Symplectic Momentum Neural Networks - Using Discrete Variational Mechanics as a prior in Deep Learning

Saul Santos  
Monica Ekal  
Rodrigo Ventura

Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisbon  
Instituto de Sistemas e Robótica, Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisbon

Abstract

With deep learning being gaining attention from the research community for prediction and control of real physical systems, learning important representations is becoming now more than ever mandatory. It is of extremely importance that deep learning representations are coherent with physics. When learning from discrete data this can be guaranteed by including some sort of prior into the learning, however not all discretization priors preserve important structures from the physics. In this paper we introduce Symplectic Momentum Neural Networks (SyMo) as models from a discrete formulation of mechanics for non-separable mechanical systems. The combination of such formulation leads SyMos to be constrained towards preserving important geometric structures such as momentum and a symplectic form and learn from limited data. Furthermore, it allows to learn dynamics only from the poses as training data. We extend SyMos to include variational integrators within the learning framework by developing an implicit root-find layer which leads to End-to-End Symplectic Momentum Neural Networks (E2E-SyMo). Through experimental results, using the pendulum and cartpole we show that such combination not only allows these models to learn from limited data but also provides the models with the capability of preserving the symplectic form and show better long-term behaviour.

Keywords: Physics-Informed learning, Variational Integrators, Deep Learning, Discrete Mechanics

1. Introduction

Even though, Neural Networks have the ability to achieve astonishing results and being practically at the forefront of areas such as Computer Vision Krizhevsky et al. (2012) or natural language Collobert and Weston (2008), these black-box parametrizations still lack of intuition about physics. In fact, traditional deep learning techniques rely on a search and evaluate procedure through a broad spectrum of candidate hypotheses and are limited to the characteristics of the data. By enforcing physical intuition to such strong models, explicitly or implicitly, is thus possible to narrow the hypothesis space to a range where these models have the ability to reproduce physically consistent results.

The application of even the state-of-the-art black box models has very frequently met with limited success in scientific domains due to their large data requirements, inability to produce physically consistent results, and their lack of generalizability to out-of-sample scenarios Willard et al. (2020). By needing large amount of training data in order to generalize well to unseen states another problem comes up which is the fact that such data can be prohibitively expensive to obtain.
In this work we are interested in combining physical priors with deep learning techniques for mechanical system modeling. Further, we extend this combination to account for numerical integration. First by combining continuous variational principles with discretization schemes by Neural ODEs Chen et al. (2018) through conventional integrators. Secondly, the novelty resides on a family of geometric integrators called Variational Integrators that have the particularity of preserving geometric structures of the continuous system Marsden and West (2001), in opposition with traditional integrators. Variational Integrators have the property of being symplectic and preserve the momentum, or its change in the presence of external forces Johnson et al. (2015). Although symplectic-momentum integrators do not preserve energy exactly they exhibit bounded energy behavior achieving near energy conservation and thus they are extremely useful for long term simulations, such as for low thrust spacecraft missions Junge et al. (2005). Our contribution handles elegantly non-separable mechanical systems as we derive efficient back-propagation to grip with the implicit equations arising from the discrete variational principles.

Figure 1: Phase Space of the simulated models for the pendulum system alongside with the ground truth fields. Integration for 4000 time-steps with time-step $h = 0.1$. NODE consist in a Neural ODE learning directly the dynamics from data with Runge kutta 4th-order and midpoint as ODE solvers. L-NODE consist of using the Lagrangian dynamics of mechanical systems as a model prior with the same ODE solvers of NODEs. SyMo results in the combination of discrete mechanics with deep learning. E2E-SyMo accounts for variational integration through a root finding implicit layer. SyMos preserve the symplectic form while the other models drift away from the ground truth.

2. Related Work

Two recent developments were key to the developed approach. Firstly, in Raissi et al. (2017) use state-of-the-art deep learning techniques for solving Nonlinear Partial Differential Equations in a learning fashion with physical plausibility and good generalization properties. Secondly, Raissi (2018) extended his work not only to learn the solution but also to discover the nonlinear partial differential equation. This lead researchers to try to mimic these approaches into a several range of applications. Specifically, Lutter et al. (2019b) propose learning architectures that impose Lagrangian
mechanics in a structured approach. This methodology is optimized to minimize the violation of the Euler-Lagrange Ordinary Differential Equation (ODE) directly from data and further applied to energy-based control problems Lutter et al. (2019a). This work is generalized to include all forms of Lagrangians by Cranmer et al. (2020) and extended to Hamiltonian mechanics in Greydanus et al. (2019).

All the methods mentioned above assume continuous-time equations of motion for dynamical systems. These equations encode the underlying physical properties, such as symmetries corresponding to conservation laws. However, when learning from discrete data these continuous models need to be discretized. With this in mind researchers started not only to combine physical priors with deep learning but also with numerical integrators. In Chen et al. (2018) proposed Neural Ordinary Differential Equations, differentiable ode solvers with $O(1)$ memory backpropagation. This lead researchers to propose algorithms that combine methods with prior knowledge about the underlying equations of motion with geometric discretization schemes. Particularly in Zhong et al. (2020) authors proposed learning the dynamics of ordinary differential equation by combining Hamiltonian Mechanics with Neural ODEs and in Chen et al. (2020) where authors leverage symplectic integration with neural networks. In Saemundsson et al. (2020) authors combine variational integrators with deep learning techniques. However, this approach assumes only separable Hamiltonians (inertia matrix does not depend on the configuration). Our work is capable of handling implicit equations arising from non-separable mechanical systems cases.

3. Background

3.1. Continuous Lagrangian Dynamics

Any mechanical system can be represented by a set of generalized coordinates, $q \in \mathbb{R}^n$, that define completely the configuration of the mechanical model. The Lagrangian mechanics define the scalar Lagrangian, $\mathcal{L}$, as the difference between the kinetic energy, $T$, and the potential energy, $V$. For rigid bodies the kinetic energy takes the well-known quadratic form $T(q, \dot{q}) = \frac{1}{2} \dot{q}^T M(q) \dot{q}$:

$$\mathcal{L} = T(q, \dot{q}) - V(q) = \frac{1}{2} \dot{q}^T M(q) \dot{q} - V(q) \quad (1)$$

where $H \in \mathbb{R}^{n \times n}$ is called generalized inertia matrix Murray et al. (1994), and by nature is represented as a positive definite matrix.

In the forced case, one can extend the Hamiltonian principle to include non-conservative forcing such as external inputs or dissipative forces by using the Lagrange-d’Alembert principle Ober-Blöbaum et al. (2011) that seeks paths satisfying:

$$\delta \int_{t_0}^{t_f} \mathcal{L}(q, \dot{q}) \, dt + \int_{t_0}^{t_f} F(q, \dot{q}, u) \, \delta dt = 0 \quad (2)$$

where the second integrand is defined as the virtual work and $\delta$ represents variations vanishing at the endpoints. Requiring that the variations of the action be zero for all $\delta q$ and integrating (2) by parts we arrive at the forced Euler-Lagrange equations

$$\frac{d}{dt} \left( \frac{\partial \mathcal{L}(q, \dot{q})}{\partial \dot{q}} \right) - \frac{\partial \mathcal{L}(q, \dot{q})}{\partial q} = F(q, \dot{q}, u), \quad (3)$$
where $F$ is the forcing function that expresses the external forces in terms of generalized coordinates and $u$ are the input controls such as motor torques.

The forced discrete Euler-Lagrange equations define an implicit equation that can be transformed into an explicit equation by taking into account the Lagrangian (1). Therefore, the obtained model can be reformulated into the forward manipulator equation,

$$\ddot{q} = f^{(a)}(q, \dot{q}, u) = H^{-1}(q) \left( F(q, \dot{q}, u) - C(q, \dot{q}) + g(q) \right). \quad (4)$$

where $C \in \mathbb{R}^n$ is called the vector of coriolis and centrifugal forces while $g(q) = \frac{\partial V(q)}{\partial q} \in \mathbb{R}^n$ is the gravitational potential vector. Equation (4) can be used to obtain a trajectory $q(t)$ starting from an initial condition $x_{t_0} = [q(t_0), \dot{q}(t_0)]$ and actuation $u$, via numerical integration.

### 3.2. Discrete Lagrangian Mechanics

In an alternative approach of numerical integration one can instead discretize the action integral forcing the errors to respect the conservation of properties. This approach is called discrete mechanics and the corresponding numerical integrators variational integrators Marsden and West (2001).

Rather than having a configuration $q$ and velocity $\dot{q}$, in the context of discrete mechanics the trajectory of a continuous-time dynamical system is approximated by choosing a discrete Lagrangian, $L_d$, that discretizes the action integral along the exact solution curve segment, $q$, i.e. $q_k \approx q(t_k)$ and $q_{k+1} \approx q(t_k + h)$ Ober-Blöbaum et al. (2011):

$$L_d(q_k, q_{k+1}, h) \approx \int_{t_k}^{t_k+h} L(q(t), \dot{q}(t)) \, dt. \quad (5)$$

Similar to the continuous case the discrete approach can also be extended to accommodate external forces by approximating the continuous forces by a left, $f_d^-$ and right discrete force, $f_d^+$.

$$f_d^+(q_k, q_{k+1}, u_k).\delta q_{k+1} + f_d^-(q_k, q_{k+1}, u_k).\delta q_k \approx \int_{t_k}^{t_k+h} F(q(t), \dot{q}(t), u(t))\delta q \, dt \quad (6)$$

where $u_k$ is the discretization of the continuous force inputs, i.e. $u_k \approx u(t_k)$.

Analogous to the continuous case and performing the calculus of variations, we arrive to the discrete equivalent of equation (7) that is known by Forced Discrete Euler-Lagrange Equations (DEL):

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) + f_d^+(q_k, q_{k-1}, u_k) + f_d^-(q_{k-1}, q_k, u_{k-1}) = 0 \quad (7)$$

where the slot derivative $D_i$ represents the derivative of the discrete Lagrangian, $L$, with respect to the $i^{th}$ argument. Variational Integrators are a class of algorithms with the intu of solving the implicit DEL equation for $q_{k+1}$.

1. The left and right forces can be thought as the continuous control force acting during the time spans $[t_{k-1}, t_k]$ and $[t_k, t_{k+1}]$ Ober-Blöbaum et al. (2011).
4. Baselines

Geometric Neural Ordinary Differential Equation: The first challenge towards leveraging Neural ODEs to learn state-space models of mechanical systems is the fact that the dynamics arising from such dynamical systems are defined by a second order ordinary differential equation. However, the dynamics can, instead, be seen as a system of coupled first-order ODEs with state \( x = [q, \dot{q}]^T \) and parameters \( \theta \):

\[
\dot{x} = f^{(a)}(x, u; \theta) = \begin{bmatrix}
\dot{q} \\
\ddot{x}
\end{bmatrix}
\]

With actuation set to be constant between time-steps the final augmented state assumes the form of

\[
\begin{bmatrix}
\dot{x} \\
\dot{u}
\end{bmatrix} = f(x, u; \theta) = \begin{bmatrix}
\dot{q} \\
0
\end{bmatrix} = f(x, u; \theta).
\]

With the regression prediction being given as an integration between two time steps

\[
\hat{x}_{t+h} = \text{Integrator}(f(x, u; \theta)).
\]

We consider observation of the form of \((x_t, u_k, x_{t+1})\). However, we rely, before feeding the neural networks with the observations, on an embedding where we convert angles \( \psi \) to the circle manifold \((\cos \phi, \sin \phi)\), hence the term geometric. The augmented state can then be used by a Neural ODE [Chen et al. (2018)] and trained by optimizing the parameters of \( f_\theta \) through minimization of the mean squared error loss \( L = \frac{1}{N} \sum_{i=1}^{N} \| \hat{x}_{i,t+h} - x_{i,t+h} \|^2 \) over integration between two adjacent time-steps.

Lagrangian Neural Ordinary Differential Equation: Here, we parametrize the potential energy \( \hat{V}(q) \) and the inertia matrix \( \hat{H}(q) \) and build the euler-lagrange equations 4 with the embedding working as input of the neural network, without changing the nature of the underlying equations, since by the chain rule gradients are calculated on the generalized coordinates. We designate these models by L-NODE hereinafter.

5. Symplectic Momentum Neural Networks

5.1. Problem Formulation

Given input and output spaces \( \mathcal{X} \times \mathcal{Y} \), we build a neural network based architecture over the \((x, y)\) pairs that encodes a function, \( g(x, y; \theta) \), that relates those pairs with the discrete Euler-Lagrange equations. Let the observations be of the form of \((q_{k-1}, q_k, u_{k-1}u_k, u_{k+1})\), where \( q_{k+1} \) are the regression targets. The input space can be defined by a set of two adjacent points in the configuration space and three adjacent discrete control inputs \( x = (q_{k-1}, q_k, u_{k-1}u_k, u_{k+1}) \in \mathcal{X} \) and the output space to be \( y = (q_{k+1}) \in \mathcal{Y} \). Our goal is to build a neural network architecture that captures dependencies between the input and output space by using the Discrete Euler-Lagrange equation as a function that correlates both spaces.

We pretend to build equation (7) based on a neural network representation. Hence, learning consists in minimizing the violation of the DEL equations. This can be obtained by adjusting the free parameters, \( \theta \) to minimize the loss function:

\[
\theta^* = \arg \min_{\theta} \left( \frac{1}{N} \sum_{i=1}^{N} \| g(x_i, y_i; \theta) \|_2^2 \right)
\]
Inference consists in clamping the value of observed variables and finding configurations of the variables \(q_{k+1}\), obtained by implicitly solving the parameterized DEL, through the Newton’s root finding algorithm:

\[
\hat{q}_{k+1} = \text{RootFind}(g(q_{k+1}; \theta^*)).
\]  

We designate this models by Symplectic Momentum Neural Networks (SyMo) henceforth.

### 5.2. Ensuring Symmetry and Positive Definiteness of the Inertia Matrix

In mechanical systems the inertia matrix, \(H\) is symmetric positive definite. Symmetry and positive semi-definitess is enforced by assuming a parameterized lower triangular matrix \(\hat{L}(q; \beta)\) by a neural network, which predicts its \(\frac{N^2 + N}{2}\) elements of its Cholesky factor with \(N\) being the number of degrees of freedom of the mechanical system, then the Cholesky decomposition of this matrix is a decomposition \(\hat{H}(q; \beta) = \hat{L}(q; \beta)\hat{L}^T(q; \beta)\) Lutter et al. (2019b). Positive definiteness is obtained if the diagonal of \(\hat{L}\) is positive. This is guaranteed by using a non-negative activation function such as the SoftPlus for the diagonal elements of \(\hat{L}\) and adding a small constant \(\epsilon\) to the diagonal elements of \(\hat{H}\).

### 5.3. Discretization

In this work we consider the midpoint rule as an approximation of the action integral

\[
\mathcal{L}_d(q_k, q_{k+1}; \theta) = hL \left( \frac{q_k + q_{k+1}}{2}, \frac{q_k + q_{k+1}}{2h}; \theta \right) \approx \int_0^h \mathcal{L}(q(t), \dot{q}(t)) \, dt.
\]  

The above approximation leads to second-order accuracy Marsden and West (2001). From now on, we will denote the collocation points by \(q_{k+1/2} = \frac{1}{2}q_k + \frac{1}{2}q_{k+1}\) and \(q_{k-1/2} = \frac{1}{2}q_{k-1} + \frac{1}{2}q_k\). For Lagrangians of Mechanical Systems (see equation (1)) and using the neural network architecture aforementioned to parameterize the inertia matrix at the collocation points \(q_{k-1/2}\) and \(q_{k+1/2}\), through the lower triangular matrix \(\hat{L}(q_{k\pm 1/2}; \theta)\), and the potential energy, \(\hat{V}(q_{k\pm 1/2}; \psi)\), the discrete Lagrangians for the two adjacent time-steps are built upon the special structure of the approximated Lagrangian integral,

\[
\hat{\mathcal{L}}_d(q_{k-1}, q_k; \theta) = h \left[ \left( \frac{q_k - q_{k-1}}{h} \right) \hat{H}(q_{k-1/2}; \beta) \left( \frac{q_k - q_{k-1}}{h} \right)^T \right] - \hat{V}((q_{k-1/2}; \psi))
\]

\[
\hat{\mathcal{L}}_d(q_k, q_{k+1}; \theta) = h \left[ \left( \frac{q_{k+1} - q_k}{h} \right) \hat{H}(q_{k+1/2}; \beta) \left( \frac{q_{k+1} - q_k}{h} \right)^T \right] - \hat{V}((q_{k+1/2}; \psi)).
\]

Similarly the collocation points for the control inputs can be denoted by \(u_{k+1/2} = \frac{1}{2}u_k + \frac{1}{2}u_{k+1}\) and \(u_{k-1/2} = \frac{1}{2}u_{k-1} + \frac{1}{2}u_k\). We can approximate the virtual work (equation 6) by the midpoint rule for control affine systems:

\[
\hat{f}_d^+ (q_k, q_{k+1}, u_k, u_{k+1}) = \frac{h}{2} \hat{F} \left( \frac{q_{k+1} - q_k}{h}, u_{k+1} \right) = \frac{h}{4} (u_{k+1} + u_k)
\]

\[
\hat{f}_d^+ (q_k, q_{k-1}, u_k, u_{k-1}) = \frac{h}{2} \hat{F} \left( \frac{q_{k} - q_{k-1}}{h}, u_{k-1} \right) = \frac{h}{4} (u_{k-1} + u_k).
\]
Formally we are now able to write the Discrete-Euler Lagrange equation in terms of the learning parameters, input and output spaces by:

$$g_{\theta} = \frac{\partial}{\partial q_k} \left[ \hat{\mathcal{L}}_d(q_{k-1}, q_k; \theta) + \hat{\mathcal{L}}_d(q_k, q_{k+1}; \theta) \right] + f^-_{d}(q_k, q_{k+1}, u_k, u_{k+1}) + f^+_{d}(q_{k-1}, q_k, u_{k-1}, u_k),$$

(18)

All the gradient operations are performed by automatic differentiation.

**Learning from Embeddings:** Considering observations in $\mathbb{R}^n$ we apply appropriated embeddings to the observations that follow angular coordinates, making the learning free of singularities. Here, we use an embedding $s(q)$ but on the collocation points, $q_{k\pm 1/2} \rightarrow s(q_{k\pm 1/2})$ to account for rotational coordinates. The embedding is not applied to translational coordinates.

6. End-to-End Symplectic Momentum Neural Networks

So far, we have established a neural architecture that takes into account the underlying discrete equations of motion arising from the discrete variational principles, and using a root finding algorithm based on the architecture to implicitly integrate the dynamics in a time marching process. However, we have not discussed yet the process of including the resulting integrators into the learning process. This is trivial by using the implicit function theorem and gives origin to End-to-End Symplectic Momentum Neural Networks (E2E-SyMo). In fact theorem 1 gives us an insight of how to compute implicitly the gradients necessary for back-propagation without the need to back-propagate through all intermediate operations of the root-finding algorithm.

**Theorem 1** \textbf{Gradient of the RootFind solution.} Let $q_{k+1} \in \mathbb{R}^n$ be the root of the physical constrained parameterized RootFind procedure based on the implicit DEL equations, $g(q_{k+1}, x; \theta) \in \mathbb{R}^n$ (equation 18), mapping $(q_{k-1}, q_k)$ to $(q_k, q_{k+1})$. The gradients of the scalar loss function $L_{\theta}$ with respect to the parameters $\theta$ are obtained by vector-Matrix products as follows:

$$\frac{\partial L}{\partial \theta} = - \frac{\partial L}{\partial q_{k+1}} \left[ \frac{\partial \mathcal{L}_d(q_k, q_{k+1}; \theta)}{\partial q_{k+1}} \frac{\partial q_{k+1}}{\partial q_k} + \frac{\partial f^-_{d}(q_k, q_{k+1}, u_k, u_{k+1})}{\partial q_{k+1}} \right]^{-1} \frac{\partial g(q_{k+1}; \theta)}{\partial \theta}$$

(19)

**Proof** Under the conditions of the implicit function theorem, we can formulate the relation between the root $q^*_{k+1}$ and the remaining variables as the graph of a function of the remaining variables, $q^*_{k+1} = f(x; \theta)$, that define the implicit DEL equations.

The theorem also tell us how to compute derivatives of $q_{k+1}(x; \theta)$ by implicit differentiation and based on that obtain the partial derivative of $q_{k+1}$ v.r.t. $\theta$.

$$g(x, q_{k+1}; \theta) = 0$$

$$\frac{\partial g(x, q_{k+1})}{\partial \theta} + \frac{\partial g(x, q_{k+1}; \theta)}{\partial q_{k+1}} \cdot \frac{\partial q_{k+1}}{\partial \theta} = 0$$

Differentiate both sides.

Using the Chain Rule.

$$- \left[ \frac{\partial g(x, q_{k+1}; \theta)}{\partial q_{k+1}} \right]^{-1} \frac{\partial g(x, q_{k+1})}{\partial \theta} = \frac{\partial q_{k+1}}{\partial \theta}$$

Rearranging the equations.
**Forward Pass.** Contrary to conventional neural networks where the output is the activation from the \(L^{th}\) layer, here, the output are the roots of the parameterized DEL equations solved by Newton’s root-finding algorithm, i.e., the output is

\[
q_{k+1} = \text{RootFind}_{q_k}(g(x, q_{k+1}; θ)).
\]

This infinite depth RootFind layer adds two new hyperparameters. Specifically, the tolerance and the maximum number of iterations of the Newton’s method. The initial guess for the algorithm is employed by explicit Euler integration, i.e, \(q^{(0)}_{k+1} = q_k + h \dot{q}_k\), with \(\dot{q}_k = \frac{1}{h}(q_k - q_{k-1})\), which is simply \(q^{(0)}_{k+1} = 2q_k - q_{k-1}\).

**Backward Pass.** The backward pass simply consists in applying the insight given by theorem 1 with gradients being calculated through automatic differentiation.

### 7. Experimental Setup

We use two simulated dynamic systems to evaluate the performance of SyMos when compared to the baselines arising from conventional integrators. Specifically, we use the physical pendulum and the cartpole as systems.

**Dataset Generation:** The initial state is composed by the configurations and velocities \(x_0 = [θ, \dot{θ}]\). We randomly generated initial conditions with a uniform distribution. The initial conditions are combined with a constant control input for each trajectory in a uniform distribution in the range of \(u ∈ [-2, 2]\). The ground truth trajectories are simulated by SciPy’s `solve_ivp` adaptive solver Virtanen et al. (2020) with method RK45 using Open AI Gym Brockman et al. (2016). In order to show that the methods that incorporate priors can learn from limited amount of data we vary the size of the training set by doubling from 8 to 128 initial state conditions. Each trajectory is integrated for 32 time steps with a time span of \(h = 0.1\) for the pendulum and \(h = 0.05\) for the cartpole.

**Methods:** For the NODE and L-NODE we choose the “RK4” and the midpoint methods of numerical integration for training and making predictions. We use the labels NODE-RK4, NODE-
Midpoint, L-NODE-RK4 and L-NODE-Midpoint to describe the integrator used. We set the size of mini-batches to be four times the number of initial state conditions. Besides the Softplus for the diagonal elements of $\dot{L}$ we use linear activations in the output layer. At the hidden level we use the hyperbolic tangent. The neural network consists of a two-hidden-layer with 128 hidden neurons for the pendulum and 256 for the cartpole.

**Metrics:** To have a fair comparison with SyMos and once learning the L-NODEs and NODEs involves velocities we set the train and test error as the Mean Squared Error (MSE) between the estimated configurations and the ground truth. To evaluate the performance of each model in terms of long term prediction, we construct the metric of integration error by using 16 random unseen initial state conditions without control actuation and integrating them for 500 time-steps. We logged the inertia and energy loss per trajectory.

**Model Training:** We train our models using Adam optimizer Kingma and Ba (2015) with 2000 epochs with initial learning rate 0.0001 for the pendulum and 0.001 for the cartpole and using the ReduceLROnPlateau scheduler with patience 50 and factor 0.7. For the E2E-SyMo we use a training tolerance of $1e^{-5}$ and a maximum number of 10 iterations. For integration we relax the tolerance to $1e^{-4}$. With SyMos, after training, we perform the root finding operation to the learned DEL equations with the same hyperparameters.

8. Results

Figure 3: Mean Squared error in the configuration space for training, testing and integration and energy and mass MSE for the integration trajectories for the pendulum. SyMos show a lower integration error.

Figure 3 shows the variation in train error, test error, integrator error, energy error and inertia error with changes in the number of initial state conditions in the training set. We can see that the incorporation of prior knowledge generally yields better train and test losses, specially for a small number of trajectories. For instance, the NODE-RK4 requires more trajectories to achieve similar results with the SyMos and L-NODE-RK4. This means that the priors provide the models with the capability of learning the dynamics with less training data. However, in terms of integration, NODE-RK4 fails to keep up with those same models. This is normal as the absence of priors do not provide the models with the capability of preserving important physical properties. SyMos have a

2. https://pytorch.org/docs/stable/generated/torch.optim.lr_scheduler.ReduceLROnPlateau.html
lower integration error which empathizes their good long-term behaviour. This is expected as the 
priors take into account the geometric structure of the original continuous time equations leading to 
better integration behaviour.

Figure 4 shows the results for the cartpole system. E2E-SyMo present the lowest test, integration 
and inertia error. Even outperforming the models with fourth-order integrators which shows how 
important is the preservation of geometric structures when integrating these models. In terms of 
energy conservation L-NODE-RK4 outperform the remainder methods. NODE-RK4 beats all the 
other models in terms of train loss but it’s outperformed in the other metrics. This shows that the 
models without a prior are prone to overfitting.

![Figure 4](image)

Figure 4: Mean Squared error in the configuration space for training, testing and integration and 
energy and mass MSE for the integration trajectories for the cartpole. SyMos show a 
better integration behaviour and inertia modeling error.

9. Conclusion

In this work we introduced Symplectic Momentum Neural Networks as architectures that incor-
porate discrete mechanics with deep learning techniques. Further, we derived an implicit layer to 
accommodate variational integrators within learning for systems where the inertia depends on the 
configuration. We compared these models against the Neural ODEs with and without prior know-
ledge about the underlying equations of motion. Our models showed better long-term behaviour and 
conservation of properties proving that these models can be used for data driven numerical integra-
tion in an efficient and interpretable way. Future work should adress the incorporation of dissipation 
into the learning framework. Code is made available in [https://github.com/ssantos97/SyMo](https://github.com/ssantos97/SyMo).

Acknowledgments

This work was supported by the LARSyS - FCT Project UIDB/50009/2020 and FCT PhD grant ref. 
PD/BD/150632/2020
References

Greg Brockman, Vicki Cheung, Ludwig Pettersson, Jonas Schneider, John Schulman, Jie Tang, and Wojciech Zaremba. Openai gym. *CoRR*, abs/1606.01540, 2016. URL http://arxiv.org/abs/1606.01540.

Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations. *Advances in Neural Information Processing Systems*, 2018.

Zhengdao Chen, Jianyu Zhang, Martín Arjovsky, and Léon Bottou. Symplectic recurrent neural networks. *International Conference of Learning Representations*, 2020. URL http://arxiv.org/abs/1909.13334.

Ronan Collobert and Jason Weston. A unified architecture for natural language processing. *Proceedings of the 25th international conference on Machine learning - ICML 08*, 2008. doi: 10.1145/1390156.1390177.

Miles Cranmer, Sam Greydanus, Stephan Hoyer, Peter Battaglia, David Spergel, and Shirley Ho. Lagrangian Neural Networks. pages 1–9, 2020. URL http://arxiv.org/abs/2003.04630.

Sam Greydanus, Misko Dzamba, and Jason Yosinski. Hamiltonian neural networks. *Advances in Neural Information Processing Systems*, 32:1–16, 2019. ISSN 10495258.

Elliot Johnson, Jarvis Schultz, and Todd Murphey. Structured linearization of discrete mechanical systems for analysis and optimal control. *IEEE Transactions on Automation Science and Engineering*, 12(1):140–152, 2015. doi: 10.1109/tase.2014.2333239.

Oliver Junge, Jerrold E. Marsden, and Sina Ober-Blöbaum. Discrete mechanics and optimal control. *IFAC Proceedings Volumes*, 38(1):538–543, 2005. doi: 10.3182/20050703-6-cz-1902.00745.

Diederik P. Kingma and Jimmy Lei Ba. Adam: A method for stochastic optimization. *3rd International Conference on Learning Representations, ICLR 2015 - Conference Track Proceedings*, pages 1–15, 2015.

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems*, volume 25, pages 1097–1105. Curran Associates, Inc., 2012. URL https://proceedings.neurips.cc/paper/2012/file/c399862d3b9d6b76c8436e924a68c45b-Paper.pdf.

Michael Lutter, Kim Listmann, and Jan Peters. Deep Lagrangian Networks for end-to-end learning of energy-based control for under-actuated systems. *IEEE International Conference on Intelligent Robots and Systems*, pages 7718–7725, 2019a. ISSN 21530866. doi: 10.1109/ROS40897.2019.8968268.

Michael Lutter, Christian Ritter, and Jan Peters. Deep Lagrangian networks: Using physics as model prior for deep learning. *7th International Conference on Learning Representations, ICLR 2019*, pages 1–17, 2019b.
J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numerica*, 10:357–514, 2001. doi: 10.1017/s096249290100006x.

Richard M. Murray, Zexiang Li, and S. Shankar Sastry. A mathematical introduction to robotic manipulation. CRC Press, 1994.

Sina Ober-Blöbaum, Oliver Junge, and Jerrold E. Marsden. Discrete mechanics and optimal control: An analysis. *ESAIM - Control, Optimisation and Calculus of Variations*, 17(2):322–352, 2011. ISSN 12928119. doi: 10.1051/cocv/2010012.

Maziar Raissi. Deep Hidden Physics Models: Deep Learning of Nonlinear Partial Differential Equations. *arXiv*, 19:1–24, 2018.

Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Physics Informed Deep Learning (Part I): Data-driven Solution of Nonlinear Partial Differential Equations. (Part I):1–22, 2017. URL http://arxiv.org/abs/1711.10566.

Steindor Saemundsson, Alexander Terenin, Katja Hofmann, and Marc Peter Deisenroth. Variational Integrator Networks for Physically Structured Embeddings. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2020. URL http://arxiv.org/abs/1910.09349.

Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nelson, Eric Jones, Robert Kern, Eric Larson, C J Carey, Ílhan Polat, Yu Feng, Eric W. Moore, Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero, Charles R. Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mulbregt, and SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17:261–272, 2020. doi: 10.1038/s41592-019-0686-2.

Jared Willard, Xiaowei Jia, Shaoming Xu, Michael S. Steinbach, and Vipin Kumar. Integrating physics-based modeling with machine learning: A survey. *ArXiv*, abs/2003.04919, 2020.

Yaofeng Desmond Zhong, Biswadip Dey, and Amit Chakraborty. Symplectic ODE-Net: Learning Hamiltonian Dynamics with Control. *International Conference on Learning Representations*, 2020. URL http://arxiv.org/abs/1909.12077.