TDHNN: Time-Dependent Hamiltonian Neural Networks

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Abstract

Deep networks embedded with physically-informed priors demonstrate remarkable results in accurately learning and predicting non-linear dynamical systems. In particular, networks designed to learn an energy constraint and exploit the Hamiltonian formalism show strong and consistent performance in learning autonomous dynamics that depend implicitly on time. Here, we extend this work to include an explicit time-dependence with the goal of providing a more general formalism to learn dynamical systems. We illustrate that the inclusion of time allows us increased flexibility at solving non-autonomous systems.

1 Introduction

Neural networks, as universal function approximators, have shown resounding success across a host of domains. However, their performance in learning physical systems has often been limited. Physicists, as a consequence, have not been encouraged by the initial excitement of machine learning. However, new research aimed at *scientific machine learning* - a branch that tackles science problems with domain-specific ML, is paving a way to address numerous challenges. One crucial method has been to incorporate prior theoretical information into the network, such as hamiltonian mechanics. This excitement has spurred others to work with lagrangians, ODEs and even graphs in order to tackle dyanamical systems. Despite their widespread adoption, a major bottleneck of many of the existing methods is the lack of an explicit time dependence. The most general form of Hamilton's equations, includes an explicit time dependence term. We show that the addition of this term, coupled with a few intuitive regularizations can induce networks to learn from both autonomous and non-autonomous settings. We extensively benchmark this addition across multiple datasets and consistently find the inclusion to be of benefit. Furthermore, we emphasise that the constraint is an easy plug-and-play addition to existing networks and illustrate how existing networks such as HNN, Symp ODEN and Hnets benefit from its inclusion.

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2 Background

2.1 Hamiltonian Neural Networks

Recently, [?] 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 $\mathbf{q} = (q_1, q_2, ..., q_M)$ and momentum $\mathbf{p} = (p_1, p_2, ..., p_M)$. 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.)

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}, \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \tag{1}$$

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 $\mathbf{S} = \left[\frac{\partial \mathcal{H}}{\partial \mathbf{p}}, -\frac{\partial \mathcal{H}}{\partial \mathbf{q}}\right]$:

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

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.

3 Method

The time-derivative of a Hamiltonian $\mathcal{H}(\mathbf{q}, \mathbf{p}, t)$ can be obtained using the chain rule:

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{q}}\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial H}{\partial \mathbf{p}}\frac{\partial \mathbf{p}}{\partial t} + \frac{\partial \mathcal{H}}{\partial t} \tag{3}$$

The underlying fact in energy preserving systems is that $H = E$ is a constant. As such, the time derivative should be set to zero. By learning the Hamiltonian and differentiating it with respect to $\mathbf{q}, \mathbf{p}$ we obtain the time derivatives of the state vectors which when replaced in the above equation yield:

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = -\frac{\partial \mathbf{p}}{\partial t}\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{q}}{\partial t}\frac{\partial \mathbf{p}}{\partial t} + \frac{\partial \mathcal{H}}{\partial t} = 0 \tag{4}$$

which leaves us with:

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial t} = 0 \tag{5}$$

To enforce this additional constraint in our networks, all we need to do is simply provide the time to the network, which extends the input dimension by 1, and allow the time component to be differentiable. We then compute the gradient and use an L1 penalty such that the final loss is:

$$\mathcal{L}_{EPNN} = \left\| \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{q}} + \frac{\partial \mathbf{p}}{\partial t} \right\| + \left\| \frac{\partial \mathcal{H}}{\partial \mathbf{p}} - \frac{\partial \mathbf{q}}{\partial t} \right\| + |\frac{\partial \mathcal{H}}{\partial t}| \tag{6}$$

4 FIRST LEVEL HEADINGS

First level headings are all caps, flush left, bold, and in point size 12. Use one line space before the first level heading and one-half line space after the first level heading.

4.1 Second Level Heading

Second level headings are initial caps, flush left, bold, and in point size 10. Use one line space before the second level heading and one-half line space after the second level heading.

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4.2 Citations, Figure, References

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All artwork must be centered, neat, clean, and legible. All lines should be very dark for purposes of reproduction, and art work should not be hand-drawn. Figures may appear at the top of a column, at the top of a page spanning multiple columns, inline within a column, or with text wrapped around them, but the figure number and caption always appear immediately below the figure. Leave 2 line spaces between the figure and the caption. The figure caption is initial caps and each figure should be numbered consecutively.

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Figure 1: Sample Figure Caption

[1] Sample of the first footnote.
[2] Sample of the second footnote.

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All tables must be centered, neat, clean, and legible. Do not use hand-drawn tables. Table number and title always appear above the table. See Table 1.

Use one line space before the table title, one line space after the table title, and one line space after the table. The table title must be initial caps and each table numbered consecutively.

Table 1: Sample Table Title

PART	DESCRIPTION
Dendrite	Input terminal
Axon	Output terminal
Soma	Cell body (contains cell nucleus)

5 SUPPLEMENTARY MATERIAL

If you need to include additional appendices during submission, you can include them in the supplementary material file. You can submit a single file of additional supplementary material which may be either a pdf file (such as proof details) or a zip file for other formats/more files (such as code or videos). Note that reviewers are under no obligation to examine your supplementary material. If you have only one supplementary pdf file, please upload it as is; otherwise gather everything to the single zip file.

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   ```

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5. Check that the content of your submission, *excluding* references, is limited to **8 pages**. The number of pages containing references alone is not limited.

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   of the authors of your paper, all
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3. The camera-ready versions of the accepted papers are 8 pages, plus any additional pages needed for references.

4. If you need to include additional appendices, you can include them in the supplementary material file.

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Acknowledgements

All acknowledgments go at the end of the paper, including thanks to reviewers who gave useful comments, to colleagues who contributed to the ideas, and to funding agencies and corporate sponsors that provided financial support. To preserve the anonymity, please include acknowledgments *only* in the camera-ready papers.

References

References follow the acknowledgements. Use an unnumbered third level heading for the references section. Please use the same font size for references as for the body of the paper—remember that references do not count against your page length total.

References

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