Neural ODEs as Feedback Policies for Nonlinear Optimal Control

Ilya Orson Sandoval ∗ Panagiotis Petsagkourakis ∗
Ehecatl Antonio del Rio-Chanona ∗

∗ Centre for Process Systems Engineering
Imperial College London, London, United Kingdom
(os220@ic.ac.uk, p.petsagkourakis@imperial.ac.uk & a.del-rio-chanona@imperial.ac.uk).

Abstract: Neural ordinary differential equations (Neural ODEs) define continuous time dynamical systems with neural networks. The interest in their application for modelling has sparked recently, spanning hybrid system identification problems and time series analysis. In this work we propose the use of a neural control policy capable of satisfying state and control constraints to solve nonlinear optimal control problems. The control policy optimization is posed as a Neural ODE problem to efficiently exploit the availability of a dynamical system model. We showcase the efficacy of this type of deterministic neural policies in two constrained systems: the controlled Van der Pol system and a bioreactor control problem. This approach represents a practical approximation to the intractable closed-loop solution of nonlinear control problems.

Keywords: Optimal Control, Feedback Policy, Reinforcement Learning, Adjoint Sensitivity Analysis, Control Vector Iteration, Penalty Methods, Nonlinear Optimization.

1. INTRODUCTION

Neural policies represent the dominant approach to parametrize controllers in Reinforcement Learning (RL) research. Their attractiveness relies on their dimensional scaling property and universal approximation capacity. However, their training procedure usually relies on inefficient sampling based strategies to estimate the gradient of the objective function to be optimized. On the contrary, when an environment model is available as a differential equation system, it is possible to leverage it for efficiency through methods based on optimal control and dynamic optimization (Ainsworth et al., 2021; Yildiz et al., 2021). In this work we explore this setting, exploiting a neural policy to parametrize a deterministic control function as a state feedback controller. This approach provides an approximation to the practically intractable optimal closed-loop policy in continuous time.

The optimization of such a controller follows the same strategy as the training of Neural Ordinary Differential Equations (Neural ODEs) (Chen et al., 2018). In our application, the weights of the network only define the control function within a predefined system, instead of defining the whole differential equation system as in NeuralODEs. To understand the training procedure, it is fruitful to overview the close connection between adjoint sensitivity analysis used in dynamical systems and the backpropagation algorithm used in neural networks. We revise the literature surrounding these topics and their use in recent applications where both fields meet.

Backpropagation may be seen as a judicious application of the chain rule in computational routines, introduced in optimal control (Griewank, 2012) and popularized within the neural network community (Rumelhart et al., 1986). The first derivations trace back to the introduction of the Kelley-Bryson gradient method to solve multistage nonlinear control problems (Dreyfus, 1962). In neural networks, it may be derived from the optimization problem where Lagrange multipliers (adjoint variables) enforcing the transitions between states (Mizutani et al., 2000).

On continuous time optimal control problems, the optimality conditions from Pontryagin’s Maximum Principle (Pontryagin et al., 1986) establish a connection between the sensitivities of a functional cost and the adjoint variables. This relationship is exploited in continuous sensitivity analysis, where it is used to estimate the influence of parameters in the solution of differential equation systems (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007). When the time is discretized in an ODE system, backpropagation is analogous to the adjoint system of the maximum principle (Serban and Hindmarsh, 2005; Jorgensen, 2007).

The discretize-then-optimize distinction has a different meaning in optimal control literature (Biegler, 2010). There it refers to direct approaches to the optimization problem, which first discretize the dynamical equations to afterwards solve the finite-dimensional nonlinear optimization. The optimize-then-discretize refers to any
The adjoint approach suggested with the introduction of Neural ODEs (Chen et al., 2018) is a modern variant of Control Vector Iteration (CVI) (Luus, 2009), a sequential indirect strategy that optimizes a fixed vector of parameters by relaxing just one of the necessary conditions of optimality \(^2\). The relaxed condition is approximated iteratively along optimization rounds where the dynamical and adjoint equations are always satisfied, as in feasible paths methods (Chachuat, 2007). An algorithmic improvement introduced by (Chen et al., 2018) is the efficient use of reverse-mode Automatic Differentiation (AD) to calculate vector-Jacobians products that appear through the differential equations defining the optimality conditions of the problem. This grants the possibility of dealing with high dimensional parameter problems efficiently, which is crucial for neural policies within dynamical systems in continuous time. Furthermore, it crucially avoids the symbolic derivations historically associated with indirect methods including CVI in the numerical optimal control literature (Biegler, 2010).

The use of neural networks within control systems was explored originally in the 90s (Chen, 1989; Miller et al., 1990) where the focus was on discrete time systems (Hunt et al., 1992). The use of neural control policies in this discrete vein has also attracted attention recently in nonlinear control (Rackauckas et al., 2020a; Adhau et al., 2021; Jin et al., 2020) and MPC (Amos et al., 2018; Karg and Lucia, 2020; Drgona et al., 2022). The gradients required for optimization are computed through direct application of AD over the evolution of a discrete system; a strategy coined as differentiable control or more generally differentiable simulations. These strategies revive some of the original ideas that brought interest to neural networks in nonlinear control (Cao, 2005) with modern computational tooling for AD calculations (Baydin et al., 2017).

Reinforcement Learning (RL) commonly leverage neural parametrization of policies within Markov decision processes (MDP) (Sutton et al., 1992) and has had a rising success with dimensionality scaling thanks to deep learning (Schmidhuber, 2015). The adaptation of RL approaches to continuous time scenarios based on Hamilton-Jacobi-Bellman formulations was originally explored in (Munos, 1997; Doya, 2000). A continuous time actor-critic variation based on discrete time data was analysed more recently in (Yildiz et al., 2021). The study of the model-free policy gradient method to continuous time was explored by (Munos, 2006). In continuous time settings with deterministic dynamics as an environment, neural policies may be trained with techniques from dynamic optimization like CVI, avoiding noisy sampling estimations as in classic RL. A comparison of the training performance improvement between deterministic model-based neural policies and model-free policy gradient was showcased in (Ainsworth et al., 2021).

With a view in practical applications, it is crucial to be able to satisfy constraints while also optimizing the policy performance. While this has been a major focus in optimal control since its inception (Bryson and Ho, 1975), there has been little attention to general nonlinear scenarios. Most works assume either linear dynamics or fixed control profiles instead of state feedback policies. In relation to model-free RL, constraint enforcement is an active area of research (Brunke et al., 2021). Recent work has explored variants of objective penalties (Achiam et al., 2017), Lyapunov functions (Chow et al., 2019) and satisfaction in chance techniques (Petsakourakis et al., 2022).

Here we develop a strategy that allows continuous time policies to solve general nonlinear control problems while satisfying constraints successfully. Our approach is based on the deterministic calculation of the cost functional gradient with respect to the static feedback policy parameters given a white-box dynamical system environment. Saturation from the policy architecture enforces hard control constraints while state constraints are enforced through relaxed logarithmic penalties and an adaptive barrier update strategy. We furthermore showcase how the inclusion of the feedback controller within the ODE definition shapes the whole phase space of the system. This Neural ODE quality is impossible to achieve in nonlinear systems with standard optimal control methods that only provide controls as a function of time.

2. PROBLEM STATEMENT

We consider continuous time optimal control problems with fixed initial condition and fixed final time. The cost functional is in the Bolza form, including both a running \((\ell)\) and a terminal cost \((\phi)\) in the functional objective \((J)\) (Bryson and Ho, 1975):

\[
\begin{align}
\min_{\theta} & \quad J = \int_{t_0}^{t_f} \ell(x(t), \sigma_\theta(x)) \, dt + \phi(x(t_f)), \\
\text{s.t.} & \quad \dot{x}(t) = f(x(t), \sigma_\theta(x), t), \\
& \quad x(t_0) = x_0, \\
& \quad g(x(t), \sigma_\theta(x)) \leq 0,
\end{align}
\]

where the time window is fixed \(t \in [t_0, t_f]\), \(x(t) \in \mathbb{R}^n\) is the state, \(\sigma_\theta(x) : \mathbb{R}^n \to \mathbb{R}^n\) is the state feedback controller and \(\theta \in \mathbb{R}^n\) are its parameters.

3. METHODOLOGY

The most common parametrization in trajectory optimization methods utilizes low-order polynomials with a predefined set of time intervals to approximate the controller as a function of time (Rao, 2009; Teo et al., 2021). In contrast, in our work the the control function is posed the output of a parametrized state feedback controller. The controller parameters are constant through all the integration time (they define statically the nonlinear feedback controller) and are the only optimization variables of the problem. This transforms the original dynamical optimization problem into a parameter estimation one (Teo et al., 2021). The approach approximates an optimal closed-loop policy, which is a continuous function that is well-defined for states outside the optimal path. This quality allows

\(\text{procedure that departs from the optimality conditions of the problem, also called indirect approaches. Since the adjoint equations are part of the optimality conditions in dynamic optimization, the classic indirect classification includes both variants in ML literature. From an optimization perspective, there is not difference in the approach that calculates the gradients since both do so through adjoints; the selection of the approach is merely practical, based on the peculiarities of each problem (Ma et al., 2021).} \)
to calculate the phase portrait of the system with the embedded control policy, as shown in section 4.

In this work, an adaptive step size ODE solver is the procedure that selects the adequate time discretization during the differential equation integration. The trade-off between computational speed and accuracy is also exclusively set by the adaptive integration method and its error tolerance (Rackauckas and Nie, 2017). This allows the integrator to account for the influence of the policy to keep a constant integration error throughout the time interval.

Once the gradient of the objective function is computed, any first-order gradient based optimization procedure can be used. Through this work we used the ADAMW optimizer (Kingma and Ba, 2015; Loeschilov and Hutter, 2019) for the preconditioning procedure. The IPOPT optimizer (Wächter and Biegler, 2006) with the limited-memory quasi-Newton approximation was used throughout the Fiacco-McCormick iterations.

3.1 Adjoint sensitivity analysis

The Euler-Lagrange equations for the Bolza problem are the backbone of the calculation of the gradients of a functional objective with respect to the policy parameters. Here we display the relevant equations for clarity and describe the precise algorithm for their numerical evaluation using automatic differentiation.

First we consider the augmented objective function with smooth Lagrange multipliers $\lambda(t) \in \mathbb{R}^{n\ast}$ (also called costate/adjoint vector) to enforce the dynamical equations as constraints,

$$L(x, \theta, \lambda) = J(x, \theta) - \int_{t_0}^{t_f} \lambda^T (\dot{x} - f(x, \theta)) \, dt.$$  

$$H(x, \theta, \lambda) = \lambda^T f(x, \theta) + \ell(x, \theta).$$

Denoting partial derivatives with subscripts, the dynamic constraints are then equivalent to

$$\dot{x}(t) = H_A(x, \theta, \lambda).$$  

(2)

The following form of multipliers $\lambda$ assure the stationary path required for first-order optimality ($dL = 0$):

$$\dot{\lambda}(t) = -H_S = -\lambda^T f_x - \ell_x,$$  

(3a)

$$\lambda(t_f) = \phi(x(t_f)).$$  

(3b)

The sensitivity of the objective function $J$ with respect to the parameters $\theta$ are

$$J_{\theta} = L_{\theta} = \int_{t_0}^{t_f} \lambda^T f_{\theta} + \ell_{\theta} \, dt = \int_{t_0}^{t_f} H_{\theta} \, dt.$$  

(4)

It is important to note that both the adjoint (3) and the cost sensitivity equations (4) require the availability of the forward path solution $x(t)$ (see 1).

As in control vector iteration (Luus, 2009), the last optimality condition is relaxed and left to be approximated iteratively by the optimization procedure over the controller parameters $\theta$:

$$H_\theta = \lambda^T f_\theta + \ell_\theta \to 0.$$  

(5)

The terms of the form $\lambda^T f_\theta$ are vector-Jacobian products that can be efficiently calculated with reverse AD (Chen et al., 2018). The precise numerical implementation is shown in algorithm 1.

The parametrization variables of the controller $\theta$ may be thought of as unconstrained time-constant variables; their optimization is a parameter estimation problem with dynamic constraints (Teo, Li, Yu, and Rehbock, 2021). Since the optimization variables are the unconstrained parameters of the policy, it is not necessary to use the more general Pontryagin’s Maximum Principle, which explicitly deal with control variable constraints. Further problem variants including minimum-time problems could also be considered without great modifications (Bryson and Ho, 1975).

Algorithm 1 Adjoint Sensitivity pseudocode

Inputs: Set of parameters $\theta$, neural controller $\pi_{\theta}$, dynamical system $x(t) = f(x, \theta)$, initial condition $x_0$, fixed time interval $[t_0, t_f]$, running cost function $\ell(x(t), \pi_{\theta}(x))$, final cost function $\phi(x).

procedure FORWARD INTEGRATION
Calculate $x(t)$ by integrating forward the dynamical system.
Store $x(t_f)$ and an interpolation of the path $x(t)$, or setup checkpoints to recalculate it on demand.  

Set the adjoint ODE: $\lambda = -H_x$ with boundary condition $\lambda(t_f) = \phi_x(x(t_f))$. \(\triangleright\) Equation 3.

Set the quadrature ODE: $J_\theta = H_\theta$ with boundary condition $J_\theta(t_f) = 0$. \(\triangleright\) Equation 4.

procedure BACKWARD INTEGRATION
Define the extended ODE system $\dot{F} := [-H_x, -H_\theta].$
Integrate $F$ backwards from $t_f$ to $t_0$.
output Last block of the extended system at the origin: $F(t_0). \triangleright J_\theta = \int_{t_f}^{t_0} -H_\theta \, dt$

3.2 Neural Policy

Given the initial condition $x_0$ and a set of parameters $\theta$, the evolution of the states $x(t)$, $\forall t \in [t_0, t_f]$ is obtained by the numerical integration of the dynamical system following the parametrized control $u(t) = \pi_\theta(x(t))$. In practice, at each point where the system requires to be evaluated by the ODE integrator, the controller will also be evaluated at the current state and its output sets the control component of the system dynamics (see section 4 for specific examples).

We use a dense neural network with parameters $\theta$ as a state feedback control policy. The controller input is the state of the system at the current time $x(t)$ and its outputs are the constrained controls $u(t) \in U \subseteq \mathbb{R}^{n\ast}$. 

$$\pi_{\theta}(t) = \pi(x(t), \theta) \in U.$$  

(6)
The controller outputs are box-constrained to $3.3 \text{Control constraints}$

The output layer of the network always has the same number of nodes as the control dimension.

$\frac{\beta(z; \delta)}{-\ln(z)}$

Fig. 1. Relaxed logarithmic penalty function (Feller and Ebenbauer, 2014). Both coefficient and relaxation parameter can be adjusted to approximate interior point penalties iteratively.

The output layer of the network always has the same number of nodes as the control dimension.

3.3 Control constraints

The controller outputs are box-constrained to $U$ directly from the nonlinearity of the last activation function of the policy. We use a custom scaled sigmoid function $\sigma(\cdot) : \mathbb{R} \to [0, 1]$ for each control component $u_i$. Then, the last layer of the policy has the functional form

$$u_i = u_i^{(lb)} + (u_i^{(ub)} - u_i^{(lb)}) \sigma(z_i),$$

where $u_i^{(lb)}$ and $u_i^{(ub)}$ are the lower and upper bounds of the control component, respectively, and $i \in [1, \ldots, n_i]$. By construction, any parameter set in the policy yields a feasible control sequence satisfying the control constraints.

3.4 State constraints

State constraints are enforced via penalty functions added to the original functional cost function as a running cost,

$$\ell(x, \pi) \to \ell(x, \pi) + \alpha P(x, \delta),$$

where the weight parameter $\alpha$ and the relaxation parameter $\delta$ are both positive. This approach purposely avoids the treatment of state constraints through additional Lagrange multipliers. This would be problematic due to alternating optimality conditions along subarcs with active constraints, unknown in number and locations $a priori$ (Bryson and Ho, 1975; Biegler, 2010).

Relaxed logarithmic penalties It is not trivial to understand the black-box relationship between the policy parameters and the specific control profiles the corresponding policy generates. This is specially problematic because unoptimized parameters may result in a state evolution that violates state constraints. Consequently, a state constraint penalty must be well defined for states outside the feasible region to correct the initial profiles. On the other hand, penalties defined exclusively outside the feasible region lack correction signals in the vicinity of the boundary and inside the allowed control region. To address this, we leverage a logarithmic relaxation that extends the penalty definition outside the feasible region while preserving an interior feedback as logarithmic barriers used in interior point methods.

We use a variant of the relaxed logarithmic barrier function introduced in (Feller and Ebenbauer, 2014) (see figure 1):

$$P(z) = \begin{cases} -\ln(z) & z > \delta, \\ \beta(z; \delta) & z \leq \delta, \end{cases}$$

with the truncated exponential relaxing function

$$\beta(z; \delta) = \exp(1 - z/\delta) - 1 - \ln(\delta).$$

The scalar $\delta \geq 0$ is called the relaxation parameter, and controls the distance from the constraint boundary where the relaxation of the barrier function starts. Note that in equation 7 the transition between both functions at $\delta$ is smooth.

The progression of barrier parameters follows Fiacco-McCormick iterations (Fiacco and McCormick, 1990) with a barrier update after several optimization iterations. The penalties are increased by tightening both the coefficient (alpha) and the relaxation parameter (delta) sequentially between optimization rounds where they are left fixed. Once the initial parameters $\theta$ are settled, the initial penalty parameters are tuned to start the first optimization round with a reasonable ratio between the original objective function and the state penalty. After each optimization procedure, the relaxation parameter $\delta$ is decreased by a constant rate until this ratio is attained again, to then proceed with the next optimization round. If at any round this reduction becomes problematic for the optimization due to the steep convergence to a logarithmic penalty, the coefficient $\alpha$ is increased instead in that occasion. The iterations are repeated until the loss function stops decreasing or a predefined number of barrier updates is reached.

3.5 Policy parametrization

For setting the initial values of the parameters of the controller we use the Glorot uniform initialization (Glorot and Bengio, 2010): biases are initialized to zero and the weights $W^{(i)}$ of layer $i$ follow a uniform distribution

$$W^{(i)} \sim U[-b, b], \quad b = G \sqrt{\frac{6}{n_{in} + n_{out}}},$$

where $n_{in}$ and $n_{out}$ are the number of input and output units in that layer, respectively. The gain $G$ is set to 1 for the output layer with sigmoid activations and 5/3 for hidden layers with tanh activations, as is commonly done in practice for this nonlinear activations. Crucially for our application, even though the Glorot initialization avoids backpropagation pathologies, the control profile that the policy produce is not necessarily a good initial guess for the optimization procedure.

3.6 Preconditioning

In this section we describe several strategies that proved useful to improve the convergence of the optimization to a feasible policy. Similarly to indirect methods in optimal control (Rao, 2009), the convergence improves when the initial parameters produces a good initial control profile. Thus, it is beneficial to optimize towards a reasonable control profile as a preconditioning step. Afterwards, the original problem can beoptimized starting from the policy parameters that reproduce the preconditioning control profile.
The optimization towards a predefined profile is a special case of the problem statement (equation 1), with a running cost that penalizes the discrepancy from the profile along the time evolution of the system, 

$$ J_{pre} = \int_{t_0}^{t_f} [\pi_0(x(t)) - u_{ref}(t)]^2 dt. $$

Since it is challenging to link the network parameter values to the control profile that the policy generates with them, initial stiffness of the policy can also be problematic. This is alleviated by applying the preconditioning procedure iteratively on gradually increasing time windows, to eventually cover the entire time span.

Moreover, a multi-start method is advisable given the high nonlinearity of the optimization problem. Generating multiple feasible control profiles instead of multiple aleatoric network parameters proved more effective to guide the initial control search.

Furthermore, solving a coarse version of the same optimal control problem (without policy) through classic methods like collocation (Rao, 2009) provides the best initial guess as a function of time $u(t)$, since it is closer to the optimal solution. A related approach that also relies on a collocation solution to guide the NeuralODE training was suggested in (Roesch et al., 2021), yet applied to identify mechanistic models in a data-driven manner instead of control problems. The collocation routines used Gauss-Lobatto quadrature with low-order polynomials over a coarse time grid covering the same time span of the original problem (Pulsipher et al., 2022).

4. CASE STUDIES

We applied the discussed techniques to a set of optimal control problems with nonlinear dynamical systems. Since the state feedback controller is well defined in continuous time and space, it is possible to trace the whole phase space of the dynamical system with the embedded controller. We show the convergence of the policy towards feasible solutions satisfying constraints through the iterative tightening of the relaxed logarithmic penalties.

4.1 Van der Pol Oscillator

We analysed the constrained van der Pol oscillator problem from (Vassiliadis et al., 1994):

$$ \begin{align*}
\min_{\theta} \quad & J = \int_{0}^{5} x_1^2 + x_2^2 + u^2 \, dt, \\
n\text{s.t.} \\
& \dot{x}_1(t) = x_1(1 - x_2^2) - x_2 + u, \\
& \dot{x}_2(t) = x_1, \\
& x_1(t) + 0.4 \geq 0, \\
& -0.3 \leq u(t) \leq 1,
\end{align*} $$

with initial condition $x(t_0) = (0,1)$. The state feedback controller was a dense neural network with 2 hidden layers of 16 nodes 

$$ u(t) = \pi_0(x_1(t), x_2(t)). $$

Intermediate layers used a hyperbolic tangent while the output layer used a sigmoid scaled to the allowed interval.

The problem was first optimized disregarding the running constraints (figure 2a), obtaining a final objective $J$ of 2.87. This optimal solution was subsequently used as the starting parameters for the constrained version of the problem, where the running penalty was added to enforce state constraints. The final constrained solution is displayed in figure 2b, where the enforced constraint on $x_1(t)$ is partially active along the optimal path. The optimum value was 2.953 in the constrained case; both optimal values match closely the results reported in (Vassiliadis et al., 1994).

Since the policy is embedded within the dynamical system as a state feedback controller, the policy is well defined for states outside the optimal trajectory and modifies the whole phase space picture.

4.2 Bioreactor

As a more challenging case study of chemical engineering relevance (Vassiliadis et al., 2021), we optimize the bioreactor model analysed in (Bradford et al., 2020). The reactor has 3 state variables and 2 control functions, which represent the biomass concentration ($C_X$), the nitrate concentration ($C_N$), the bioproduct concentration ($C_q$), the light intensity ($I$) and the nitrate inflow rate ($F_N$) of the system, respectively:

$$ \begin{align*}
\frac{dC_X}{dt} &= \frac{u_m C_X I}{1 + k_s + \frac{I}{k_l}} C_N + K_N - u_d C_X, \\
\frac{dC_N}{dt} &= -Y_X \frac{u_m C_X I}{1 + k_s + \frac{I}{k_l}} C_N + K_N + F_N, \\
\frac{dC_q}{dt} &= \frac{k_m C_X I}{1 + k_s + \frac{I}{k_l}} - \frac{k_d C_q}{C_N + K_{NP}},
\end{align*} $$

with the initial condition 

$$ [C_X(0), C_N(0), C_q(0)] = [1, 150, 0]. $$

The rest of the parameters are arranged in table 1 in the appendix.

The main objective is to maximize the bioproduct $C_q$ at the end of the batch time $T$. Additionally, there are 2 running state constraints and 1 final state constraint conditions that must be satisfied, as well as 2 control constraints:

$$ \begin{align*}
C_N &\leq 800, \quad \forall t \in (0, t_f), \\
0.011 C_X - C_q &\leq 0.3, \quad \forall t \in (0, t_f), \\
C_N &\leq 150, \quad t = t_f, \\
120 &\leq I \leq 400, \quad \forall t \in (0, t_f), \\
0 &\leq F_N \leq 40, \quad \forall t \in (0, t_f).
\end{align*} $$

As before, the controller has 2 hidden layers of 16 nodes, with 3 input and 2 output nodes 

$$ I(t), F_N(t) = \pi_0(C_X(t), C_N(t), C_q(t)). $$

5. CONCLUSION

In this work, we explored how neural feedback policies within a white-box dynamical model may be used to solve
Fig. 2. Phase portraits of the Van der Pol system with the embedded neural controller. The portrait on the left corresponds to an unoptimized policy while the portrait on the right corresponds to the optimized policy. The transition between portraits shows how the system dynamics change after the controller has been optimized and complies with the state constraints (shown as the black region).

![Phase portraits](image)

Fig. 3. Constraint enforcement through relaxed logarithmic penalty tightening. As the $\delta$ parameter is reduced, penalties tend to the classic logarithmic penalties from interior point methods. Higher values of delta are useful to deal with infeasible paths generated by unoptimized policies in the initial iterations.

![Constraints](image)

nonlinear optimal control problems in continuous time. We also showcased practical approaches to satisfy both state and control constraints with the optimized policy, which are crucial for real world applications and an active area of research. The approach takes motifs from reinforcement learning by leveraging a neural network as a nonlinear controller, within an environment defined by a deterministic dynamical system. We relied on adjoint sensitivity analysis to handle the large number of parameters required by the neural policy. This approach takes advantage of the specific ODE model form for a precise gradient calculation that avoids sampling completely. In contrast to open-loop methods in optimal control, the state feedback policy can be evaluated for any state outside the optimal trajectory. Our policies provide the whole phase space of the controlled nonlinear system, approximating the intractable closed-loop solution of the nonlinear optimal control problem.

Table 1. Bioreactor parameters (Bradford et al., 2020).

| Parameter | Value   |
|-----------|---------|
| $u_m$     | 0.0572  |
| $u_d$     | 0       |
| $K_N$     | 393.1   |
| $Y_{N/X}$ | 504.5   |
| $k_m$     | 0.00016 |
| $k_d$     | 0.281   |
| $k_s$     | 178.9   |
| $k_i$     | 447.1   |
| $k_{sq}$  | 23.51   |
| $k_{iq}$  | 800     |
| $K_{N_p}$ | 16.89   |
ACKNOWLEDGEMENTS
The authors would like to thank Christopher Rackauckas and the Julia language community for helpful discussions on the numerical implementation of this work. We are grateful to Miguel de Carvalho and Fabian Thiemann for their helpful reviews and comments.

REFERENCES
Achiam, J., Held, D., Tamar, A., and Abbeel, P. (2017). Constrained policy optimization. In D. Precup and Y.W. Teh (eds.), Proceedings of the 34th International Conference on Machine Learning, volume 70 of Proceedings of Machine Learning Research, 22–31. PMLR.

Adhau, S., Naik, V.V., and Skogestad, S. (2021). Constrained Neural Networks for Approximate Nonlinear Model Predictive Control. In 2021 60th IEEE Conference on Decision and Control (CDC), 295–300. IEEE, Austin, TX, USA. doi: 10.1109/CDC5484.2021.9683320.

Ainsworth, S., Lowrey, K., Thicketstun, J., Harchaoui, Z., and Srinivasa, S. (2021). Faster policy learning with continuous-time gradients. In A. Jadbabaie, J. Lygeros, G.J. Pappas, P. A. Parrilo, B. Recht, C.J. Tomlin, and M.N. Zeilinger (eds.), Proceedings of the 3rd Conference on Learning for Dynamics and Control, volume 144 of Proceedings of Machine Learning Research, 1054–1067. PMLR.

Amos, B., Jimenez, I., Sacks, J., Boots, B., and Kolter, J.Z. (2018). Differentiable MPC for End-to-End Planning and Control. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), Advances in Neural Information Processing Systems, volume 31, 8289–8300. Curran Associates, Inc.

Baydin, A.G., Pearlmutter, B.A., Radul, A.A., and Siskind, J.M. (2017). Automatic differentiation in machine learning: a survey. 18(1), 5595–5637.

Biegler, L.T. (2010). Nonlinear Programming: Concepts, Algorithms, and Applications to Chemical Processes. Society for Industrial and Applied Mathematics. doi: 10.1137/1.9780898719385.

Bradford, E., Imsland, L., Zhang, D., and del Rio Chanona, E.A. (2020). Stochastic data-driven model predictive control using gaussian processes. Computers & Chemical Engineering, 139, 106844. doi: 10.1016/j.compchemeng.2020.106844.

Brende, L., Gref, M., Hall, A.W., Yuan, Z., Zhou, S., Panerati, J., and Schoellig, A.P. (2021). Safe Learning in Robotics: From Learning-Based Control to Safe Reinforcement Learning. arXiv:2108.06266 [cs, ess].

Bryson, A.E. and Ho, Y.C. (1975). Applied optimal control: optimization, estimation, and control. Taylor & Francis, rev. print edition. OCLC: 19270190.

Cao, Y. (2005). A formulation of nonlinear model predictive control using automatic differentiation. 15(8), 851–858.

Chachuat, B. (2007). Nonlinear and dynamic optimization: From theory to practice.

Chen, F.C. (1989). Back-propagation neural network for nonlinear self-tuning adaptive control. In Proceedings. IEEE International Symposium on Intelligent Control 1989, 274–279. IEEE Comput. Soc, Press, Albany, NY, USA. doi:10.1109/ISIC.1989.238682.

Chen, R.T.Q., Rubanova, Y., Bettencourt, J., and Duvenaud, D.K. (2018). Neural Ordinary Differential Equations. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), Advances in Neural Information Processing Systems 31, 6571–6583. Curran Associates, Inc.

Chow, Y., Nachum, O., Faust, A., Duenez-Guzman, E., and Ghavamzadeh, M. (2019). Lyapunov-based safe policy optimization for continuous control.

Daulbaev, T., Katrutsa, A., Markeeva, L., Gusak, J., Cichocki, A., and Oseledets, I. (2020). Interpolation Technique to Speed Up Gradients Propagation in Neural ODEs. 33.

Doya, K. (2000). Reinforcement Learning in Continuous Time and Space. Neural Computation, 12(1), 219–245. doi:10.1162/089976600300015961.

Dreyfus, S. (1962). The numerical solution of variational problems. 5(1), 30–45.

Drgona, J., Tuor, A., and Vrabie, D. (2022). Learning Constrained Adaptive Differentiable Predictive Control Policies With Guarantees. arXiv:2004.11184 [cs, ess].

Feller, C. and Ebenbauer, C. (2014). Continuous-time linear MPC algorithms based on relaxed logarithmic barrier functions. IFAC Proceedings Volumes, 47(3), 2481–2488. doi:10.3182/20140824-6-ZA-1003.01022.

Fiacco, A.V. and McCormick, G.P. (1990). Nonlinear Programming: Sequential Unconstrained Minimization Techniques. Society for Industrial and Applied Mathematics. doi:10.1137/1.9781611971316.

Glorot, X. and Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In Y.W. Teh and M. Titterington (eds.), Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, volume 9 of Proceedings of Machine Learning Research, 249–256. JMLR Workshop and Conference Proceedings.

Griewank, A. (2012). Who invented the reverse mode of differentiation? In M. Grötschel (ed.), Optimization stories, volume 21st International Symposium on Mathematical Programming, chapter Computing Stories, 389–400. Documenta Mathematica.

Hunt, K., Sbarbaro, D., Zbikowski, R., and Gawthrop, P. (1992). Neural networks for control systems—A survey. Automatica, 28(6), 1083–1112. doi:10.1016/0005-1098(92)90053-I.

Jin, W., Wang, Z., Yang, Z., and Mou, S. (2020). Ponthier-gin differentiable programming: An end-to-end learning and control framework. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin (eds.), Advances in Neural Information Processing Systems, volume 33, 7979–7992. Curran Associates, Inc.

Jorgensen, J.B. (2007). Adjoint sensitivity results for predictive control, state- and parameter-estimation with nonlinear models. In 2007 European Control Conference (ECC), 3649–3656. IEEE, Kos. doi: 10.23919/ECC.2007.7068974.

Karg, B. and Lucia, S. (2020). Efficient representation and approximation of model predictive control laws via deep learning. IEEE Transactions on Cybernetics, 50(9), 3866–3878. doi:10.1109/TCYB.2020.2999556.

Kingma, D.P. and Ba, J. (2015). Adam: A method for stochastic optimization. In ICLR (Poster).
