Joint Differentiable Optimization and Verification for Certified Reinforcement Learning

Yixuan Wang 1  Chao Huang 2  Zhaoran Wang 1  Zhuoran Yang 3  Qi Zhu 1

Abstract

In model-based reinforcement learning for safety-critical control systems, it is important to formally certify system properties (e.g., safety, stability) under the learned controller. However, as existing methods typically apply formal verification after the controller has been learned, it is sometimes difficult to obtain any certificate, even after many iterations between learning and verification. To address this challenge, we propose a framework that jointly conducts reinforcement learning and formal verification by formulating and solving a novel bilevel optimization problem, which is differentiable by the gradients from the value function and certificates. Experiments on a variety of examples demonstrate the significant advantages of our framework over the model-based stochastic value gradient (SVG) method and the model-free proximal policy optimization (PPO) method in finding feasible controllers with barrier functions and Lyapunov functions that ensure system safety and stability.

1. Introduction

Reinforcement learning (RL) has shown great promises in controller synthesis for complex systems, typically by maximizing a total reward function that encodes the desired control goal (Sutton & Barto, 2018). However, there is significant hesitation in applying RL to safety-critical systems (Knight, 2002) such as autonomous vehicles and avionics because of the uncertain and potentially dangerous safety impact (Xiang & Johnson, 2018; Ivanov et al., 2021). It is thus important to provide formal guarantees on system properties such as safety and stability under the learned controller before deploying it, i.e., certify the controller. A common approach to guarantee these properties is to find a corresponding certificate, e.g., a barrier function for safety (Prajna & Jadbabaie, 2004) and a Lyapunov function for stability (Lyapunov, 1992).

In this work, we focus on learning a certified controller for systems with unknown parameters in their model. In the traditional way, this is typically done in a two-step ‘open-loop’ process: 1) first, model-based reinforcement learning (MBRL) is utilized to learn the system model parameters and the controller simultaneously, and then 2) formal verification methods are applied to find certificates for different properties by solving optimization problems with approaches such as semi-definite programming (SDP). However, for such open-loop paradigm, it is sometimes difficult to find any feasible certificate even after many iterations of learning and verification steps, and the failed verification results often are not leveraged sufficiently in the learning of a new controller. Thus, integrating controller synthesis and certificate generation in a more holistic manner has received increasing attention recently.

Pioneering works on control-certificate joint learning mainly focus on systems with known models, i.e., explicit models with no unknown parameters (Jin et al., 2020; Qin et al., 2021; Wang et al., 2021). Those methods typically collect samples from the system space and transform the certificate conditions into loss functions and solve them via supervised learning methods such as regression. However, they can be hardly used to address systems with unknown parameters due to the nature of supervised learning, and the certificates obtained in those works are often tested/validated via sampling-based approaches without being formally verified.

Contribution of this Work: To address these challenges, we propose a certified RL method with joint differentiable optimization and verification for systems with unknown model parameters. As shown in Fig. 1, our approach seamlessly integrates RL optimization and formal verification by formulating and solving a novel bilevel optimization problem, which generates an optimal controller together with its certificates, e.g., barrier functions for safety and/or Lyapunov functions for stability. The upper-level problem in the bilevel optimization tries to learn the controller parameters \(\theta\) and the unknown system model parameters \(\alpha\) by maximizing the total reward for the controller via MBRL; while the lower-level problem tries to verify system prop-
Our work is related to the joint learning of controller and verification by leveraging neural networks to represent barrier functions and Lyapunov functions (Jin et al., 2020; Dawson et al., 2022; Qin et al., 2021). These approaches first translate the certificate conditions into loss functions, sample and label data points from the system state, and then learn the certificate in a supervised learning manner. They, however, require a known system dynamics model and cannot be directly applied to systems models with unknown parameters, which is the case our approach addresses. Moreover, the neural network-based certificates generated by these approaches are often tested/validated through sampling based methods and are not formally verified, while our approach provides formal and deterministic guarantees.

Our work is also related to closed-loop controller learning methods, such as falsification guided controller synthesis. Falsification-based methods try to search for counterexamples to improve controller synthesis or certificate searching (Fremont et al., 2020). And some works (Chen et al., 2020; Peruffo et al., 2020; Dai et al., 2021) build falsification on the verification modules that can provide formal guarantees for the final output. Different from the counter examples provided in these works, the verification module in our approach provides gradient feedback that can more directly guide the controller synthesis to find verifiable parameter configurations. Most recently, the work in (Wang et al., 2021) integrates control learning with verification in a closed-loop manner by computing the forward reachable set to construct a controller with reach-avoid property, however, that work still assumes a known system model and is not differentiable.

Finally, our work leverages SVG (Heess et al., 2015) in MBRL, and is a first-order, end-to-end differentiable approach with the computation of analytic gradient of the RL objective and the consideration of gradient from verification feedback. As another category of MBRL, Dyna-Style algorithms (Sutton, 1991) can be viewed as zero-order optimization approaches without analytic gradient. They generate imaginary data without interacting with the environment and learn the controller with these data in a model-free manner.
3. Problem Formulation

We consider a continuous system whose dynamics can be expressed as an ordinary differential equation (ODE):

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

where \( x \in X \subset \mathbb{R}^n \) is a vector denoting the system state within the state space \( X \) and \( u \in U \subset \mathbb{R}^m \) is the control input variable. \( f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n \) is a locally Lipschitz-continuous function ensuring that there exists a unique solution for the system ODE. \( \alpha \in \mathbb{R}^n \) and \( \beta \in [\underline{\beta}, \bar{\beta}] \) is a vector denoting the unknown system model parameters that are within a lower bound \( \underline{\beta} \) and an upper bound \( \bar{\beta} \). The system has an initial state set \( X_0 \subset X \), an unsafe state set \( X_u \subset X \) and a goal state set \( X_g \subset X \). Without the loss of generality, \( X_g \) is assumed as the origin point in this paper. These sets are semialgebraic, which can be expressed as:

\[
\begin{align*}
X_0 &= \{x|\xi_i(x) \geq 0, i = 1, \cdots, s\}, \\
X_u &= \{x|\xi_s(x) \geq 0, i = s + 1, \cdots, s + q\}, \\
X &= \{x|\psi_i(x) \geq 0, i = s + q + 1, \cdots, s + q + r\}.
\end{align*}
\]

The partial derivatives \( f_x \) and \( f_u \) can be computed with the parameters \( \alpha \). We abbreviate partial differentiation or gradient using subscripts, e.g., \( \frac{\partial f(x,u;\alpha)}{\partial x} \equiv f_x \) with gradient or derivative denoting in front.

Such a continuous system can be controlled by a feedback controller \( \pi(x; \theta) : X \rightarrow U \), which is parameterized by \( \theta \) in the following way. Given any time \( \forall t \geq 0 \), the controller \( \pi \) reads the system state \( x(t) \) at \( t \), and computes the control input as \( u = \pi(x(t); \theta) \). Overall, the system evolves by following \( \dot{x} = f(x, \pi(x; \theta)) \) with \( \pi \).

A flow function \( \varphi(x(0), t) : X_0 \times \mathbb{R}_+ \rightarrow X \) maps some initial state \( x(0) \) to the system state \( \varphi(x(0), t) \) at time \( t \), \( \forall t \geq 0 \). Mathematically, \( \varphi \) satisfies 1) \( \varphi(x(0), 0) = x(0) \), and 2) \( \varphi \) is the solution of the \( \dot{x} = f(x, u) \). Based on the flow definition, the system safety and stability properties and their corresponding certificates, e.g., barrier function and Lyapunov function, are defined as follows.

Definition 3.1. (Infinite-time Safety Property) Starting from any initial state \( x(0) \in X_0 \), the system defined in (1) is considered as meeting the safety property if and only if its flow never enters into the unsafe set \( X_u \):

\[ \forall t \geq 0, \varphi(x(0), t) \notin X_u. \]

Such safety property can be formally guaranteed if the controller \( \pi \) can obtain its barrier function.

Definition 3.2. (Exponential Condition based Barrier Function) \( \text{Kong et al., 2013} \) Given a controller \( \pi(x; \theta) \), \( B(x; \beta^B) \) is a safety barrier function parameterized by \( \beta^B \) with \( \lambda \in R \) if:

\[
\begin{align*}
B(x; \beta^B) &\leq 0, \quad x \in X_0, \\
B(x; \beta^B) &> 0, \quad x \in X_u, \\
\frac{\partial B}{\partial x} \cdot f(x, \pi(x; \theta); \alpha) - \lambda B(x; \beta^B) &\leq 0, \quad x \in X.
\end{align*}
\]

Remark 3.3. A barrier function essentially indicates that the system flow function starting from \( X_0 \) will always have non-positive value and thus never enter unsafe state set \( X_u \). Exponential condition based barrier function in Definition 3.2 is extended from the original barrier function definition that is only based on the Lie derivative (for the third inequality) as following (Prajna & Jadbabaie, 2004):

\[ \frac{\partial B}{\partial x} \cdot f(x, \pi(x; \theta); \alpha) \leq 0, \quad x \in X. \]

Exponential condition based barrier function is less conservative than the original barrier function when its \( \lambda < 0 \).

Definition 3.4. (Stability Property) Starting from any initial state \( x(0) \in X_0 \), the system defined in (1) is stable around the goal set \( X_g \) if there exists a KL function \( \tau (\text{Khalil, 2002}) \) such that for any \( x(0) \in X_0 \),

\[ \|\varphi(x(0), t)\|_{X_g} \leq \tau(\|x(0)\|_{X_g}, t), \]

where \( \|x\|_{X_g} = \inf_{x_g \in X_g} \|x - x_g\| \), with \( \|\cdot\| \) denoting the Euclidean distance.

Stability can be formally guaranteed if there exists a Lyapunov function for controller \( \pi \).

Definition 3.5. (Lyapunov Function) \( V(x; \beta^V) \) is a Lyapunov function of controller \( \pi(x; \theta) \) if:

\[ V(x; \beta^V) \geq 0, \quad x \in X, \]

\[ \frac{\partial V}{\partial x} \cdot f(x, \pi(x; \theta); \alpha) \leq 0, \quad x \in X. \]

Considering the safety and stability certificates in this work, we formulate the certified control learning problem we address as the following:

Problem 3.6. (Certified Control Learning) Given a continuous system defined as (1), learn a controller \( \pi(x; \theta) \) that formally satisfies the safety and/or stability property with its barrier function \( B(x; \beta^B) \) and/or Lyapunov function \( V(x; \beta^V) \) as certificates.

4. Our Approach for Certified Differentiable Reinforcement Learning

In this section, we present our certified differentiable reinforcement learning framework to solve the Problem 3.6.
We first introduce a novel bilevel optimization formulation for Problem 3.6 in Section 4.1, by treating the learning of control and system model parameters as an upper-level MBRL problem and formulating the verification as a lower-level SDP problem. We then solve the bilevel optimization problem with the Algorithm 1 introduced in Section 4.2, which leverages the gradients of the slack variable and the value function, and includes techniques for variable transformation, safety shielding, and parameter identification. Finally, we conduct theoretical analysis on the optimality of our approach in Section 4.3.

### 4.1. Bilevel Optimization Problem Formulation

**Definition 4.1.** A polynomial \( p(x) \) is a sum-of-squares (SOS) if there exist certain polynomials \( f_1(x), f_2(x), \ldots, f_m(x) \) such that \( p(x) = \sum_{i=1}^{m} f_i(x)^2 \). In such case, it is easy to get \( p(x) \geq 0 \).

The three conditions in a barrier function can be relaxed into three SOS programmings based on Putinar’s Positivstellensatz theorem (Nie & Schweighofer, 2007) as:

\[
\begin{align*}
-B(x) - \sum_{i=1}^{s} \sigma_i(x) \cdot \xi_i(x) & \in \Sigma[x], \\
B(x) - \sum_{i=s+1}^{s+q} \sigma_i(x) \cdot \zeta_i(x) & \in \Sigma[x], \\
-\frac{\partial B}{\partial x} : f(x, \pi(x)) + \lambda B(x) - \sum_{i=s+q+1}^{s+q+r} \sigma_i(x) \psi_i(x) & \in \Sigma[x].
\end{align*}
\]

Here, \( \sigma_i \in \Sigma[x], i = 1, \ldots, s+q+r, \) and \( \Sigma[x] \) denotes the SOS ring that consists of all the SOSs over \( x \). \( \xi_i(x) \geq 0, \zeta_i(x) \geq 0, \psi_i(x) \geq 0 \) are the semi-algebraic constraints on \( X_0, X_u, \) and \( X \), respectively. If such SOS programmings can be solved, i.e., a feasible barrier function \( B(x) \) exists, the system is proved to be always safe under controller \( \pi \).

Similarly, a Lyapunov function can also be formulated into two SOS programmings as the following, and if a solution is obtained, the system stability can be guaranteed:

\[
\begin{align*}
V(x) - \sum_{i=1}^{r} \sigma_i(x) \cdot \psi_i(x) & \in \Sigma[x], \\
-\frac{\partial V}{\partial x} : f(x, \pi(x)) - \sum_{i=r+1}^{2r} \sigma_i(x) \psi_i(x) & \in \Sigma[x].
\end{align*}
\]

**Remark 4.2.** Systems with non-polynomial univariate basic elementary functions, such as \( \sin(x), \cos(x), 1/x, \sqrt{x}, \exp(x), \log(x) \) and their compositional functions, can be equivalently transformed into polynomial systems with additional variable introduced in (Liu et al., 2015). Thus, their barrier and Lyapunov functions can also be relaxed into SOS programmings.

With the above SOS programmings, we formulate an optimization problem for the certified control learning as:

\[
\max_{\theta, \alpha} \mathbb{E}[V(x(0))] \\
\text{s.t. } h^i(x; \theta, \alpha, \beta) \in \Sigma[x]
\]

(4)

Here, \( V(x(0)) \) is the value function on the initial state \( x(0) \in X_0 \) in RL. \( h^i(x; \theta, \alpha, \beta) \) is the SOS programming as in Eq (2)(\( i = 1, 2, 3 \)) and Eq (3)(\( i = 1, 2 \)), with \( \theta, \alpha, \beta \) as the vector of controller parameters, unknown system parameters, and parameters for certificates (barrier and/or Lyapunov functions), respectively. As RL builds on the discrete-time MDPs, we need to discretize continuous dynamics \( f \) to compute \( \mathbb{E}[V(x(0))] \) by simulating different traces with the controller. Specifically, in RL, \( V(x) \) satisfies the Bellman equation as:

\[
V(x) = r(x, \pi(x)) + \gamma V'(x'),
\]

where \( r \) is a reward function at the state-action pair \( (x, \pi(x)) \), encoding the desired learning goal for the controller, \( x' \) is the next system state, and constant factor \( \gamma < 1 \).

Next, we are going to show how to transform an SOS into an SDP, which is used in our framework.

**Theorem 4.3.** Given a polynomial \( h(x) \) in SOS with the degree bound \( 2D \), we have:

\[
h(x; \theta, \alpha, \beta) \in \Sigma[x] \iff \begin{cases}
h(x; \theta, \alpha, \beta) = w(x)^T Q(\theta, \alpha, \beta) w(x) \\
Q(\theta, \alpha, \beta) \succeq 0
\end{cases}
\]

Here, \( w(x) = (1, x_1, \ldots, x_n, x_1^2, \ldots, x_n^2) \) is a vector of monomials, and \( Q \) is a \( d^Q \times d^Q \) positive semi-definite matrix, where \( d^Q = (D+n) \), called Gram matrix of \( h(x) \).

The optimization problem in (4) can then be written as:

\[
\max_{\theta, \alpha} \mathbb{E}[V(x(0))] \\
\text{s.t. } h^i(x; \theta, \alpha, \beta) = w(x)^T Q^i(\theta, \alpha, \beta) w(x) \\
Q^i(\theta, \alpha, \beta) \succeq 0
\]

(5)

To make \( h(x) = w(x)^T Q w(x) \), we need to list all the equations for coefficients in each monomial. Given an upper bound of degree \( 2D \) of the polynomial \( h(x) \), let \( a = (a_1, a_2, \ldots, a_n), b = (b_1, b_2, \ldots, b_n), d = (d_1, d_2, \ldots, d_n), (a_i, b_i, d_i \in \mathbb{N}) \) be the \( n \)-dimensional vectors indicating the degree of \( x = (x_1, x_2, \ldots, x_n) \). Let \( h(x) = \sum_{\|a\|_1 \leq 2D} h_a x_a \), where \( \| \cdot \|_1 \) is the 1-norm operator and \( h_a(\theta, \alpha, \beta) \) is the coefficient of \( x_a = \prod_{i=1}^{n} x_i^{a_i} \). Let \( Q = Q_{bd} \), where \( \{Q_{bd}\} \) represents the entry corresponding
to $x_0$ and $x_1$ in the base vector $w(x)$. Then, by equating the coefficients for all the monomials, we have

$$h(x; \theta, \alpha, \beta) = w(x)^T Q(\theta, \alpha, \beta) w(x)$$

$$\iff \forall |a|_1 \leq 2D, h_u(\theta, \alpha, \beta) = \sum_{b+d=a} Q_{bd}$$

as the equality constraints. Along with $Q \succeq 0$, the optimization problem in (4) can now be written as an SDP problem:

$$\max \mathbb{E}[\mathcal{V}(x(0))]$$

$$\text{s.t. } h_u^*(\theta, \alpha, \beta) = \sum_{b+d=a} Q_{bd}, \forall |a|_1 \leq 2D,$$

(5)

$$Q^i(\theta, \alpha, \beta) \geq 0.$$ 

To leverage the gradient from the verification results and form an end-to-end differentiable framework, the above problem can now be further written as our bilevel optimization problem by introducing a slack variable $c$. Specifically, the upper problem tries to solve:

$$\max \mathbb{E}[\mathcal{V}(x(0)); \theta, \alpha] - \lambda (c^*(\theta, \alpha))^2 - \|\alpha - \alpha_0\|^2,$$

where $c^*(\theta, \alpha)$ is the solution to a lower-level problem:

$$\min c$$

$$\begin{cases}
    h^i_u(\theta, \alpha, \beta) \leq \sum_{b+d=a} Q_{bd} + c, \forall |a|_1 \leq 2D, \\
    h^i_u(\theta, \alpha, \beta) \geq \sum_{b+d=a} Q_{bd} - c, \forall |a|_1 \leq 2D, \\
    Q^i(\theta, \alpha, \beta) \geq 0, \\
    c \geq 0,
\end{cases}$$

(6)

where for barrier function, $i = (1, 2, 3)$, and for Lyapunov function, $i = (1, 2, 3)$. $\alpha_0 \in \mathbb{R}^p$ is the ground truth value of the unknown system model parameter vector and needs to be estimated in learning. $\lambda \geq 0$ is a penalty multiplier. Overall, the lower-level SDP problem tries to search for a feasible solution for the certificates while reduce the slack variable $c$. The upper-level problem tries to maximize the value function in RL, reduce the penalty from the lower-level slack variable, and learn the uncertain parameters. In this way, by differentiating the lower-level problem, the gradient $c^*_\theta$ of $c^*$ with respect to $\theta$ can be combined with the gradient of MBRL in the upper-level problem, and the entire bilevel optimization problem is fully differentiable.

4.2. Algorithm for Solving the Bilevel Optimization

We develop the Algorithm 1 to solve the bilevel optimization problem in (6). The inputs to Algorithms 1 include the system model with unknown parameters, step length, shielding set, and the form of polynomials for the certificates and the controller. The outputs contain the learned controller and its certificates (barrier and/or Lyapunov function). There are four major modules in Algorithm 1, including the variable transformation for system model, shielding-based safety-assured simulation, parameter identification, and computing the gradients for RL and certificates, as detailed below.

**Variable Transformation:** If the system model contains non-polynomial univariate basic elementary functions such as $\sin(x)$, $\cos(x)$, $\exp(x)$, $\log(x)$, $\frac{1}{x}$, $\sqrt{x}$, we can equivalently transform them into polynomial terms with additional variables introduced. Take $\dot{x} = \sin(x)$ as an example, let $m = \sin(x), n = \cos(x)$, then we have $\dot{x} = m, \dot{n} = \cos(x)\dot{x} = nm, \dot{n} = -\sin(x)\dot{x} = -m^2$ as a polynomial system.

**Shielding-based Safe Learning:** We compute a shielding set $\mathcal{S}$ to ensure the system safety during learning, by stopping the current learning process if the system is within $\mathcal{S}$. Specifically, we can construct the set $\mathcal{S}$ offline based on the definition that the system may enter the unsafe state set $X_u$.

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**Algorithm 1 End-to-end MBRL with Certification**

1. **Input:** Nominal continuous dynamics $\dot{x} = f(x, u; \alpha)$ and its discretized form $f^d$, unknown system model parameters $\alpha \in [\alpha, \bar{\alpha}]$, barrier function $B(x) = \beta^B \cdot w^B(x)$, Lyapunov function $V(x) = \beta^V \cdot w^V(x)$, controller $\pi = \theta \cdot w^\theta(x)$, step length $l$, shielding set $\mathcal{S}$.

2. **if** $f$ contains non-polynomial term **then**

3. **Conduct variable transformation.**

4. **end if**

5. Initialize $\theta = 0, \beta^B = 0, \beta^V = 0$.

6. **repeat**

7. Trajectory $=[]$

8. **for** $t = 1 \text{ to } T$ **do**

9. **if** $x(t) \in \mathcal{S}$ **then**

10. Early stop and start over again.

11. **end if**

12. **Apply control input** $\pi(x(t); \theta)$.

13. **Trajectory.append**($\{x(t), \pi(x(t); \theta), r(x, \pi(x(t))\}$).

14. **end for**

15. $V^x' = 0, V^\theta' = 0$.

16. **for** $t = T \text{ down to } 0$ with Trajectory do

17. $\alpha \leftarrow \alpha + \gamma \frac{\partial \mathcal{V}_x}{\partial \theta}$.

18. $V_x = r_x + r_u x + \gamma \mathcal{V}_x(f^d + f^d_u x)$.

19. $V_\theta = r_u \pi \theta + \gamma \mathcal{V}_x f^d u + \gamma V' \theta$ based on Eq (7).

20. **end for**

21. Solve lower-level SDP; compute $c^*, \beta^*$.

22. Compute gradient $c^*_\theta = \mathcal{R}(\mathcal{c}, \mathcal{b}^*, \mathcal{s}(\mathcal{A}, \mathcal{d}, \mathcal{e}) \cdot \mathcal{C}_\theta$ based on Eq (8).

23. $\theta \leftarrow \theta + l(V_\theta - 2\lambda c^* \cdot c^*_\theta)$.

24. Increase $\lambda$.

25. **until** $c^* = 0$

26. **Output:** $\pi(x; \theta), B(x; \beta^B), V(x; \beta^V)$. 

---
for the next step when it is in $S$:

$$S = \{ x \mid \min_{\alpha} \min_{x_u \in X_u} \| x' - x_u \| = 0 \}$$

with respect to the state $x$ and the controller parameters $\theta$:

$$V_x = r_x + r_u \pi_x + \gamma V_x'(f_x^d + f_u^d \pi_x),$$
$$V_\theta = r_u \pi_\theta + \gamma V_\theta' f_u^d \pi_\theta + \gamma V_\theta,$$

where every subscript is a partial derivative. $E[V(x(0))]$ will be increased by updating $\theta$ with the direction as gradient $V_\theta(x(0))$. For the implementation, we can collect a trajectory $\{x(0), u(0), r(0), \cdots, x(T), u(T), r(T)\}$ of the discrete-time system by the controller, let $V_x' x(0) = 0, V_\theta' = 0$ and roll back to the initial state $x(0)$, and obtain the gradient $V_\theta(x(0))$ according to Eq (7).

Computing the Certification Gradient: To solve problem (6) in an end-to-end manner, the slack variable $c^*$ should be differentiable to the controller parameters $\theta$ as it connects the two sub-problems. The lower-level SDP belongs to the disciplined parameterized programming problem where the optimization variables are $c, \beta$ and the parameters are $\theta$. And the lower-level problem defined in (6) can be viewed as a function mapping of $\theta$ to the optimal solution $(c^*, \beta^*)$, e.g. $F: \theta \rightarrow (c^*, \beta^*)$. According to (Agrawal et al., 2019), function $F$ can be expressed as the composition $R \circ \phi \circ C$, where $C$ represents the canonicalizer mapping of $\theta$ to a cone problem $(A, e)$, which is then solved by a cone solver $\phi$ and returns $(\bar{c}^*, \bar{\beta}^*)$. Finally, the retriever $R$ translates the cone solution $(\bar{c}^*, \bar{\beta}^*)$ to the original solution $(c^*, \beta^*)$. Thus, according to the chain rule, we have

$$c^*_\beta = \mathcal{R}_{(c^*, \beta^*)} \cdot s_{(A,e)} \cdot C_\theta$$

as a part of the gradient in the upper-level objective. Overall, the controller can be updated as $\theta \leftarrow \theta + l (V_\theta - 2c^* \cdot \phi_\theta)$. As the termination condition in Algorithm 1, $c^* \cdot 0$ indicates that the SDP problem (5) has a feasible solution $\beta^*$ given the current $\theta$, meaning that there exists a certificate for the learned controller.

4.3. Theoretical Analysis

**Proposition 4.5.** Suppose that there exists a step length $l$ satisfying the Wolfe conditions (Wolfe, 1969) for the value gradient $V_\theta$ and the verification gradient $c^*_\beta$, at the $k$-th update. Then Algorithm 1 will reach a stationary point for problems (6).

$E[V(x(0); \theta, \alpha)] - \lambda (c^*(\theta, \alpha))^2$ can be viewed as an unconstrained optimization problem over $\theta$. For this unconstrained problem, because we can compute its closed-form gradient as $V_\theta$ and $c^*_\beta$, we can choose the step length $l$ by the Wolfe conditions, which lead problem (6) to a stationary point when given a $\lambda$. The detailed proof can be found in the Appendix A.

Although reaching a stationary point does not necessarily mean $c^* = 0$ in problem (6) and thus does not necessarily
Table 1. Certification results by our approach and the baseline SVG method for the four examples. B for barrier function, L for Lyapunov function, D for the polynomial degree of the certificate function that is obtained or tried, ✓ means that a certified controller is found and × means that it is not found. We can see that our approach is able to find certified controller for all four examples, while the baseline SVG method fails in more than half of the cases (with certificate function degree up to 8).

| EXAMPLE | OURS | BASELINE SVG |
|---------|------|--------------|
| PJ      | B(D=2) ✓ | ×            |
| BALL    | L(D=2) ✓ | L(D=4) ✓     |
| PENDULUM| L(D=2) ✓ | L(D=8) ×     |
| LK      | L(D=2) ✓, B(D=4) ✓ | L(D=2) ✓, B(D=8) × |

5. Experimental Results

With experiments on four example systems, we compare our approach with two baseline methods: 1) a model-based SVG method for RL, with shielding and parameter identification similar to our approach, but without verification feedback in the loop (i.e., verification is done each iteration after the controller is updated, as in typical open-loop methods); and 2) a model-free PPO method for RL, without verification in the loop, shielding, and parameter identification. Table 1 summarizes the certification results of our approach and the baseline SVG method on the four examples, and we will discuss each of them in details below, as the baseline SVG is our main comparison target. We will also show comparison with the PPO method later on these examples (but only on convergence rate and final performance, as it is challenging to generate certificates for model-free PPO). More details of the experiments can be found in the Appendix A.

5.1. PJ (Safety)

We consider a modified example from (Prajna & Jadababaie, 2004), where \( x_1 = \alpha_1 x_2, x_2 = \alpha_2 x_1^2 + u, \alpha = (\alpha_1, \alpha_2) \in [-1.5, 1.5]^2 \) with the ground truth value as \((1, 1)\), system state \( x = (x_1, x_2) \), initial state space \( X_0 = (x_1 - 1.5)^2 + x_2^2 \leq 0.25 \), unsafe state space \( X_u = (x_1 + 0.8)^2 + (x_2 + 1)^2 \leq 0.25 \), and state space

\[ X = [-100, 100]^2 \]

We focus on the system safety in this example and thus are only interested in the barrier certificate. Fig. 2 shows the simulated system trajectories by the learned controllers from our approach and from the baseline SVG. It also shows the 0-level contour plot of the barrier function (in purple) from our approach. We can see that the controller learned by the SVG after 100 iterations is unsafe (entering the unsafe region in red) and thus there is no safety certificate. Our approach is safe during and after learning with shielding and the learned certificate. Moreover, in our approach, unknown system parameter \( \alpha \) quickly converges to its ground truth value within several iterations.

5.2. Ball (Stability)

We consider another modified example from (Prajna et al., 2005), where \( x_1 = -x_1^3 + \alpha_1 x_1 x_3, x_2 = -x_2 - x_1^2 x_2, x_3 = \alpha_2 x_1^2 x_3 + u, \alpha_1 \in [-4, 0], \alpha_2 \in [0, 5] \), and their ground truth value are \(-1\) and 3, respectively. System state \( x = (x_1, x_2, x_3) \), initial state space \( X_0 = (x + 1)^2 + (y + 1)^2 + (z + 1)^2 \leq 0.25 \), and the state space \( X = [-3, 0]^3 \). The aim of control design is to obtain a feedback controller for stabilizing the system to the origin, and thus we only focus on the Lyapunov certificate for stability. The simulated controlled trajectories of our approach and of baseline SVG are shown in Fig. 3 with several random initial states. Fig. 3 also shows the quadratic Lyapunov function generated from our approach. The baseline SVG fails to generate a quadratic Lyapunov function for the entire learning process but can synthesize one with the degree order of 4, as in Table 1.
Figure 3. Left: Simulated system trajectories on \((x_1, x_2)\) under the learned controllers from our approach and from SVG for the Ball example. Right: Generated Lyapunov certificate function from our approach on \((x_1, x_2)\).

Figure 4. Left: Simulated system trajectories on \((\varphi, \dot{\varphi})\) under the learned controllers from our approach and from SVG for the Inverted Pendulum example. Right: Generated Lyapunov certificate function from our approach on \((\varphi, \dot{\varphi})\).

5.3. Inverted Pendulum (Stability)

We use the inverted pendulum as another example that considers Lyapunov certificate function for system stability. The example can be expressed with a second-order ODE: \(\ddot{\varphi} = -\frac{g}{m} \sin(\varphi) - \frac{d}{m} \dot{\varphi} + \frac{u}{m} \), where \(\varphi\) is the angle deviation error. \(x = (\varphi, \dot{\varphi})\) is the system state, \(m = 1, l = 1, d = 0.1\). Unknown parameter \(g \in [9, 10.5]\) with the ground truth value as 9.8. \(X_0 = \{x | \varphi^2 + \dot{\varphi}^2 \leq 1\}\), \(X = \{x | \varphi^2 + \dot{\varphi}^2 \leq 2\}\). Due to the \(\sin\) function in the model, we conduct the variable transformation, with \(p = \sin(\varphi)\) and \(q = \cos(\varphi)\), such that pendulum dynamics can be transformed into a 4-dimensional polynomial system. Fig. 4 shows the simulated trajectories by the controllers from our approach and from the baseline SVG, as well as the Lyapunov function generated from our approach. Baseline SVG fails to generate a Lyapunov function with the polynomial degree up to 8 during the entire learning process, as in Table 1.

Figure 5. Left: Simulated system trajectories on \((y, v_y)\) under the controllers from our approach and from baseline SVG for the Lane Keeping example. Right: Barrier function and Lyapunov function value generated by our approach, along with the trajectories.

5.4. Lane Keeping (Safety and Stability)

Finally, we consider a simplified lane keeping example (Chen et al., 2014), where we try to derive barrier and Lyapunov certificate functions for safety and stability. The system model can be expressed as \(\dot{x} = Ax + Bu\), where \(x = (y, v_y, \psi_e, r)^T\) is the state vector with lateral displacement error \(y\), lateral velocity \(v_y\), yaw angle error \(\psi_e\) and yaw rate \(r\). Control input \(u\) represents the steering angle at the front tire. Matrix \(A\) and \(B\) are defined as

\[
A = \begin{bmatrix}
0 & 1 & v_x & 0 & 0 \\
0 & -1 & \frac{b C_{a_t} - a C_{a_t}}{m v_x} & \frac{b C_{a_t} - a C_{a_t}}{v_x} & \frac{-a^2 C_{a_t} + b^2 C_{a_t}}{l_s v_x} + \alpha_2 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 
\end{bmatrix},
\]

\[
B = \begin{bmatrix}
0 & C_{at} \\
0 & \frac{a C_{at}}{l_s} \\
0 & \frac{a C_{at}}{l_s} \\
0 & \frac{a C_{at}}{l_s} 
\end{bmatrix}^T,
\]

where \(v_x\) is the longitudinal vehicle velocity. \(\alpha_1 \in [-15, 5], \alpha_2 \in [-10, -1]\) are the unknown parameters with ground truth value of \(-10.5\) and \(-5.61\). Any other elements are constant values of the vehicle. \(X_0 = \{x | (y - 0.4)^2 + (v_y - 2)^2 + (\psi_e - 0.5)^2 + r^2 \leq 0.04\}\), \(X = \{x | (y - 2)^2 + (v_y - 2)^2 + \psi_e^2 + (r - 1)^2 \leq 1\}\), \(X = \{y^2 + v_y^2 + \psi_e^2 + r^2 \leq 9\}\). Fig. 5 shows the simulated system trajectories under the controllers from our approach and from baseline SVG. It also shows the barrier function value and the Lyapunov function value generated by our approach, along with the trajectories over time. SVG can generate a quadratic Lyapunov function but fails to find a barrier function, as in Table 1.

Learning Reward Comparison: We also compare the learning rewards of our approach, SVG and model-free PPO in Fig. 6 for all the examples. Our approach overall
achieves better reward learning than the two baselines in convergence rate and final performance.

6. Conclusion

In this paper, we present a joint differentiable optimization-verification framework for certified reinforcement learning, with the formulation and solving of a novel bilevel optimization problem, leveraging the gradients from the certificates and the value function. Experimental results demonstrate the advantage of our approach over SVG and PPO in finding controllers with feasible certificates for guaranteeing system safety and stability. In future work, we plan to improve the efficiency of our approach, which is currently limited by the scalability of sum-of-squares programming.

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A. Appendix

A.1. Proofs

Proof of Proposition 4.5

Let $g(\theta_k) = -\mathbb{E}[\mathcal{V}(x(0); \theta_k, \alpha)] + \lambda_k c^2(\theta_k)$, which is the negative value of the objective in the bilevel problem (6), and thus it needs to be minimized. Let $p_k = -g_{\theta_k}$ denote the line search direction as the gradient. According to the second Wolfe condition with two constant numbers $0 < d_1 < d_2 < 1$, we have

$$(g_{\theta_{k+1}} - g_{\theta_k})^T p_k \leq (d_2 - 1) g_{\theta_k}^T p_k.$$ 

Assume that the gradient $g_{\theta}$ of $g(\theta)$ is Lipschitz continuous, which implies that there exist a constant value $L$ such that

$$\frac{g_{\theta_{k+1}} - g_{\theta_k}}{\theta_{k+1} - \theta_k} = \frac{g_{\theta_{k+1}} - g_{\theta_k}}{l_k p_k} \leq L,$$

$$(g_{\theta_{k+1}} - g_{\theta_k})^T p_k \leq l_k L \|p_k\|^2,$$

where $l_k$ is the step length. Combine the two inequalities, we can get

$$l_k \geq \frac{d_2 - 1}{L} \frac{g_{\theta_k}^T p_k}{\|p_k\|^2}.$$ 

According to the first Wolfe condition, we can obtain

$$g(\theta_{k+1}) \leq g(\theta_k) - d_1 \frac{1 - d_2 (g_{\theta_k}^T p_k)^2}{L} \|p_k\|^2,$$

$$g(\theta_{k+1}) \leq g(\theta_k) - d \|g_{\theta_k}\|^2,$$

where $d = \frac{d_1(1-d_2)}{L}$. We can then extend the inequality to the initial value as

$$g(\theta_{k+1}) \leq g(\theta_0) - d \sum_{i=0}^{k} \|g_{\theta_i}\|^2.$$ 

Since we are considering the episodic RL and $c^*$ is bounded from the lower-level SDP, function $g$ is bounded, and thus there is positive number $N$ such that

$$\sum_{k=0}^{\infty} \|g_{\theta_k}\|^2 < N \implies \lim_{k \to \infty} \|g_{\theta_k}\| = 0,$$

which indicates the problem eventually reaches a stationary point.

Proof of Theorem 4.6

Because problem (5) can be viewed as a constrained problem with constraint $c(\theta) = 0$, suppose that $\bar{\theta}$ is a global solution of problem (5) with $c(\bar{\theta}) = 0$ (meaning that there exists a feasible certificate), and name the objective function of problem (6) $\max_{\theta, \alpha} \mathbb{E}[\mathcal{V}(x(0); \theta, \alpha)] - \lambda c^2(\theta) - \|\alpha - \alpha_0\|_2^2$ as $g(\theta)$, we then have

$$g(\bar{\theta}) \geq g(\theta) \forall \theta, c(\theta) = 0.$$ 

Since $\theta_k$ maximizes $g(\theta, \lambda_k)$ for each iteration $k$, we then have $g(\theta_k, \lambda_k) \geq g(\bar{\theta}, \lambda_k)$, resulting in the following inequality:

$$\mathbb{E}[\mathcal{V}(x(0); \theta_k, \alpha)] - \lambda_k c^2(\theta_k) \geq \mathbb{E}[\mathcal{V}(x(0); \bar{\theta}, \alpha)] - \lambda_k c^2(\bar{\theta}) = \mathbb{E}[\mathcal{V}(x(0); \bar{\theta}, \alpha)],$$

and thus,

$$c^2(\theta_k) \leq \frac{\mathbb{E}[\mathcal{V}(x(0); \theta_k, \alpha)] - \mathbb{E}[\mathcal{V}(x(0); \bar{\theta}, \alpha)]}{\lambda_k}.$$
Suppose that $\theta^*$ is a limit point of the sequence $\{\theta_k\}$, so that there exists an infinite sub-sequences $K$ such that

$$\lim_{k \in K} \theta_k = \theta^*.$$

When $k \to \infty$, we then have

$$c^2(\theta^*) = \lim_{k \in K} c^2(\theta_k) \leq \lim_{k \in K} \frac{E[V(x(0); \theta_k, \alpha)] - E[V(x(0); \tilde{\theta}, \alpha)]}{\lambda_k}.$$

For $E[V(x(0); \theta_k, \alpha)]$ and $E[V(x(0); \tilde{\theta}, \alpha)]$, since they follow the same distribution on $x(0) \in X_0$, and we deal with the episodic setting in RL, their difference is thus bounded. Because we have $\lambda_k \to \infty$ when $k \to \infty$, so $c(\theta^*) = 0$, meaning that $\theta^*$ is the feasible solution of the SDP problem (5).

Moreover, follow the inequality of $\theta_k$ with $k \to \infty$, we have

$$\lim_{k \in K} E[V(x(0); \theta_k, \alpha)] - \lambda_k c^2(\theta_k) \geq E[V(x(0); \tilde{\theta}, \alpha)],$$

$$E[V(x(0); \theta^*, \alpha)] - \lambda_k c^2(\theta^*) \geq E[V(x(0); \tilde{\theta}, \alpha)],$$

$$E[V(x(0); \theta^*, \alpha)] \geq E[V(x(0); \tilde{\theta}, \alpha)].$$

Since $\theta^*$ is a feasible solution with $c(\theta^*) = 0$, whose objective is not smaller than that of the global solution $\tilde{\theta}$, we can conclude that $\theta^*$ is a global solution as well, as claimed in Theorem 4.6.

A.2. More Experiment Details

Example 1: PJ

We design a linear controller as $\pi(\theta) = \theta_1 x_1 + \theta_2 x_2$ with parameters $[\theta_1, \theta_2]$. The barrier function is assumed to be a quadratic function.

With our approach, the learned controller is $\pi = -2x_1 - 1.8x_2$, with the barrier function certificate as $B(x) = 62.1 + 79.6x_1 + 67.8x_2 + 27x_1^2 + 37x_1x_2 - 0.57x_2^2$.

Example 2: Ball

We design a linear controller as $\pi(\theta) = \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$. We assume that the Lyapunov function can be expressed as $V = \beta_1 x_1^2 + \beta_2 x_2^2 + \beta_3 x_3^2$, with $\beta_1, \beta_2, \beta_3 \geq 0$ to ensure that the Lyapunov function is positive.

With our approach, the learned controller is $\pi = 2 \times 10^{-4} x_1 - 0.072 x_2 - 1.98 x_3$, with the Lyapunov function certificate as $V = 81x_1^2 + 0.017x_2^2 + 27x_3^2$.

Example 3: Inverted Pendulum

We design a linear controller as $\pi(\theta) = \theta_1 \varphi + \theta_2 \dot{\varphi} + \theta_3 \sin(\varphi) + \theta_4 \cos(\varphi)$. The quadratic Lyapunov function can be expressed as $V(\beta) = \beta \cdot [\varphi, \dot{\varphi}, p, q, \varphi^2, \dot{\varphi}^2, \varphi^2, \dot{\varphi}^2, p^2, q^2]^T$, where $p = \sin(\varphi), q = 1 - \cos(\varphi)$.

With our approach, the learned controller is $\pi = -0.95 \varphi - 3.36 \dot{\varphi} + 2.94 \sin(\varphi) + 0.1 \cos(\varphi)$, with $\beta = [-2.1e^{-4}, -1.6e^{-4}, 3.2e^{-3}, 0.54, 2.8e^{-3}, -7.7e^{-4}, 2.6e^{-4}, 0.477, 1.6e^{-4}, -3.43e^{-4}, -1.43e^{-2}, 0.43, 3.88, 3.448]$ for the Lyapunov function certificate.

Example 4: Lane Keeping

With our approach, the learned controller is $\pi = \theta^T x$, where $\theta = [-1.48, 0.12, -2.75 - 1.27]^T$. The barrier function certificate is $B(x) = \beta^T_B \epsilon(x)$, where $\beta_B = [0.84, -1.13, 0.33, -0.26, -1.24, -7.7e^{-4}, -9.23e^{-2}, -2.8e^{-2}, 1.1e^{-2}, 7.9e^{-4}, -5.1e^{-2}, -5.7e^{-2}, 5.5e^{-9}, -3.9e^{-10}]^T$ and $c(x) = [1, y, v_y, \psi_e, r, y v_y, y \psi_e, y r, v_y \psi_e, v_y r, \psi_e r, y^2, y^3, y^4]^T$. The Lyapunov function certificate is $V(x) = \beta^T \epsilon(x)$ where $\beta = [0.61, 0.18, 5.42, 0.85, -0.32, 2.65, 0.82, -0.75, -0.68, 2.48]^T$ and $m(x) = [y^2, v_y^2, \psi_e^2, r^2, y v_y, y \psi_e, y r, v_y \psi_e, v_y r, \psi_e r]^T$.

With the baseline SVG method, the learned controller is $[-0.67, -0.25, -4.85, -0.54084192]x$. This controller has a valid quadratic Lyapunov function, but the method fails to generate a feasible barrier certificate.