

DPhil: Thesis

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1 Introduction

The Euler-Lagrange formulation equates to:

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q}$$

where:

$$L = T - U$$

In the example of a pendulum:

$$T = 1/2mv^2 = 1/2m(l\dot{\theta})^2 = 1/2ml^2\dot{\theta}^2$$

$$U = mgh = mgl(1 - \cos \theta)$$

$$L = 1/2ml^2\dot{\theta}^2 - mgl(1 - \cos \theta)$$

Placing the above into the euler-lagrange form gives us:

LHS:

$$\frac{\partial L}{\partial \dot{q}} = ml^2 \dot{\theta}$$

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}} \right) = ml^2 \ddot{\theta}$$

RHS:

$$\frac{\partial L}{\partial q} = -mgl \sin \theta$$

Therefore:

$$\ddot{\theta} = \frac{g}{l} \sin \theta$$

Now, to transition to the Hamiltonian version:

We can write the hamiltonian as the sum of the energies:

$$H = T + U$$

$$H = p^2/2m + U$$

$$H = -L + 2K$$

$$H = -L + mv^2$$

$$H = -L + p^2/m = -L + p * (m\dot{q})/m = -L + p\dot{q}$$

$$p = \frac{\partial L}{\partial \dot{q}}$$

2 Literature Review

2.1 Artificial Intelligence

- Humans have long tried to understand how the mind works - from a biological perspective it is clear that connectomics paves a pathway to understanding how we think - With the advent of computers and 'large' processing power, many researchers began to ask whether the human mind can be replicated using a computer. - Early work by walter and warren was the first to point out a means to build neural network logic. - Followed by Hebbian - Then an AI winter - Geof Hinton backprop - slew of advents in neural processing, convnets, rnns, graphs, tensor nets, deep RL, - all seeking to solve more tasks/increase generalizability.

- to date, there has been no general purpose solution (AGI) for a vast array of tasks e.g. a human can learn to create art, sit math exams, play sports, yet a robot so far can only do one of these tasks well. - Numerous limitations in terms of processing power and memory access still exist

- Despite these limitations, neural networks have brought about significant advancements to society in robotics, self driving cars, cancer detection.

- In what follows, we outline some of the major advances, those which have been fundamental pillars to research conducted during this phd. We follow no particular order.

2.2 Inductive Biases

An inductive bias in machine learning is prior information used to guide model building. In simple linear regression, for example, we assume the distribution of the noise in our data follows a Gaussian. This is a natural inductive bias because prior to seeing any data, we have assumed our noise model follows this form. In neural networks, architectures with variable depth, form and activations for example, serve as inductive biases. In essence, we encode initial assumptions about the complexity of data via inductive biases.

A feedforward deep neural network naturally encodes 'nonlinearity' as a prior and arguably makes the least assumptions about the underlying data. Convolutional Neural Networks assume spatial representations can be captured. Recurrent Neural Networks assume temporal data as inputs.

In what follows, we highlight some of the recent advances in inductive biases, particularly as they relate to solving problems in physics.

2.3 Graph Neural Networks

Graph Neural Networks are neural networks which use graphs as inputs. As such, they can be used to understand and learn the relationships which exist between the nodes of a graph. More formally, a graph is a tuple (Vertices, Edges, Globals). These are attributes of the graph where the nodes contain information, edges contain relationship weights and globals consist of macro variables general to all graphs.

interaction-physics based problems naturally benefit from graphs. We see that HOGNs and OGNs achieve great results in rolling out trajectories of N body systems.

Although they account for a new set of relational inductive biases, graphs still involve complex message passing schemes that involve significant fine-tuning. In addition, they assume data streams are already structured. However, graphs have shown significant promise in physics e.g. in explaining the phase transition of glassy materials. Their use in physics opens up a tried-and-tested pathway to solve more complex problems particularly in accounting for material interactions.

They're even shown to model complex fluid like systems from visual data.

Most systems to date have looked at graphs for classical physics but literature from 2004 suggests graphs, inherent in their relational structure, can also capture Ising-like hamiltonian structure.

2.4 Symplectic Biases

Symplecticity refers to the concept of volume-preservation. Riemannian** Core to our beliefs in physical systems is the notion of energy conservation, indirectly accounted for by symplecticity.

2.5 Integrative Biases

- ODEnet - new paper by tegmark

2.6 Physics priors

- tegmark paper - ai feynman - models trying to learn diffeqs -

A brief look at residual nets illustrates that these iterative methods look like euler discretization steps. Adding more layers and taking smaller steps can result in a parametrization of a continuous dynamics:

$$\frac{dh}{dt} = f(h(t), t, \theta)$$

Essentially the neural network hidden layers contain the components of the differential equation. The input layer $h(0)$ gives us an IVP which we can evolve to time T . But this is a 'continuous-depth' network and we need a way to backprop. The method to backprop is *adjoint sensitivity method* which computes gradients by solving a second, augmented ODE back in time.

Neural networks have shown remarkable success at solving an array of problems in vision, robotics and healthcare. However, these networks still struggle to learn the basic laws of physics. [?] show that we can take a physical system (i.e. position and momentum values or images of a moving pendulum) and map it to a latent space which can encode the dynamics of the system. One way to learn these dynamics is to train the network to learn a latent space which is equivalent to the rate of change of momentum/position. However, [?] show that using this simple approach is not enough in being able to accurately predict energy conserving phase space trajectories. Instead, they show that if we treat the latent space as a vector field (symplectic gradient) or as a parametric function for the hamiltonian then we can differentiate it with respect to the input (p and q) and obtain energy conservation laws. In this way, the neural network is parametrized to encode the hamiltonian of the system.

An alternative approach to this method is that of variational integrator networks proposed by [?]. Inspired by neural-ODE's, they propose a neural net whose architecture matches the discrete equation of motion governing the dynamical system. Essentially, the embedding learned by the network is a dynamical system itself. They use a variational integration discretization - this method

only introduces 3rd order errors w.r.t energy and closely resembles the continuous time dynamics. The approach follows the neural ODE approach with two changes, the ODE we model is the Euler-Lagrange from free-form dynamical system. In addition the discretization is a VI.

3 related work reviews

4 Physics Priors

Broadly, the intersection of physics and AI falls into one of two domains, physics for AI or AI for physics. The former uses techniques from physics to develop and improve learning algorithms in general, for example xx. The latter uses existing learning approaches (with adaptations) to predict physics, for example ML for materials. In this review, we focus our attention on the latter.

Physicists have long been interested in using learning tools to predict physics based systems. Some of these include predicting magnetic properties of 2-D materials, predicting the time evolution of N-body systems and even using AI to understand phase transitions. However, numerous challenges still remain in terms of data-efficient learning, reducing computational cost, improving predictive accuracy and learning better representations of the underlying physical process. Researchers have identified methods to address these challenges, but arguably the most promising hinges on physics-informed priors embedded in learning. It has been shown that models enriched with physically-informed priors i.e. models which consist of some knowledge about the physical system apriori, significantly outperform traditional methods in terms of data-efficiency and predictive accuracy. This has sparked a sharp interest in building both task-specific and general physics priors to improve learning. In this section, we summarize some of the core developments over time in physics informed inductive biases.

4.1 gradient learning

The notion of embedding physically-informed inductive biases in neural networks can be found in numerous early work aimed at modelling materials [?, ?, ?, ?, ?]. For example, early efforts by Witkoskie and Doren [?] demonstrate that in contrast to directly learning a potential energy surface, the inclusion of gradient learning can drive a network to accurately model the forces. This addition means that we supplement the learning process with additional information and hence improve the learnt potential surface.

4.2 Hamiltonian Neural Networks

ing neural networks to accurately learn classical dynamics from data problems has been Hamiltonian Neural Networks [?]. In demonstrated that dynamic predictions through time can be improved using Hamiltonian Neural Networks

(HNNS) which endow models with a Hamiltonian constraint. The Hamiltonian is an important representation of a dynamical system because it is one of two approaches that generalizes classical mechanics. The Hamiltonian \mathcal{H} is a scalar function of position $\mathbf{q} = (q_1, q_2, \dots, q_M)$ and momentum $\mathbf{p} = (p_1, p_2, \dots, p_M)$. In representing physical systems with a Hamiltonian, one can simply extract the time derivatives of the inputs by differentiating the Hamiltonian with respect to its inputs (see Eqn. 1.)

$$\frac{d\mathbf{q}}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \quad (1)$$

As a consequence, it is noted in [?] that by accurately learning a Hamiltonian, the system's dynamics can be naturally extracted through backpropagation. This information allows us to build two 1st-order differential equations which can be used to update the state space, (\mathbf{q}, \mathbf{p}) . Equation 2 shows this integral, in which we define the symplectic gradient $\mathbf{S} = \left[\frac{\partial \mathcal{H}}{\partial \mathbf{p}}, -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \right]$:

$$(\mathbf{q}, \mathbf{p})_{t+1} = (\mathbf{q}, \mathbf{p})_t + \int_t^{t+1} \mathbf{S}(\mathbf{q}, \mathbf{p}) dt \quad (2)$$

It can be shown that the Hamiltonian in many systems also represents the total energy of the system. Therefore, the Hamiltonian is a powerful inductive bias that can be utilised to evolve a physical state while maintaining energy conservation.