Pontryagin Differentiable Programming: An End-to-End Learning and Control Framework

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Abstract
This paper develops a Pontryagin differentiable programming (PDP) methodology to establish a unified end-to-end learning framework, which solves a large class of learning and control tasks. The proposed PDP framework distinguishes itself from existing ones by two key techniques: first, by differentiating the Pontryagin’s Maximum Principle, the PDP framework allows for an end-to-end learning of any parameterized system, even though differentiation with respect to an unknown objective function is not readily attainable; and second, based on control theory, the PDP framework incorporates both the forward and backward propagations by constructing two separate control systems, which are then efficiently solved using techniques in control domain. Three learning modes of the proposed PDP framework are investigated to address three types of learning problems: inverse optimization, system identification, and control/planning, respectively. Effectiveness of this framework in each learning mode has been validated in the context of pendulum systems.

1 Introduction
An abundance of learning tasks can be formulated as problems of modeling/designing control systems. Those problems usually focus on two components: the system dynamical model, which governs the evolution rule of the system state given an input; and the control law, which describes how the inputs are produced. For example, training a deep neural network (Chen et al., 2018) can be viewed as achieving a dynamical model with the system states being the hidden values of neurons; reinforcement learning problems can be looked at as finding an optimal control policy for a system to maximize a notion of accumulative reward (Sutton and Barto, 2018); and inverse reinforcement learning (Ng et al., 2000) is basically reconstructing a control law, specifically an control objective function, in order to emulate or match behavioral observations. With significant progress achieved in various challenging domains, existing learning techniques usually rely on a large number of samples (Mnih et al., 2013, 2015; Oh et al., 2016). To attain sample-efficient learning, a trend of work attempts to exploit structural priors of a system, but normally restricted to using simple models due to their attainable differentiation (Deisenroth and Rasmussen, 2011; Heess et al., 2015; Schneider, 1997). This has motivated us to establish an end-to-end framework that can learn a more general class of models by unitizing structural and differential patterns in control theory.
1.1 Background and Related Work

Learning tasks can be treated as problems of achieving specific control systems. Based on which component is parameterized in a control system, existing learning problems can be categorized as below.

- **System identification** focuses on finding a dynamical equation using observed/labeled data. Parameterized models considered include transfer functions (Johansson, 1993; Ljung and Glad, 1994), ordinary differential equations (Chen et al., 2018), and (deep) neural networks (Gonzalez and Yu, 2018; Wang, 2017). The learning is usually established by minimizing the reproduction error between the model output and observed data. Recently, Koopem operator theory (Koopman, 1931) is employed to transform the learning process into a linear programming in an observable space (Proctor et al., 2018; Williams et al., 2015).

- **Control and planning** aims to find an optimal control law such that the behavior of a control system optimizes a certain control objective given by some notion of accumulative reward/cost. Closely related to this category are techniques of reinforcement learning, most of which seek a fixed reactive control policy (that is, a direct mapping from system state to control input) using a policy class such as linear functions or neural networks (Lillicrap et al., 2015; Mnih et al., 2013; Sutton et al., 2000).

- **Inverse optimization** aims to obtain an underlying control objective, which can be viewed as a high-level control law, from observed demonstrations. Related techniques include inverse reinforcement learning (Ng et al., 2000; Ziebart et al., 2008), inverse optimal control (Jin et al., 2019; Keshavarz et al., 2011), and imitation learning (Abbeel and Ng, 2004; Syed et al., 2008). By parameterizing the objective function as a weighted sum of features, these methods optimize the learning goal, such as maximizing entropy/margin or minimizing optimality violations, over the unknown weights.

Among varying learning techniques, a growing number of results have demonstrated that leveraging available structures in a system can lead to improved learning efficiency and generalization. Specifically, two benefits can be achieved by resorting to the structures of control systems. First, through system models, sample complexity can be reduced and high-dimensional tasks can be efficiently learned. For instance, to address poor sample complexity of model-free reinforcement learning (Mnih et al., 2013, 2015), model-based counterparts first learn the system dynamical model, and then integrate the learned model into the process of finding optimal control policies (Abbeel et al., 2006; Deisenroth and Rasmussen, 2011; Schneider, 1997). Second, by exploiting the structural models and differential patterns in control systems, new automatic differentiation techniques can be developed to allow for efficient learning of more complex tasks. For example, in (Amos et al., 2018; Okada et al., 2017; Tamar et al., 2016), differentiation techniques are developed to enable a joint learning of system dynamics and control objective function.

Another related line of studies focuses on understanding deep learning from the perspective of optimal control theory. As suggested by these works, a multi-layer neural network can be viewed as a dynamical system where the values of the neurons and the network weights are regarded as the state and input of a control system, respectively. Training a deep neural network then becomes solving an optimal control problem, whose optimality condition is characterized by the Pontryagin’s Maximum Principle (PMP) (Boltyanski et al., 1960; Pontryagin, 2018). A practical training algorithm for deep learning can then be obtained by approximating the optimal solution given by the PMP via various numerical approximation (Chernousko and Lyubushin, 1982; Krylov and Chernousko, 1972). See, e.g., (Benning et al., 2019; Li and Hao, 2018; Li et al., 2017; Liu and Markowich, 2019; Weinan, 2017; Weinan et al., 2019; Zhang et al., 2019) for more details of these work, and see (Liu and Theodorou, 2019) for a recent survey on the connection between deep learning and optimal control theory.

Related to our work are the recent techniques developed in (Okada et al., 2017; Pereira et al., 2018), where a Path Integral Network is proposed to learn the path integral optimal control systems. The path integral
formation characterizes a special class of optimal control systems where the dynamical model is an affine function of the input and the control objective is quadratic to input (Kappen, 2005). Such path integral formation can be covered by the proposed PDP framework, where we focus on more general optimal control systems. In (Amos et al., 2018), a Model Predictive Control (MPC) framework is developed based on iterative Linear Quadratic Regular (iLQR) method (Li and Todorov, 2004). Differentiation in such framework is not directly performed over the parameterized dynamical model and control objective but its local LQR approximation. Differently, by differentiating the PMP, the proposed PDP framework directly achieves the gradient with respect to the unknown dynamics and control objective. Moreover, by connecting the differential PMP to control establishment, we develop an auxiliary control system in backward pass of the learning framework, which handles the differentiation efficiently using techniques in control domain. Such a scheme and formulation does not appear in existing literature.

1.2 Contributions

In this paper, we propose a Pontryagin differentiable programming (PDP) framework which unifies multiple learning and control tasks under one end-to-end PDP framework as shown in Fig.1. By parameterizing different components of a control system, such as the dynamical model, control policy, and/or control objective function, the PDP framework is able to efficiently solve different learning problems, e.g., system identification, control and planning, and inverse problems. This will be achieved by two key techniques: first, we differentiate the Pontryagin’s maximum principle to enable an end-to-end learning of any parameterized component in a system; and second, based on control theory, we construct an auxiliary control system in the backward pass of the PDP framework, as shown in Fig. 1, and this allows an efficient computation using techniques in control domain. Three learning modes of the proposed PDP framework are investigated to address three types of problems: model identification, control and planning, and inverse optimization, respectively.

2 Problem Formulation

We consider a general form of an optimal control system $\Sigma(\theta)$ which is parameterized by a tunable $\theta \in \mathbb{R}^r$ in both system dynamical model and control objective function,

$$
\Sigma(\theta) : \begin{align*}
\text{dynamics: } & \quad x_{t+1} = f(x_t, u_t, \theta) \quad \text{with } x_0, \\
\text{control objective: } & \quad J(\theta) = \sum_{t=0}^{T-1} c_t(x_t, u_t, \theta) + h(x_T, \theta). 
\end{align*}
$$

(1)

Here, $x_t \in \mathbb{R}^n$ is the system state; $u_t \in \mathbb{R}^m$ is the system input; $f : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^r \mapsto \mathbb{R}^n$ is the dynamical model and assumed to be twice-differentiable; $t = 0, 1, \cdots, T$ denote the time steps with $T$ being the overall time horizon; and $c_t : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^r \mapsto \mathbb{R}$ and $h : \mathbb{R}^n \times \mathbb{R}^r \mapsto \mathbb{R}$ denote the running and final costs/rewards, respectively, both assumed twice-differentiable.
For each choice of $\theta$, the corresponding optimal control system $\Sigma(\theta)$ generates a sequence of inputs such that its trajectory of states-inputs
\[ \xi_\theta = \{x_{0:T}, u_{0:T-1}\} \] optimizes its control objective $J(\theta)$. Thus for each $\theta$, there exists a system trajectory denoted by $\xi_\theta$. To evaluate such a trajectory $\xi_\theta$, one usually introduces a scalar-valued loss function
\[ L(\xi_\theta, \theta), \] which is differentiable with respect to $\xi_\theta$ and $\theta$. Such loss function is usually specified according to specific missions. The problem of interest is to find an optimal $\theta^*$ to solve the optimization problem
\[ \min_{\theta} L(\xi_\theta, \theta) \quad \text{subject to} \quad \xi_\theta \text{ is generated by } \Sigma(\theta). \] (4)

2.1 Specialization of Learning Modes

We next show that how the above problem in (4) can be specially tailored for various learning tasks. Each of the specializations is called a learning mode.

Learning Mode 1: Inverse Optimization. We consider that $\theta$ is in the control objective $J$ and the dynamical model $f$, as written in (1). We specifically define the loss function $L(\xi_\theta, \theta)$ in (3) to be
\[ L = \mathbb{E}_{\xi^o} l(\xi_\theta, \xi^o), \] (5)
where $\xi^o = \{x_{0:T}^o, u_{0:T-1}^o\}$ is the observed trajectory that is subject to certain population model, and $l$ is a differentiable scalar-valued penalty function to quantify the inconsistency of the trajectory $\xi_\theta$ of $\Sigma(\theta)$ with the observed $\xi^o$, e.g., let $l = \|\xi_\theta - \xi^o\|^2$. Then, the problem in (4) formulates the class of inverse optimization problems, whose goal is to learn an optimal control system $\Sigma(\theta)$ that are consistent with the observed data. This type of problems is studied in inverse optimal control (Jin et al., 2019), inverse reinforcement learning (Ng et al., 2000), and imitation learning (Abbeel and Ng, 2004).

Learning Mode 2: System Identification. We consider a special form of $\Sigma(\theta)$, where $\theta$ only parameterizes the dynamics $f$ while the control objective $J$ is set to a constant scalar, e.g., $h = 0$ and $c = 0$. Under this case, the system trajectory $\xi_\theta$ in (2) with any inputs $u_{0:T-1}^h$ can optimize $J$; in other words, the input $u_t$ can be chosen arbitrarily. Then $\Sigma(\theta)$ represents a class of dynamical models; that is,
\[ \Sigma(\theta) : \quad \text{dynamics: } x_{t+1} = f(x_t, u_t, \theta) \quad \text{with } x_0 \text{ and provided } u_{0:T}. \] (6)
Given any input sequence $u_{0:T-1}$, the above $\Sigma(\theta)$ outputs the trajectory $\xi_\theta = \{x_{0:T}^\theta(u_{0:T-1})\}$. We define the loss function $L(\xi_\theta, \theta)$ in (3) to be
\[ L = l(\xi_\theta, \xi^o), \] (7)
where $\xi^o = \{x_{0:T}^o(u_{0:T-1})\}$ is the observed data of an unknown (black box) system under the same inputs $u_{0:T-1}$, and $l$ is a differentiable scalar-valued penalty function to quantify the reproduction error between the outputs of $\Sigma(\theta)$ and $\xi^o$, e.g., let $l = \|\xi_\theta - \xi^o\|^2$. Then, (4) formulates the problem of system identification, whose goal is to learn a dynamical model to emulate the block-box system (Gonzalez and Yu, 2018; Proctor et al., 2018).

Learning Mode 3: Control and Planning. We consider the system $\Sigma(\theta)$ whose control objective $J$ is set to a constant scalar (e.g., $h = 0$ and $c = 0$) and dynamics $f$ is exactly known (e.g., learned via Learning
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Mode 2); that is, there is no \( \theta \) in \( f \). Instead of externally providing inputs \( u_{0:T-1} \), we here use \( \theta \) to parameterize a control input function \( u_t = u(t, \theta) \). The system \( \Sigma(\theta) \) thus is

\[
\begin{align*}
\Sigma(\theta): & \quad \text{dynamics: } x_{t+1} = f(x_t, u_t) \quad \text{with} \quad x_0, \\
& \quad \text{control inputs: } u_t = u(t, \theta).
\end{align*}
\]

The parameterized control input function \( u_t = u(t, \theta) \) can be Chebyshev or Lagrange polynomials, which are normally used in the collocation methods (Elmaghraby et al., 1995; Patterson and Rao, 2014; Vlassenbroeck and Van Dooren, 1988). Given \( u_t = u(t, \theta) \), \( \Sigma(\theta) \) in (8) will have a trajectory \( \xi_\theta = \{x^0_{0:T}, u^0_{0:T-1}\} \). To achieve an optimal control/planning performance, we define the loss \( L(\xi_\theta, \theta) \) in (3) to be

\[
L = \sum_{t=0}^{T-1} l(x^0_t, u^0_t) + l_f(x^0_T),
\]

where \( l \) and \( l_f \) are the running and final costs (or negative rewards), respectively, which are specified by the designer or learned via Learning Mode 1. The problem in (4) then formulates the type of optimal control/planning problems, whose goal is to find an optimal parameter \( \theta^* \), or equivalently an sequence of control inputs \( u^*_t = u(t, \theta^*) \) for \( t = 0, 1, \cdots, T-1 \), which minimizes the accumulative loss in (9). Techniques related to this type of problems include optimal control (Patterson and Rao, 2014), trajectory optimization (Ratliff et al., 2009), and reinforcement learning (Deisenroth and Rasmussen, 2011).

3 Key Idea for End-to-End Learning

For the general formulation in (4), the end-to-end learning aims to solve the problem by applying the gradient descent technique to the system as a whole (Muller et al., 2006), that is,

\[
\theta_{k+1} = \theta_k - \eta_k \frac{dL}{d\theta}|_{\theta=\theta_k}.
\]

Here \( k = 0, 1, \cdots \) is the iteration index; \( \frac{dL}{d\theta}|_{\theta=\theta_k} \) is the gradient of the loss with respect to \( \theta \) and evaluated \( \theta_k \); and \( \eta_k \) is the learning rate (or step size) (Zeiler, 2012). By chain rule, one has

\[
\frac{dL}{d\theta}|_{\theta=\theta_k} = \frac{\partial L}{\partial \xi}|_{\xi=\xi_{\theta_k}} \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} + \frac{\partial L}{\partial \theta}|_{\theta=\theta_k}.
\]

In order to achieve the gradient quantity \( \frac{dL}{d\theta}|_{\theta=\theta_k} \), one needs \( \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} \), which is however unknown. The key idea to solve the problem in (4) by obtaining \( \frac{dL}{d\theta}|_{\theta=\theta_k} \) is an end-to-end learning scheme presented in Fig. 2. Here, the learning update in (10) at each iteration consists of two passes, namely, a forward pass, where the current \( \xi_{\theta_k} \) is obtained from the current system \( \Sigma(\theta_k) \), and the corresponding loss \( L(\xi_{\theta_k}, \theta_k) \) is evaluated, and a backward pass, where the gradient quantities \( \frac{\partial L}{\partial \theta}|_{\theta=\theta_k} \) and \( \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} \) are computed.

In the forward pass, \( \xi_{\theta_k} \) can be obtained by solving an optimal control problem for \( \Sigma(\theta_k) \) using existing optimal control solvers such as ILQR algorithm (Li and Todorov, 2004), single or multiple shooting methods (Bock and Plitt, 1984), and collocation methods (Patterson and Rao, 2014), or using Learning Mode 3 as we will discuss later. In the backward pass, \( \frac{\partial L}{\partial \theta}|_{\theta=\theta_k} \) and \( \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} \) are straightforward to compute from the given loss function \( L(\xi_{\theta_k}, \theta) \). The main technical challenge, however, lies in obtaining the gradient \( \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} \) since \( \xi_{\theta} \) depends on \( \theta \) through the operation of solving an optimal control problem in the forward pass. Although differentiation through the operation in the forward pass is an option to obtain \( \frac{\partial \xi_{\theta_k}}{\partial \theta}|_{\theta=\theta_k} \), when the optimal control system \( \Sigma(\theta_k) \) is of small size, it will incur huge memory and computational costs and become intractable when the optimal control system is high-dimensional. In the subsequent section, we will solve
In order to achieve the gradient \( \frac{\partial L}{\partial \theta} |_{\theta=\theta_0} \) by developing two techniques: one is the differential PMP and the other is an auxiliary control system \( \Sigma (\xi_\theta) \), as shown in Fig. 2.

4 Key Techniques: Differential PMP & Auxiliary Control System

For any choice of \( \theta \), we define the following discrete-time Hamiltonian function for the optimal control system \( \Sigma (\theta) \) in (1),

\[
H(x_t, u_t, \lambda_{t+1}; \theta) = c_t(x_t, u_t; \theta) + f(x_t, u_t; \theta)' \lambda_{t+1}
\]

with \( t = 0, 1, \cdots, T - 1 \). Here \( \lambda_{t+1} \) is called the costate for the optimal control system. According to the Pontryagin’s Maximum Principle (PMP) (Pontryagin, 2018), the system’s optimal trajectory \( \xi_\theta = \{x^0_{0:T}, u^0_{0:T-1}\} \) in (2) must satisfy the following optimality conditions

\[
x^t_{t+1} = f(x^t_t, u^t_t; \theta),
\]

\[
\lambda^t_\theta = \frac{\partial H}{\partial x^t_t} = \frac{\partial c_t}{\partial x^t_t} + \frac{\partial f'}{\partial x^t_t} \lambda_{t+1},
\]

\[
0 = \frac{\partial H}{\partial u^t_t} = \frac{\partial c_t}{\partial u^t_t} + \frac{\partial f'}{\partial u^t_t} \lambda_{t+1}
\]

for \( t = 0, 1, \cdots, T - 1 \), and

\[
\lambda^T_\theta = \frac{\partial h}{\partial x^T_T}.
\]

for \( t = T \). Here, \( \lambda^t_{0:T} \) are the costate trajectory associated with the optimal trajectory \( \xi_\theta = \{x^0_{0:T}, u^0_{0:T-1}\} \). For notation simplicity, we above use \( \frac{\partial g}{\partial x_t} \) to denote the derivative of any differentiable function \( g(x) \) with respect to \( x \) and evaluated at \( x_t \), that is, \( \frac{\partial g}{\partial x_t} = \frac{\partial g}{\partial x} |_{x=x_t} \), and \((\cdot)'\) to denote the matrix transpose operation.

In order to achieve the gradient \( \frac{\partial L}{\partial \theta} \), we differentiate the above PMP equations (13)-(16) on both sides with respect to the parameter \( \theta \), respectively. This leads to the following differential Pontryagin’s Maximum Principle (or differential PMP for short)

\[
\frac{\partial x^t_{t+1}}{\partial \theta} = F_t \frac{\partial x^t_t}{\partial \theta} + G_t \frac{\partial u^t_t}{\partial \theta} + E_t,
\]

\[
\frac{\partial \lambda^t_\theta}{\partial \theta} = H^T_t \frac{\partial x^t_t}{\partial \theta} + H^{uu}_t \frac{\partial u^t_t}{\partial \theta} + F_t \frac{\partial \lambda^t_{t+1}}{\partial \theta} + H^c_t,
\]

\[
0 = H^{uu}_t \frac{\partial x^t_t}{\partial \theta} + H^{uu}_t \frac{\partial u^t_t}{\partial \theta} + G_t \frac{\partial \lambda^t_{t+1}}{\partial \theta} + H^c_t
\]

for \( t = 0, 2, \cdots, T - 1 \), and

\[
\frac{\partial \lambda^T_\theta}{\partial \theta} = H^T_T \frac{\partial x^T_T}{\partial \theta} + H^c_T.
\]
We next show how to efficiently solve them. Thus one can use the auxiliary control system where we view \( \bar{\lambda} \) as the new 'state', \( \bar{u}_t \) as the new 'control inputs', and \( \bar{x}_t \) as the new 'costate' at time step \( t \). Then one can construct the following auxiliary control system denoted by \( \Sigma(\xi_\theta) \),

\[
\Sigma(\xi_\theta): \quad \text{dynamics: } \bar{x}_{t+1} = F_t \bar{x}_t + G_t \bar{u}_t + E_t \quad \text{with} \quad \bar{x}_0 = 0,
\]

\[
\bar{J} = \sum_{t=0}^{T-1} \left[ \frac{1}{2} \begin{bmatrix} \bar{x}_t^T & \bar{u}_t & \bar{\lambda}_t \end{bmatrix}^T \begin{bmatrix} H_{tx} & H_{tu} & H_{t\bar{\lambda}} \\ H_{ux} & H_{uu} & H_{u\bar{\lambda}} \\ H_{\bar{\lambda}x} & H_{\bar{\lambda}u} & H_{\bar{\lambda}\bar{\lambda}} \end{bmatrix} \begin{bmatrix} \bar{x}_t \\ \bar{u}_t \\ \bar{\lambda}_t \end{bmatrix} \right] + \frac{1}{2} \bar{x}_T^T H_{xx} \bar{x}_T + H_{xc} \bar{x}_T.
\]

Note right away that \( \Sigma(\xi_\theta) \) is of the linear quadratic regular (LQR) form; that is, its system dynamical model is linear and the control objective function is quadratic. Moreover, the system dynamics and control objective in \( \Sigma(\xi_\theta) \) are time-variant and determined by the data of the trajectory \( \xi_\theta = \{ x_{0:T}, u_{0:T-1} \} \) of \( \Sigma(\theta) \), which is obtained in the forward pass. Let \( \{ \bar{x}_{0:T}, \bar{u}_{0:T-1} \} \) denote a stationary solution to the auxiliary control system \( \Sigma(\xi_\theta) \), that is, \( \{ \bar{x}_{0:T}, \bar{u}_{0:T-1} \} \) satisfies the first-order optimality conditions of the constrained optimization in \( \Sigma(\xi_\theta) \). Since the PMP of \( \Sigma(\xi_\theta) \) is exactly (17)-(20), then

\[
\left\{ \frac{\partial x_{0:T}}{\partial \theta}, \frac{\partial u_{0:T-1}}{\partial \theta} \right\} = \frac{\partial \xi_\theta}{\partial \theta}.
\]

Thus one can use the auxiliary control system \( \Sigma(\xi_\theta) \) to achieve the gradient quantities \( \frac{\partial \xi_\theta}{\partial \theta} \) in the backward pass of the learning, as shown in Fig. 2. In recognition that \( \Sigma(\xi_\theta) \) is of LQR form, the following lemma
provides a recursive method to solve for \( \{ \tilde{x}_{0:T}, \tilde{u}_{0:T-1}^\theta \} \), which is motivated by the Riccati recursion in optimal control theory (Liberzon, 2011).

**Lemma 4.1.** If \( H_t^{uu} \) defined in (22) is invertible, i.e., \( \det H_t^{uu} \neq 0 \), for all \( t = 0, 2, \ldots, T - 1 \), define the following recursions for \( t = T - 1, \ldots, 1 \):

\[
P_t = Q_t + A_t'(I + P_{t+1}R_t)^{-1}P_{t+1}A_t, \tag{28}
\]

\[
p_t = A_t'(I + P_{t+1}R_t)^{-1}(p_{t+1} + P_{t+1}r_t) + q_t. \tag{29}
\]

with \( P_T = H_T^{xx} \) and \( p_T = H_T^{xe} \). Here, \( A_t = F_t - G_t(H_t^{uu})^{-1}H_t^{xe} \), \( R_t = G_t(H_t^{uu})^{-1}G_t' \), \( Q_t = H_t^{xx} - H_t^{xe}(H_t^{uu})^{-1}H_t^{xe} \), \( r_t = E_t - G_t(H_t^{uu})^{-1}H_t^{xe} \), \( q_t = H_t^{xe} - H_t^{xe}(H_t^{uu})^{-1}H_t^{ue} \), and all the other matrices are defined in (21-23). Then, the stationary solution \( \{ \tilde{x}_{0:T}^\theta, \tilde{u}_{0:T-1}^\theta \} \) to the auxiliary control system \( \Sigma(\xi_\theta) \) in (26) can be obtained by iteratively solving following equations from \( t = 0 \) to \( t = T \) with \( \tilde{x}_0 = 0 \):

\[
\tilde{u}_t^\theta = -(H_t^{uu})^{-1}(H_t^{ux}\tilde{x}_t + H_t^{ue})
- (H_t^{uu})^{-1}G_t'(I + P_{t+1}R_t)^{-1}(P_{t+1}A_t\tilde{x}_t^\theta + P_{t+1}r_t + p_{t+1}), \tag{31}
\]

\[
\tilde{x}_{t+1}^\theta = F_t\tilde{x}_t^\theta + G_t\tilde{u}_t^\theta + E_t. \tag{32}
\]

Lemma 4.1 states that the stationary solution \( \{ \tilde{x}_{0:T}^\theta, \tilde{u}_{0:T-1}^\theta \} \) to the auxiliary control system \( \Sigma(\xi_\theta) \) can be solved in two steps: first, calculate matrices \( P_t \) and \( p_t \) via the recursions backward in time; and second, obtain \( \frac{\partial \xi_\theta}{\partial \theta} \) by iteratively solving (31) and (32) forward in time.

## 5 Algorithms for Different Learning Modes

Based on the previous developed techniques, we next show how to adapt the end-to-end PDP framework in Fig. 2 to different learning modes formulated in Section 2. For each learning mode, we focus on how to establish the auxiliary control system \( \Sigma(\xi_\theta) \) corresponding to the parameterized control system \( \Sigma(\theta) \).

### 5.1 Learning Mode 1: Inverse Optimization

Problems of inverse optimization consider a parameterized control system \( \Sigma(\theta) \) in (1) and loss function in (5). Under the PDP framework in Fig. 2, we set \( \Sigma(\xi_\theta) \) by (26). The algorithm is summarized in Algorithm 1.

**Algorithm 1:** End-to-end inverse optimization

**Input:** learning rate \( \{ \eta_k \}_{k=0,1,\ldots} \); observed dataset \( \{ \xi^o \} \)

**Initialization:** \( \theta_0 \)

for \( k = 0, 1, 2, \ldots \) do

- Obtain \( \xi_{\theta_k} \) from the system \( \Sigma(\theta_k) \) in (1) (using optimal control solvers or Learning Mode 2);
- Obtain \( \frac{\partial \xi}{\partial \theta} \big|_{\theta=\theta_k} \) from the auxiliary control system \( \Sigma(\xi_{\theta_k}) \) in (26) (using Lemma 4.1);
- Obtain \( \frac{\partial L}{\partial \xi} \big|_{\xi=\xi_{\theta_k}} \) from the given loss function in (5);
- Apply the chain rule (11) to obtain \( \frac{\partial L}{\partial \theta} \big|_{\theta=\theta_k} \);

\[
\theta_{k+1} = \theta_k - \eta_k \frac{\partial L}{\partial \theta} \big|_{\theta=\theta_k};
\]

end
5.2 Learning Mode 2: System Identification

Problems of system identification consider the parameterized control system \( \Sigma(\theta) \) in (6) and loss function in (7). Under the PDP framework in Fig. 2, we set up the auxiliary control system \( \Sigma(\xi_\theta) \) by only considering the first equation (17) in the differential PMP while letting \( \frac{\partial u^\theta_t}{\partial \theta} = 0 \). This is because first, \( \Sigma(\theta) \) in (6) is resulted from letting \( J \) be a constant, the other equations (18-20) of the differential PMP are thus trivialized; and second, \( \frac{\partial u^\theta_t}{\partial \theta} = 0 \) due to external inputs \( u_{0:T-1} \). Thus, the auxiliary control system \( \Sigma(\xi_\theta) \) corresponding to \( \Sigma(\theta) \) in (6) is

\[
\Sigma(\xi_\theta): \text{ dynamical model: } \bar{x}^\theta_{t+1} = F_t \bar{x}^\theta_t + E_t \quad \text{ with } \bar{x}_0 = 0. 
\]

By iteratively solving the above auxiliary control system \( \Sigma(\xi_\theta) \) from \( t = 0 \) to \( t = T \), one can obtain the resulting trajectory \( \bar{x}^\theta_{0:T} \), which is exactly \( \frac{\partial \xi_\theta}{\partial \theta} \). In summary, the algorithm for system identification is presented by Algorithm 2.

Algorithm 2: End-to-end system identification

Input: learning rate \( \{\eta_k\}_{k=0,1,\ldots} \), observe data \( \xi^o \) under inputs \( u_{0:T-1} \)

Initialization: \( \theta_0 \)

for \( k = 0, 1, 2, \ldots \) do

Obtain \( \xi_{\theta_k} \) by iteratively solving \( \Sigma(\theta_k) \) in (6) given inputs \( u_t \) for \( t = 0, \ldots, T \);

Obtain \( \frac{\partial u_{\theta_k}}{\partial \theta} \) by iteratively solving the auxiliary control system \( \Sigma(\xi_{\theta_k}) \) in (33) for \( t = 0, \ldots, T \);

Obtain \( \frac{\partial L}{\partial \xi} |_{\xi = \xi_{\theta_k}} \) from the given loss function in (7);

Apply the chain rule (11) to obtain \( \frac{dL}{d\theta} |_{\theta = \theta_k} \);

\( \theta_{k+1} = \theta_k - \eta_k \frac{dL}{d\theta} |_{\theta = \theta_k} \);

end

5.3 Learning Mode 3: Control and Planning

The type of control and planning problems considers the parameterized control system \( \Sigma(\theta) \) in (8) with the loss function in (9). Under the PDP framework in Fig. 2, the auxiliary control system \( \Sigma(\xi_\theta) \) is set by only using the first equation (17) in the differential PMP, as the other equations are trivialized. Since the inputs are now parameterized using a control input function \( u_t = u(t, \theta) \), the quantity \( \bar{u}^\theta_t = \frac{\partial u_t}{\partial \theta} \) in (17) is given by \( \frac{\partial u(t, \theta)}{\partial \theta} \). Thus, the auxiliary control system \( \Sigma(\xi_\theta) \) corresponding to \( \Sigma(\theta) \) in (8) is

\[
\Sigma(\xi_\theta): \text{ dynamical model: } \bar{x}^\theta_{t+1} = F_t \bar{x}^\theta_t + G_t \bar{u}^\theta_t \quad \text{ with } \bar{x}_0 = 0, \quad \text{control inputs: } \bar{u}^\theta_t = \frac{\partial u(t, \theta)}{\partial \theta}. 
\]

By iteratively solving the above auxiliary control system \( \Sigma(\xi_\theta) \) from \( t = 0 \) to \( t = T \), one can obtain the trajectory

\[
\{\bar{x}^\theta_{0:T}, \bar{u}^\theta_{0:T-1}\} = \left( \frac{\partial x^\theta_{0:T}}{\partial \theta}, \frac{\partial u^\theta_{0:T-1}}{\partial \theta} \right) = \frac{\partial \xi_\theta}{\partial \theta}. 
\]
In summary, the overall algorithm for learning and control is presented by Algorithm 3.

**Algorithm 3: End-to-end control and planning**

**Input:** $x_0$ and learning rate $\{\eta_k\}_{k=0,1,\ldots}$

**Initialization:** $\theta_0$

for $k = 0, 1, 2, \ldots$ do

- Obtain $\xi_{\theta_k}$ by iteratively solving $\Sigma(\theta_k)$ in (8) for $t = 0, \ldots, T$;
- Obtain $\frac{\partial L}{\partial \xi}|_{\xi = \xi_{\theta_k}}$ by iteratively solving the auxiliary control system $\Sigma(\xi_{\theta_k})$ in (34) for $t = 0, \ldots, T$;
- Obtain $\frac{\partial L}{\partial \xi}|_{\xi = \xi_{\theta_k}}$ from the given loss function in (9);
- Apply the chain rule (11) to obtain $\frac{dL}{d\theta}|_{\theta = \theta_k}$;

$\theta_{k+1} = \theta_k - \eta_k \frac{dL}{d\theta}|_{\theta = \theta_k}$;

end

5.4 Combining Different Learning Modes

In addition to using different learning modes to solve different types of learning tasks, one can combine different modes in a single learning task. For example, when solving reinforcement learning problems, one can call Learning Mode 2 to first learn a dynamical model, then integrate the learned model in Learning Mode 3 for obtaining the optimal control inputs. In inverse problems such as inverse optimal control and inverse reinforcement learning, one can first learn a dynamical model using Learning Mode 2, then use such learned model as the initial guess to Learning Mode 1. Besides, in the forward pass of Learning Mode 1, one can call Learning Mode 3 to solve optimal control problems. When solving control/planning problems, one can use a loss function that is learned by Learning Mode 1. Another application is the MPC-based reinforcement learning. In such case, one can combine Learning Mode 1 and Learning Mode 2 to learn a MPC controller, and then execute the learned MPC controller by calling Learning Mode 3.

6 Experiments

In this section, we conduct the experiments to validate capability of the proposed PDP framework under different learning modes. In Learning Mode 1, we show the efficiency of the proposed PDP framework in solving imitation learning problems in the context of LQR and pendulum systems, respectively. In Learning Mode 2, we apply the framework to identify the unknown parameters of a pendulum model. In Learning Mode 3, we demonstrate the capability of the PDP framework to achieve the optimal control solution to a pendulum wing-up control system.

We have openly released all codes of the proposed techniques in this paper, including the optimal control solvers. The codes are implemented in both Python and MATLAB. Please access at: https://github.com/wanxinjin.

6.1 Learning Mode 1: Imitation Learning

We apply Learning Mode 1 of the PDP framework to solve the problems of imitation learning. We use the parameterized optimal control system $\Sigma(\theta)$ in (1) to represent both an expert and a learner, while the parameter of the expert, denoted as $\theta^*$, is unknown to the learner. The learner has only access to the trajectories/demonstrations $\xi_o = \xi_{\theta^*}$ of the expert. The goal is to train the learner to search for its own parameter $\theta$ such that its final trajectory can mimics the expert’s demonstrations. The loss function is defined in (5) (here $l = \|\xi_\theta - \xi_o\|_2^2$), and we allow the expert’s demonstrations have different initial states $x_0$.
or horizons $T$. To facilitate analysis of results, we also introduce the index

$$e_\theta = \|\theta - \theta^*\|^2$$

(36)
to quantify the difference between the learned parameter and ground truth.

**LQR systems:** We first consider LQR systems. Both the expert and learner are represented by LQR systems. The dynamics is $f(x_t, u_t) = Ax_t + Bu_t$, and the control objective is defined by running cost $c(x, u) = x'Qx + u'Ru$ and final cost $h(x_T) = x_T'Q_f x_T$. The learner and expert share all information of the LQR system except for the parameter $	heta = \{A, R\}$. The expert has a nominal parameter $\theta^* = \{\text{ones}(2), 1\}$, which is unknown to the learner. The shared information is $B = [2, 1]'$, and $Q = Q_f = I_2$ ($2 \times 2$ identity).

We let the expert generate a batch of trajectories $\xi_o$ with different horizons $T$ and $x_0$. Here we collect eight expert trajectories, based on which we train the learner by minimizing the loss in (5) with respect to $\theta = \{A, R\}$. In Algorithm 1, we set the learning rate $\eta_0 = 10^{-3}$ with a decay rate 0.99. We set up six trials with random initial guesses $\theta_0$, and for each trial the learning results versus iteration are plotted in Fig. 3.

From Fig. 3a, we see that given random initial guess, the imitation loss is diminishing quickly and converges to zeros, indicating successful imitation. Fig. 3b shows that the parameter of the learner converges to that of the expert.

**Pendulum systems:** In this case, we solve imitation learning using pendulum systems. The pendulum dynamics is

$$\dot{\alpha} = -\frac{g}{l} \sin(\alpha) + \frac{d}{ml^2} \dot{\alpha} + \frac{1}{ml^2} \tau,$$

(37)
where $\alpha$ is the angle between the pendulum and direction of gravity ($g$ is the gravity constant); $m$ and $l$ are its mass and length, respectively; $\tau$ is the torque input applied at the pivot, and $d$ is the damping coefficient. In the pendulum model, we define its state $x = [\alpha, \dot{\alpha}]'$, input $u = \tau$, and discretize the continuous model (37) with time interval $\Delta = 0.05s$, i.e., $x_{t+1} = x_t + \Delta f(x_t, u_t)$. Let $\Sigma(\theta)$ in (1) denote the pendulum optimal control system, where

$$c(x, u) = \omega_1 (\alpha - \pi)^2 + \omega_2 \dot{\alpha}^2 + \tau^2 \quad \text{and} \quad h(x) = (\alpha - \pi)^2 + \dot{\alpha}^2$$

(38)
are the running and final costs in the control objective $J$, respectively. The parameter $\theta$ in $\Sigma(\theta)$ is

$$\theta = [m, l, d, w_1, w_2]'$$

(39)
where $m, l$, and $d$ are the parameters in the pendulum dynamics, and $w_1, w_2$ are parameters in the control objective.
Suppose that an expert has \( \theta^* = [2, 1, 0.5, 3, 1]' \), and the expert generates eight trajectories \( \xi^o \) with different horizons \( T \) and initial states \( x_0 \). Given these expert trajectories, we train the learner by minimizing the loss in (5). We set the learning rate \( \eta_0 = 10^{-3} \) with a decay rate 0.99 in Algorithm 1, and perform six trials with random initial guesses \( \theta_0 \). For each trial the learning results versus iteration are plotted in Fig. 4. As shown by Fig. 4a, the imitation loss in (5) decreases towards zero. Fig. 4b shows that the learner’s parameter, from different initial guess, all converge to \( \theta^* \).

Comparisons: In the context of pendulum imitation learning, we compare the proposed technique with the differentiable MPC method (Amos et al., 2018) in terms of running efficiency. Comparison results are presented in Fig. 5. The results indicate that the proposed PDP technique is faster than the differentiable MPC in both forward and backward passes. Such running efficiency is attributed to two factors: first, contrary to the differentiable MPC using iLQR approximation, the PDP technique solve both the forward and backward passes directly; and second, due to the control establishment in backward pass, the PDP framework solves the gradient quantities using recursions in Lemma 4.1, which is in contrast to solving a high-dimensional linear equation in the differentiable MPC.

Figure 5: Runtime (per iteration) comparison between the proposed PDP and differentiable MPC (Amos et al., 2018) for different time horizons in pendulum optimal control system. Note that y-axis is log-scale, and the runtime is averaged over 100 iterations. Both methods are implemented in Python and run on the same machine using only CPUs.

### 6.2 Learning Mode 2: System Identification

Here we use Learning Mode 2 of the proposed PDP framework to learn system dynamical models. The experiment is still in the context of pendulum systems. Suppose that there is a real pendulum whose model structure in (37) is available to the designer (e.g., obtained from principles of physics) except for its parameter \( \theta^* = [m, l, d]' = [1, 1, 0.1]' \). We use the proposed PDP framework to identify the unknown parameter.
First, we collect $x_{0:T}$ from the real system by providing random inputs $u_{0:T-1}$. We perform this for eight times which leads to eight datasets. Given such data, we apply Algorithm 2 to learn the parameterized dynamical model by minimizing the loss in (7) (here $l = \|\xi_\theta - \xi^n\|^2$). Here the learning rate is set by $\eta_0 = 10^{-3}$ with a decay rate 0.99. We set up six trials with random initial guesses $\theta_0$, and for each trial the results versus iteration are plotted in Fig. 6. We also use the index defined in (36) to show the convergence of learned $\theta$ to the ground truth $\theta^*$.

As shown in Fig. 6a, given random initial guess $\theta_0$, the identification loss (defined in (7)) decreases quickly and finally diminishes to (near) zero, indicating that the learned model successfully simulates the data of the real system. Fig. 6b shows that $e_\theta$ quickly converges to zero, thus the parameter $\theta^*$ of the real system is successfully identified.

### 6.3 Learning Mode 3: Optimal Control

In this part, we apply Learning Mode 3 of the PDP framework to perform optimal control to the above pendulum system learned by Learning Mode 2 in the previous part. We first define the loss function in (9), which is the control objective (another way to specify the objective function is via imitation learning using Learning Mode 1). Suppose that our goal is to control the pendulum from initial state $x_0 = [0, 0]'$ to the swing-up state $x_{goal} = [\pi, 0]'$ with time horizon $T = 20$ (1s). We thus specify the loss function in (9) to be

$$L = \sum_{t=0}^{T-1} (\|x_t - x_{goal}\|^2 + 0.01u_t^2) + \|x_T - x_{goal}\|^2. \quad (40)$$

Next, we choose a parameterized input function $u(t, \theta)$. Motivated by the collocation methods (Elnagar et al., 1995; Patterson and Rao, 2014), we choose the $K$-degree Lagrange polynomial (Abramowitz and Stegun, 1948) with $K + 1$ collocation points evenly populated over the time horizon, that is

$$\text{collocation points: } \{(t_0, u_0), (t_1, u_1), \ldots, (t_K, u_K)\}, \quad (41)$$

where $t_m = mT/K$, $m = 0, 1, \ldots, K$. The parameterized control inputs thus are

$$u(t) = \sum_{j=0}^{K} u_j b_j(t), \quad \text{with } b_j(t) = \prod_{0 \leq m \leq K, m \neq j} \frac{t - t_m}{t_j - t_m}. \quad (42)$$

Here, $b_j(t)$ is called Lagrange basis, and $\theta = [u_0, \ldots, u_K]'$.

We apply Algorithm 3 to minimize the control objective in (40) with respect to the parameter $\theta$. Here, we set the learning rate $\eta_0 = 10^{-3}$ with a decay rate 0.99, and the initial guess $\theta_0$ is given randomly. We use different degrees of the Lagrange polynomials, $K = 1, 2,$ and 3, and the corresponding results are presented in Fig. 7a. For reference, we also plot the optimal loss given by an optimal control solver. The results in 7a shows that by parameterizing the control input $u(t, \theta)$ using Lagrange polynomials of different degrees, each
case can converge to a loss that is very near to the optimal loss. We notice that among the three polynomial parameterizations, the polynomial of degree 3 achieves a loss closest to the optimal loss. This makes sense because it has the highest representation capability compared to the other two (however, degree polynomial may lead to over parameterization).

Having the learned parameter $\theta^*$, we plot the corresponding control inputs $u(t, \theta^*)$ in Fig. 7b. For reference, we also show the optimal control inputs given by an optimal control solver. We note that $u(t, \theta^*)$ with the polynomial of degree 3 is almost the same with optimal control inputs of ground truth (i.e., obtained from optimal control solver). This demonstrates the validity of the proposed PDP technique in solving optimal control problems.

7 Conclusions and Future Work

This paper develops a Pontryagin differentiable programming (PDP) methodology which establishes an unified end-to-end framework to solve a general class of learning tasks. This is achieved by two proposed techniques: one is the differential Pontryagin’s Maximum Principle, which allows for an end-to-end learning of any components in a control system; and the other is the integration of control establishment in the learning, where the differentiation in backward pass thus is efficiently solved by techniques in control domain. Under this PDP framework, three learning modes are investigated to address three types of learning tasks: inverse problems, system identification, and control/planning, respectively.

We emphasize utility of the PDP framework, where the proposed three learning modes can be used as building blocks for more complex learning tasks. For example, in human-machine systems, inverse optimization (Learning Mode 1) and planning (Learning Mode 2) are usually involved. In model predictive control, inverse optimization (Learning Mode 1) can be used to design the MPC controller, and its execution can be conducted using Learning Mode 3. We leave the explorations and extensions of the PDP framework in our future work. Also, we will explore convergence properties of the PDP methodology in the future work.

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Appendix

A Proof of Lemma 4.1

We substitute the following notations $\bar{x}_t^\theta = \frac{\partial x_t^\theta}{\partial \theta}$, $\bar{u}_t^\theta = \frac{\partial u_t^\theta}{\partial \theta}$, $\bar{\lambda}_t^\theta = \frac{\partial \lambda_t^\theta}{\partial \theta}$ into the differential PMP equations (17)-(20), where $\bar{\lambda}_{1:T}^\theta$ is the costates associated with the optimal trajectory $\{\bar{x}_t^\theta, \bar{u}_t^\theta\}$ resulting from solving the optimal control system $\Sigma(\xi^\theta)$ in (26). From (19), we solve $\bar{u}_t^\theta$ as

$$
\bar{u}_t^\theta = -(H_i^{uu})^{-1}(H_i^{ux} \bar{x}_t^\theta + G_i' \bar{\lambda}_t^\theta + 1 + H_i^{ue})
$$

(43)

By substituting (43) into (17) and (18) and also considering the definitions in (30), we have

$$
\bar{x}_{t+1}^\theta = A_t \bar{x}_t^\theta - R_t \bar{\lambda}_{t+1}^\theta + r_t
$$

(44)

$$
\bar{\lambda}_t^\theta = Q_t \bar{x}_t^\theta + A'_t \bar{\lambda}_{t+1}^\theta + q_t
$$

(45)

for $t = 0, 1, \ldots, T - 1$ and

$$
\bar{\lambda}_T^\theta = H_T^{xx} \bar{x}_T^\theta + H_T^{xe}.
$$

(46)

for $t = T$. Next, we will prove that there exists matrices $P_t$ and $p_t$ such that

$$
\bar{\lambda}_t^\theta = P_t \bar{x}_t^\theta + p_t.
$$

(47)

Proof by induction: (46) shows that (47) holds for $t = T$ with $P_T = H_T^{xx}$ and $p_T = H_T^{xe}$. Assume (47) holds for $t + 1$, thus by manipulating (44) and (45), we have

$$
\bar{\lambda}_t^\theta = \left( Q_t + A'_t (I + P_{t+1} R_t)^{-1} P_{t+1} A_t \right) \bar{x}_t^\theta + A'_t (I + P_{t+1} R_t)^{-1} (p_{t+1} + P_{t+1} r_t) + q_t
$$

(48)

which indicates that (47) holds for $t$. Substituting (47) into (44) and also considering (43) will lead to (31). (32) are directly resulted from (17). We complete the proof.