
List 4: Reinforcement Learning.

Deep learning control of physics-informed neural networks for fast actuation in uncertain environments

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1 Introduction

Why is this problem important to solve? Scientific Machine Learning (SciML) has arisen as a replacement to traditional numerical discretization methods. The main driving force behind this replacement is neural networks (NNs), largely due to their success in natural language processing (NLP) and computer vision (CV) problems [1]. As a vehicle to approximate the solution to a given partial differential equation (PDE) or ordinary differential equation (ODE), NNs offer a mesh-free approach via auto differentiation, and break the curse of dimensionality [2]. Combining scientific computing and ML, SciML offers the potential to improve "predictions beyond state-of-the-art physical models with smaller number of samples and generalizability in out-of-sample scenarios" [3].

Physics-informed neural networks (PINNs) are networks that solve supervised learning tasks while respecting the properties of physical laws [4]. Since their introduction, PINNs have been leveraged to solve a wide swath of problems including, but not limited to, inverse problems [2, 5–9], fractional differential equations [10], and stochastic differential equations [11–14]. Some recent work has begun exploring the application of PINNs with regards to optimal control problems [15–18]. However, these prior approaches tackle control problems by merely feeding control data to a PINN.

Describe an important research problem. A new framework of PINNs presented in this paper, hereafter known as Control PINNs, offers a novel approach to solving open loop and closed loop optimal control problems. Control PINNs simultaneously solve the learning tasks of both the system state, and its respective optimal control, without the need for a priori controller data nor an external controller. Moreover, Control PINNs can find optimal control solutions to complex computational scientific problems more efficiently. Furthermore, Control PINNs can be utilized as agents in deep reinforcement learning (DRL) [19]. In DRL, finding the state of a robot after a given action may require solving a number of physical equations (e.g. equation of motion and balance of force). This issue can be circumvented by leveraging PINNs as an agent because PINNs penalize any deviation from given physical constraints.

We begin in section 2 by providing a literature review of background information and prior approaches. Section 3 covers the methodology of the novel approach that this paper offers as contribution. Section 4 validates the methodology via implementation of an analytical toy problem. Section 5 details a road map for future work.

2 Background

2.1 Optimal Control

Hairer and Wanner provide an overview of control problems, and more specifically, optimal control problems in [20]. It is common for optimal control theory problems to be presented as ordinary differential equations of the form $y' = f(y, u)$ where $u(x)$ represents a set of controls and is applied such that a given constraint, say $0 = g(y, u)$, is satisfied by the solution while simultaneously minimizing a given cost function [20].

2.2 Physics-Informed Neural Networks

Cuomo *et al.* provide a comprehensive overview of Physics-Informed Neural Networks (PINNs) in [19]. This survey paper sheds light on how most literature involving PINNs deals with customizing PINNs "through different activation functions, gradient optimization techniques, neural network structures, and loss function structures" [19]. *The following excerpt from [19] highlights the important link between PINNs and reinforcement learning:*

"PINNs can be used as a tool for engaging deep reinforcement learning (DRL) that combines reinforcement learning (RL) and deep learning. RL enables agents to conduct experiments to comprehend their environment better, allowing them to acquire high-level causal links and reasoning about causes and effects [21]. The main principle of reinforcement learning is to have an agent learn from its surroundings through exploration and by defining a reward [22]. In the DRL framework, the PINNs can be used as agents. In this scenario, information from the environment could be directly embedded in the agent using knowledge from actuators, sensors, and the prior-physical law, like in a transfer learning paradigm" [19].

Raissi *et al.* introduce the novel physics informed neural networks (PINNs) in [4]. Raissi *et al.* define PINNs to be networks that solve supervised learning tasks while respecting the properties of physical laws. In [4], PINNs are utilized to solve data-driven problems, and data-driven discovery of partial differential equations.

In their introductory paper of [4], PINNs function by minimizing a mean-squared-error loss function involving both data from the boundary conditions, and the enforced physical equations of the given problem. The general algorithm for a Physics-Informed Neural Network (PINN) is as follows below in algorithm 1.

Algorithm 1: The PINN algorithm for solving differential equations [2]

Result: Minimize loss function $L(\theta; T)$

1. Construct neural network $\hat{u}(x; \theta)$ with parameters θ .
 2. Specify two training sets T_f and T_b for the equation and boundary/initial conditions.
 3. Specify a loss function by summing the weighted L^2 norm of both the PDE equation and boundary condition residuals.
 4. Train the neural network to find the best parameters θ^* by minimizing the loss function $L(\theta; T)$.
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Willard *et al.* provide a structured overview of physics-based modeling approaches with machine learning (ML) techniques [3]. Moreover, Willard *et al.* summarize current areas of application with regard to science-guided ML [3]. Willard *et al.* describe current methodologies of constructing physics-guided ML models and hybrid physics-ML frameworks [3]. Consequently, Willard *et al.* have compiled a taxonomy of existing techniques, and as such have shed light on knowledge gaps and provided a foundation for new ideas to spring forth.

68 According to Willard *et al.*, the five classes of methodologies to merge principles of physics-based
69 modeling with ML are: 1.) Physics-guided loss function 2.) Physics-guided initialization 3.) Physics-
70 guided design of architecture 4.) Residual modeling 5.) Hybrid physics-ML models.

71 In [23], Nellikkath and Chatzivasileiadis show that by “combining the [Karush-Kuhn-Tucker] condi-
72 tions with the neural network, the physics-informed neural network achieves higher accuracy while
73 utilizing substantially fewer data points.” Moreover, the duo expanded on their previous work in [23]
74 regarding “worst-case guarantees to cover the physics-informed neural networks (PINNs), and [...]”
75 show that PINNs result in lower worst-case violations than conventional neural networks.”

76 2.3 Optimal Control with Physics-Informed Neural Networks

77 This section describes prior approaches to solve the proposed problem. In [15], Hwang *et al.* propose
78 a two stage framework for solving PDE-constrained control problems using operator learning. They
79 first train an autoencoder model, and then infer the optimal control by fixing the learnable parameter
80 and minimizing their objective function. One strength of their approach is the ability to apply their
81 framework to both data-driven and data-free cases. The main downside to their approach is the two
82 stage nature of the framework, as the control is found only after a surrogate model has been trained.
83 Success is measured through tracking the “values of relative errors on test data in each experiment,”
84 in addition to visual inspection of the trained solution operators [15].

85 In [16], Chen *et al.* train an input convex recurrent neural network. Subsequently, they then solve
86 a convex model predictive control (MPC) problem. The main strength of the approach in [16] is
87 the guarantee of an optimal solution, thanks to the convex nature of the trained model. The main
88 limitation is similar to [15, 16], in that they employ a two stage framework of system identification and
89 controller design [16]. Success is evaluated by the “performance of both algorithms on three randomly
90 selected fixed random seeds for four tasks” [16]. The average performance, with corresponding
91 standard deviation, is then visually plotted for visual confirmation of success.

92 In [17], Antonelo *et al.* introduce a new framework called Physics-Informed Neural Nets for Control
93 (PINC). PINC uses data from the control action u , and initial state $y(0)$, to solve an optimal control
94 problem. One strength of this approach is the ability to “run for an indefinite time horizon [...] without
95 significant deterioration of network prediction” [17]. A significant limitation of this approach is
96 offline learning the control separately from the solution operator. In other words, PINC is essentially
97 a PINN that is amenable to being trained on data of the controller data, instead of learning the optimal
98 control itself. Success is evaluated through Mean Squared Error (MSE) validation error for the Van
99 der Pol Oscillator problem.

100 In [18], Mowlavi and Nabi conduct an evaluation of the comparative performance between traditional
101 PINNs and classic direct-adjoint-looping (DAL) to solve optimal control problems. Similar to
102 Antonelo *et al.* [17], Mowlavi and Nabi separate the optimal control problem into two sub-problems.
103 At each state of the system, the PDE is solved with one neural network. That information is then used
104 by another neural network to solve for the optimal control at that given state of the PDE. Afterwards,
105 the adjoint PDE (lambda term) is solved in backwards time [18].

106 The strength of Mowlavi’s and Nabi’s approach is achieving one of their main goals of comparing
107 “the pros and cons of the PINN and DAL frameworks for solving PDE-constrained optimal control
108 problems, so that the novel PINN approach can be placed in the context of the mature field of PDE-
109 constrained optimization” [18]. Success is measured via validation and evaluation steps. Validation is
110 done by monitoring residual, boundary, and initial loss components with a known a priori solution.
111 Evaluation is done by comparing the control cost objective with an a priori solution found by a
112 high-fidelity numerical solver.

113 One limitations of this approach is using the more easily solvable steady state Navier Stokes, instead
114 of unsteady state Navier Stokes. Moreover, manual derivation is used in their DAL approach, which is
115 unnecessary because DAL can use automatic differentiation (AD). Consequently, to a certain extent,
116 [18] is solving the optimal control problems manually. Furthermore, the control of the system is

being dampened over time. This is suspicious, as it might mean this dampening approach was added post hoc because of struggling results. It should be noted that the adjoint PDE is not being solved in their cost function, and thus the respective adjoint formulas are not present in said cost function. This brings us to the the main contributions of this paper.

What limitations of prior work would be addressed by your new approach? The proposed framework in this paper goes beyond the framework in [15–17], because Control PINNs do not rely on data from the controller. Moreover, instead of evaluating PINNs in the "context of the mature field of PDE-constrained optimization," [18] this paper proposes a framework that can be considered a new taxonomical entity within the genus of PINNs. The main contribution of Control PINNs is that an unknown controller u can be solved at the same time as the complex dynamical state of y .

How would you evaluate your new approach? This novel approach will be evaluated in three different ways. Firstly, an architect will be designed and then trained as a neural network while monitoring the loss function. Secondly, comparison of model results and reference solutions will be carried out for a problem with a known analytical solution. Thirdly, for problems with no known solution, the model results will be compared to simulation results using numerical analysis techniques. In other words, offline data generation for the controller can be collected for varying values of t and x (time and space). Then, this high precision data set can be plotted and validated with the solution found using a Mathematica solver.

Explain the key intuition behind your approach and why you think it is likely to be effective. Deep reinforcement learning (DRL) involves a feedback loop between an agent and an environment. The agent performs an action in the environment, which prompts a new updated state of the agent, and sometimes a given reward. This feedback loop forms the basis of an agent's policy. Correct policies that offer a reward for an agent's action strengthen the neural connectivity in certain action-state pathways [24]. By imparting known physical properties into the agent's neural network, you can supercharge these pathways to more efficiently reach a state of convergence.

Reinforcement learning (RL) is the intersection of control theory and machine learning. As a result, RL learns control strategies to interact with a complex environment [24]. RL has proven itself successful in tackling fluid mechanic problems [25–30]. Intuitively, if both RL and PINNs are successful in the field of SciML, then combining them offers an interesting avenue for research. Control PINNs can be thought of as Deep Model Predictive Control, in the sense that they can solve difficult optimal nonlinear problems [24]. With this in mind, for a given problem Q-learning can learn a policy based on the Control PINN. In other words, the quality of the both the controller, and state of the system, provided by the Control PINN, can be systematized such that the best quality of action-state can be carried out. Before leveraging a Control PINN as an agent in a DRL framework, it first must be demonstrated that it can solve optimal/open loop control problems. The methodology in section 3 lays the ground work for Control PINNs to solve an analytical toy problem.

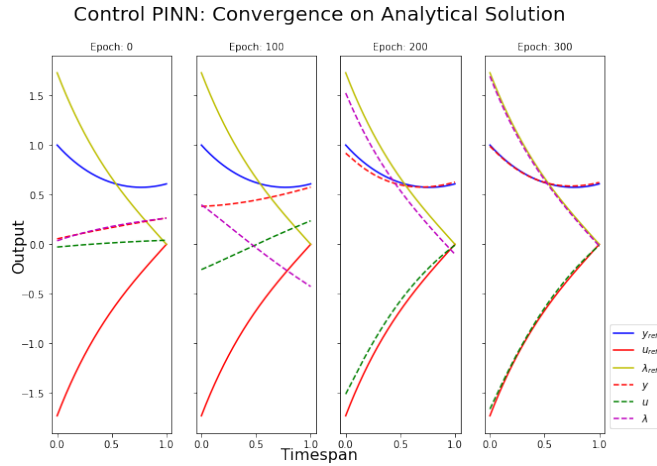


Figure 1: Results of the analytical problem. The optimal solutions of the system state, controller, and system push back on the controller are denoted by y_{ref} , u_{ref} , and λ_{ref} . Their respective predicted solutions found by the Control PINN model are denoted by y , u , and λ .

3 Methodology

We denote by $y(t)$ the solution of the ODE, and by $u(t)$ the control function. We seek to solve the control problem [31]:

$$\begin{aligned} \min_{u(t)} \Psi(y) &= \int_0^{t_f} g(y(t), u(t)) dt + w(y(t_f)) \\ \text{subject to } y' &= f(y, u), \forall t \in [0, t_f], \quad y(0) = y_0. \end{aligned} \quad (1)$$

The optimality conditions are:

$$y'(t) = f(y(t), u(t)), \forall t \in [0, t_f]; \quad y(0) = y_0^*; \quad (2a)$$

$$\lambda'(t) = -f_y^T(y(t), u(t)) \lambda(t) - g_y^T(y(t), u(t)), \forall t \in [t_f, 0]; \quad (2b)$$

$$\lambda(t_f) = w_y^T(y(t_f));$$

$$0 = -f_u(y(t), u(t)) \lambda(t) - g_u^T(y(t), u(t)), \forall t \in [0, t_f]. \quad (2c)$$

The process of solving the control problem detailed in eq. (1) is outlined in algorithm 2. The last three terms in eq. (3) can be thought of respectively as the system state, the system controller, and the push back on the controller by the system. In the context of autonomous vehicles, the system state can be thought of as the velocity and direction of the vehicle. By the same token, the system controller would be the software that governs the steering wheel and speed. Likewise, the system push back would be the feedback of the vehicle in response to the software's choices of direction and speed (e.g. the vehicle's shocks and brake pads).

What are the technical challenges with solving this problem? The main technical challenge involves learning the state of a dynamical system while at the same time finding its optimal control. Moreover, there is a tension between enforcing the boundary conditions and adhering to the constraints imposed by the physical laws. This is addressed by a scaling term in the loss function. Furthermore, as Control PINN is applied to increasingly more complex problems, some times a known unique solution may not be available. Such a solution would mainly be used for validation purposes.

Algorithm 2: The procedure to train a Control PINN model

Result: Training of a Control PINN that learns the optimal solution and the optimal control function for the given problem in (1)

1. Construct a network with inputs t, x (time and space), and outputs y, u , and λ (system state, system control, and system push back on control)
2. Via auto differentiation and back-propagation, compute the following derivatives of the output w.r.t the input: $\frac{\delta y}{\delta x}, \frac{\delta y}{\delta t}, \frac{\delta f}{\delta y}, \frac{\delta f}{\delta t}, \frac{\delta \lambda}{\delta t}, \frac{\delta f}{\delta u}, \frac{\delta g}{\delta y}, \frac{\delta g}{\delta u}$
3. With snapshots of the exact solution denoted by $y^*(t)$, minimize the loss function:

$$\begin{aligned} L &= \sum_i (t_{i+1} - t_i) \|y(t_i) - y^*(t_i)\|^2 \\ &+ \sum_i (t_{i+1} - t_i) \|D_t y(t_i) - f(y(t_i), u(t_i))\|^2 \\ &+ \sum_i (t_{i+1} - t_i) \|D_t \lambda(t_i) + f_y^T(y(t_i), u(t_i)) \lambda(t_i) + g_y^T(y(t_i), u(t_i))\|^2 \\ &+ \sum_i (t_{i+1} - t_i) \|f_u(y(t_i), u(t_i)) \lambda(t_i) + g_u^T(y(t_i), u(t_i))\|^2. \end{aligned} \quad (3)$$

A visual representation of the Control PINN Architecture is found in fig. 2. Adaptive moment estimation (Adam) is used as the optimizer. The activation function of Exponential Linear Unit (ELU) is used. The neural density is 100 neurons per layer. There are ten hidden layers that proceed the input layer that takes in time (t) and space (x). The information of the system state (y) is passed

190 to the controller (u) both directly and indirectly by a skip connection and several hidden layers,
 191 respectively. The aggregate information of the system state (y) and controller (u) is handled similarly
 192 in the context of the system's push back on the controller (λ). This architecture enables for the
 193 automatic differentiation of second order and mixed derivatives. This is necessary to impose the
 194 custom loss function detailed in algorithm 2.

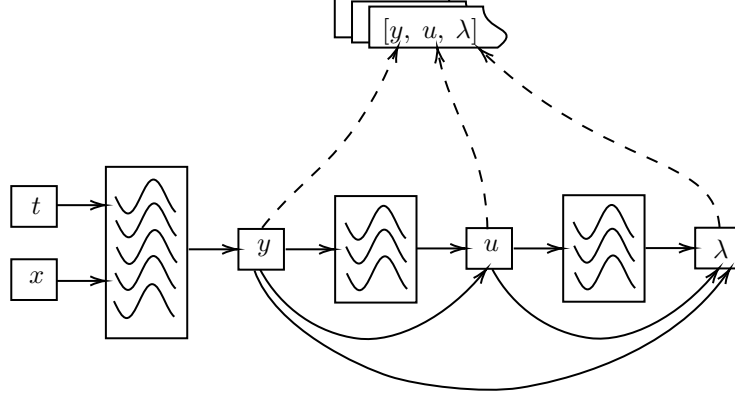


Figure 2: Visual Representation of Control PINN Architecture

195 4 Analytical Toy Problem

196 As a proof of concept, and to provide a foundation for methodology validation, let us consider the
 197 below test problem from [32]:

$$t_f = 1, \quad w(y(t_f)) = 0, \quad y(0) = y_0 = 1 \quad (4a)$$

$$f(y(t), u(t)) = \frac{1}{2}y(t) + u(t), \quad f_y(y(t), u(t)) = \frac{1}{2}, \quad f_u(y(t), u(t)) = 1 \quad (4b)$$

$$g(y(t), u(t)) = y^2(t) + \frac{1}{2}u^2(t), \quad g_y(y(t), u(t)) = 2y(t), \quad g_u(y(t), u(t)) = u(t) \quad (4c)$$

$$\lambda'(t) = -\frac{1}{2}\lambda(t) - 2y(t), \quad \forall t \in [0, 1]; \quad \lambda(t_f) = 0 \quad (4d)$$

$$0 = -\lambda(t) - u(t), \quad \forall t \in [0, 1] \quad (4e)$$

198 The optimal solution is: $y^*(t) = \frac{2e^{3t} + e^3}{e^{3t/2}(2 + e^3)}$, $u^*(t) = \frac{2(e^{3t} - e^3)}{e^{3t/2}(2 + e^3)}$, $\lambda^*(t) = -u^*(t)$. We can
 199 then check that the analytical solution found by the Control PINN satisfies the optimality equations
 200 listed above. After a couple hundred epochs, the Control PINN converges on the optimal solution.
 201 This is shown in fig. 1, wherein y_{ref} , u_{ref} , and λ_{ref} respectively represent the reference solution for
 202 the system state y , the reference solution for the system controller u , and the reference solution of the
 203 system push back on the controller λ . Please refer to the following hyperlink to see an animation of
 204 the [Control PINN model converging on the optimal solution](#).

205 5 Future Steps

206 Now that Control PINNs have been demonstrated as a proof-of-concept with an analytical toy
 207 problem, the next steps would involve increasing the problem complexity. For example, please
 208 refer to the following hyperlinks to see preliminary results for both a [1-dimensional heat problem](#),
 209 and a [2-dimensional spatio temporal predator-prey model \(reaction diffusion\)](#). From there, Control
 210 PINNs can be implemented as a closed loop problem in the form of Navier Stokes flow control, or
 211 COVID-19 contact tracing. Starting with the most simple problem, and then adding more complex
 212 building blocks, offers a road map for leveraging Control PINNs as an agent for Deep Reinforcement
 213 Learning (DRL). For example, the results of the permutation invariant cart-pole swing up problem in
 214 [33] could then be compared to a Control PINN DRL implementation.

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