whether for all $x \in \mathcal{X}_0$ we have $g^{\text{inv}}(x) \geq 0$ and for all $x \in \mathcal{X}_u$ we have $g^{\text{inv}}(x) < 0$, respectively, follows immediately from the conditions they encode.

Therefore, the three checks together verify that (1) Inv is closed under the system dynamics whenever the sampled weight vector is in $W^\pi_\epsilon$, (2) Inv contains all initial states, and (3) Inv contains no unsafe states. As these are the 3 defining properties of $W^\pi_\epsilon$-safe positive invariants, Algorithm 1 is correct and the theorem claim follows.

**B Safe exploration reinforcement learning algorithm**

Algorithm 2 shows our sketch of how standard RL algorithms, such as policy gradient methods and deep Q-learning, can be adapted to a safe exploration setup by using the safe weight sets computed by our method.

**C Experimental details**

In this section, we describe the details of our experimental evaluation setup. The code and pre-trained network parameters are attached in the supplementary materials. Each policy is a ReLU network consisting of three layers. The first layer represents the input variables, the second one is a hidden layer with 16 neurons, and the last layer are the output variables. The size of the first and the last layer is task dependent and is shown in Table 2. The $W^\pi_\epsilon$-safe positive invariant candidate network differs from the policy network in that its weights are deterministic, it has a different number of hidden units and a single output dimension. Particularly, the invariant networks for the linear dynamical system and the inverted pendulum have 12 hidden units, whereas the invariant network for the collision avoidance task has 32 neurons in its hidden layer. The policy networks are trained with a $\mathcal{N}(0, 0.1)$ (from second layer on) and $\mathcal{N}(0, 0.05)$ (all weights) prior for the Bayesian weights, respectively. MILP solving was performed by Gurobi 9.03 on a 4 vCPU with 32GB virtual machine.

Linear dynamical system The state of the linear dynamical system consists of two variables $(x, y)$. The update function takes the current state $(x_t, y_t)$ with the current action $u_t$ and outputs the next
Table 2: Number of dimensions of the policy network for the three experiments.

| Experiment             | Input dimension | Hidden size | Output dimension |
|------------------------|-----------------|-------------|-----------------|
| Linear dynamical system| 2               | 16          | 1               |
| Inverted pendulum      | 2               | 16          | 1               |
| Collision avoidance    | 3               | 16          | 3               |

states \((x_{t+1}, y_{t+1})\) governed by the equations

\[
y_{t+1} = y_t + 0.2 \cdot \text{clip}_{\pm 1}(u_t)
\]
\[
x_{t+1} = x_t + 0.3y_{t+1} + 0.05 \cdot \text{clip}_{\pm 1}(u_t),
\]

where the function \(\text{clip}_{\pm 1}\) is defined by

\[
\text{clip}_{\pm z}(x) = \begin{cases} 
-z & \text{if } x \leq -z \\
z & \text{if } x \geq z \\
x & \text{otherwise.}
\end{cases}
\]

The set of unsafe states is defined as \(\{(x,y) \in \mathbb{R}^2 \mid |(x,y)|_\infty \geq 1.2\}\), and the initial states as \(\{(x,y) \in \mathbb{R}^2 \mid |(x,y)|_\infty \leq 0.6\}\).

**Inverted pendulum** The state of the inverted pendulum consists of two variables \((\theta, \dot{\theta})\). The non-linear state transition is defined by

\[
\dot{\theta}_{t+1} = \text{clip}_{\pm 8}(\dot{\theta}_t + \frac{-3g \cdot \text{angular}(\theta_t + \pi)}{2l} + \frac{7.5 \cdot \text{clip}_{\pm 1}(u_t)}{(m \cdot l^2)}) + \delta_t,
\]
\[
\theta_{t+1} = \theta_t + \dot{\theta}_{t+1} \cdot \delta_t,
\]

where \(g = 9.81, l = 1, \delta_t = 0.05\) and \(m = 0.8\) are constants. The function \(\text{angular}\) is defined using the piece-wise linear composition

\[
\text{angular}(x) = \begin{cases} 
\text{angular}(x + 2\pi) & \text{if } x \leq \pi/2 \\
\text{angular}(x - 2\pi) & \text{if } x > 5\pi/2 \\
\frac{x - 2\pi}{\pi/2} & \text{if } 3\pi/2 < x \leq 5\pi/2 \\
2 - \frac{x}{\pi/2} & \text{if } \pi/2 < x \leq 3\pi/2.
\end{cases}
\]

The set of initial states are defined by \(\{(\theta, \dot{\theta}) \in \mathbb{R}^2 \mid |\theta| \leq \pi/6 \text{ and } |\dot{\theta}| \leq 0.2\}\). The set of unsafe states are defined by \(\{(\theta, \dot{\theta}) \in \mathbb{R}^2 \mid |\theta| \geq 0.9 \text{ or } |\dot{\theta}| \geq 2\}\).

**Collision avoidance** The state of the collision avoidance environment consists of three variables \((p_x, a_x, a_y)\), representing the agent’s vertical position and the vertical and the horizontal position of an intruder. The intruder moves toward the agent, while the agent’s vertical position must be controlled to avoid colliding with the intruder. The particular state transition is given by

\[
p_{x,t+1} = p_{x,t} + u_t
\]
\[
a_{x,t+1} = a_{x,t}
\]
\[
a_{y,t+1} = a_{y,t} - 1.
\]

Admissible actions are defined by \(u_t \in \{-1, 0, 1\}\). The set of initial states are defined as \(\{(p_x, a_x, a_y) \in \mathbb{Z}^3 \mid |p_x| \leq 2 \text{ and } |a_x| \leq 2 \text{ and } a_y = 5\}\). Likewise, the set of unsafe states are given by \(\{(p_x, a_x, a_y) \in \mathbb{Z}^3 \mid |p_x - a_x| \leq 1 \text{ and } a_y = 5\}\).