

Parsimonious neural networks learn classical mechanics and can teach it

Saaketh Desai and Alejandro Strachan
School of Materials Engineering and Birck Nanotechnology Center
Purdue University, West Lafayette, Indiana, 47907 USA

We combine neural networks with genetic algorithms to find parsimonious models that describe the time evolution of a point particle subjected to an external potential. The genetic algorithm is designed to find the simplest, most interpretable network compatible with the training data. The parsimonious neural network (PNN) can numerically integrate classical equations of motion with negligible energy drifts and good time reversibility, significantly outperforming a generic feed-forward neural network. Our PNN is immediately interpretable as the position Verlet algorithm, a non-trivial integrator whose justification originates from Trotter's theorem.

Machine learning (ML) can provide predictive models in applications where data is plentiful and the underlying governing laws are either unknown or do not exist [1–3]. These approaches are playing an increasing role even in the physical sciences where data is generally limited but underlying laws (sometimes approximate) exist. Recent successes include recognizing phases of matter [4], predicting protein folding [5], and identifying novel compounds with desired properties [6–9]. ML models have also shown the ability to guide first principles simulations of materials by accurately predicting density functionals for electronic structure calculations [10] and interatomic forces for molecular dynamics (MD) simulations [11–13]. To different degrees, these examples build on the partial knowledge of underlying physics to improve accuracy and/or to reduce the amount of data needed. One of the major drawbacks of the use of ML in the physical sciences is that, in general, models do not *learn* underlying physics such as constraints or symmetries, which limits their ability to generalize. In addition, ML models also lack interpretability. That is, machine learning approaches generally neither learn physics nor can they explain their predictions. In many fields, these limitations are compensated by copious amounts of data but this is often not possible in fields such as materials science where acquiring data is expensive and time consuming. In this letter, we combine neural network (NN) training with stochastic optimization to find the most parsimonious models consistent with the underlying training data, in our case the dynamics of a particle under a highly non-linear potential. We find that the resulting models are not only interpretable but also satisfy non-trivial underlying symmetries of the physical system. This second feature makes the parsimonious neural networks (PNNs) significantly more accurate than generic NN models. The use of stochastic optimization in conjunction with backpropagation methods to obtain robust and/or simple neural networks has been explored in detail in the past [14–17]. We extend these ideas to learn physics from data.

There are many powerful examples of the use of ML techniques in the science and engineering. Neural networks have been used to both parametrize and solve differential equations such as the Navier Stokes equation [18,19], where the network is trained to predict the parameters for the differential equation and its solution subject to soft constraints attempting to satisfy underlying physics. Neural networks have also proven useful to solve Hamilton's equations of motion [20], with recurrent architectures also beginning to show promise for such problems [21,22]. In these cases, the researcher needs to know, at least in part, the underlying physics to construct the models, mostly to incorporate the physics as a numerical constraint on the ML model via an objective

function, guiding the model towards conforming to the underlying physics. In contrast, we are interested in learning the underlying physics from data. We thus build on and extend the concept of PNNs to develop the simplest possible model consistent with the data. In this first example, we are interested in learning the equations of motion that govern the Hamiltonian dynamics of a particle under a highly non-linear external potential. Our hypothesis is that by requiring parsimony (e.g. minimizing adjustable parameters or pursuing linear relationships between variables) the resulting model will not only be easy to interpret but will be forced to tease out the symmetries of the problem. We find that the resulting PNN not only lends itself to interpretation (as Newton’s laws) but also provides a significantly more accurate description of the dynamics of the particle as compared to a flexible feed forward neural network. This is due to the PNN learning the underlying symmetries of the system, in our example time reversibility. Our work is similar in spirit to prior work in identifying invariants in dynamical systems via sparse regression [23], where the sparse regression model uses a library of candidate functions to construct invariants (e.g. Lagrangians and Hamiltonians) that best describe the input data, matching partial derivatives of invariants to the numerical derivatives of the variables. Sparse regression techniques have also proved useful in identifying partial differential equations from data [24]. Our PNN model, by virtue of being based on deep neural networks, explores a greater function space (approximately 4 billion functions in this work) and eliminates the need for estimating numerical derivatives or matching a library of candidate functions.

In this first example of physically motivated PNNs our objective is to discover the most parsimonious model capable of describing the dynamics of a particle under a non-linear interatomic potential. The training data is obtained from trajectories of a point particle of mass $m = 26.982$ amu, under an external Lennard-Jones potential with parameters $\epsilon = 0.5$ eV and $\sigma = 2.5$ Å, obtained numerically using the velocity Verlet scheme, see Supplementary Material for details. The 40,000 data points generated correspond to energies of -0.999ϵ , -0.895ϵ , -0.797ϵ and -0.733ϵ , split into input and output arrays consisting of the position and velocity at time t and $t + \Delta t$ respectively, where Δt is a small increment in time such as the timestep used to integrate the equations of motion ($\Delta t = 0.11962 \sqrt{\frac{\epsilon}{m\sigma^2}}$ in this work). The data is split into training and validation sets in an 80:20 ratio, with an additional test set of 10,000 points generated independently at an energy of -0.884ϵ .

Before describing the PNN model, we establish a baseline by training a standard feed forward neural network (Fig. 1) on our data. This network consists of three hidden layers consisting of 20, 100 and 20 neurons respectively, with the rectified linear (*relu*) activations applied to the hidden layers and linear activations applied to the output layer. We use mean squared error (MSE) as the loss function and the Adam optimizer [25] with a learning rate of 10^{-3} . The network is trained using the Keras package [26] and all data and models are available via a Jupyter notebook on nanoHUB.org. We find the network to be capable of matching the training/validation/test data reasonably well, with root mean squared errors (RMSEs) on the training, validation and test sets for the position and velocity on the order of 10^{-5} (see Supplementary Material for details). However, the network has poor predictive power and using the network iteratively to find the temporal evolution of the particle results in significant drifts in total energy, Fig. 1(b), and a lack of time reversibility, Fig. 1(c). Reversibility is judged by applying the NN sequentially 1000 times, followed by time reversal by changing the sign of the particle's velocity and applying the NN for a second set of 1000 steps. These results highlight the difficulty of the problem at hand. The underlying Hamilton's equations for classical mechanics represent a stiff set of differential equations and small errors in each timestep accumulate rapidly resulting in diverging trajectories. We find that deeper architectures for the feed-forward network do not improve the MSE, reversibility or energy conservation. Needless to say, the resulting networks are not interpretable.

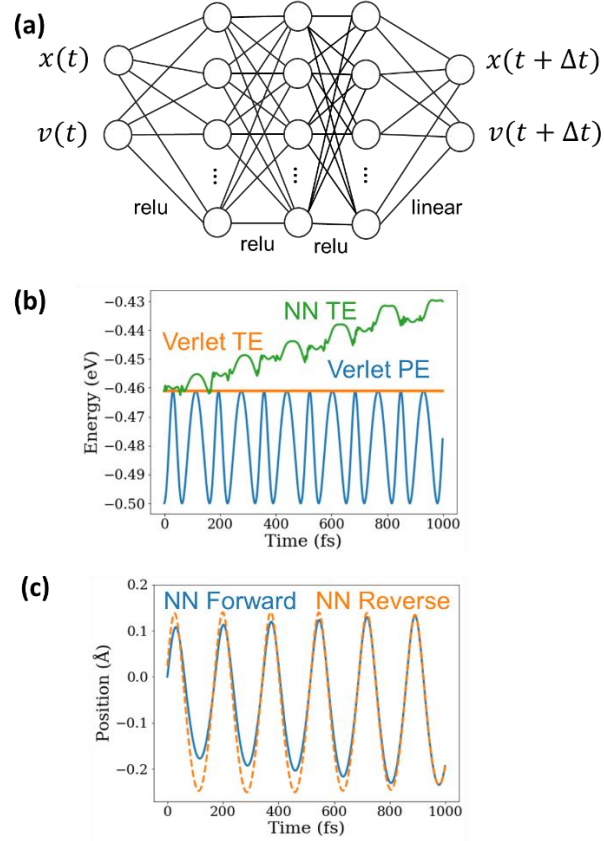


Figure 1: (a) Standard feed forward neural network, attempting to predict positions and velocities one step ahead (b) Energy drift for the feed forward NN compared to the Verlet algorithm (c) Forward and reverse trajectories generated by the feed forward NN, showing the lack of reversibility

Having established the shortcomings of the feed-forward neural network, we now switch to parsimonious neural networks (PNN), which seek to predict positions and velocities one time-step ahead of the input given. We hypothesize that seeking the simplest possible model will force the model to exploit the symmetries of the system which, in turn, will result in energy conservation and preserve time-reversibility. Finding such models is non-trivial and the development of algorithms to integrate equations of motion with good energy conservation and time reversibility has a rich history [27–31]. An example of such algorithms are the popular Verlet family of integrators [27,28] that are both reversible and symplectic [32] and whose justification lies in Trotter’s theorem [33].

We begin with a generic neural network shown in Figure 2 and use genetic algorithms to find the corresponding PNN. The initial neural network consists of two hidden layers with two neurons each and two outputs, the position and velocity of the particle at time $t + \Delta t$. The two hidden layers are connected by a “force sub-net”, a network trained to predict the force on the atom given its position. Our use of a pre-trained “force sub-net” is motivated by the prior success of neural networks in predicting interatomic forces in a wide variety of materials significantly more complex than our example [34–36]. Our focus is on learning classical dynamics. The use of a force sub-net only incorporates the physical insight that the force is an important quantity and that it depends only on the positions of the atoms. As a second baseline before moving on to PNNs, even with the addition of the pre-trained force sub-net, a regular feed-forward network, performs as poorly as the standard feed-forward network in Figure 1, see Supplementary Material for details and Figure S1.

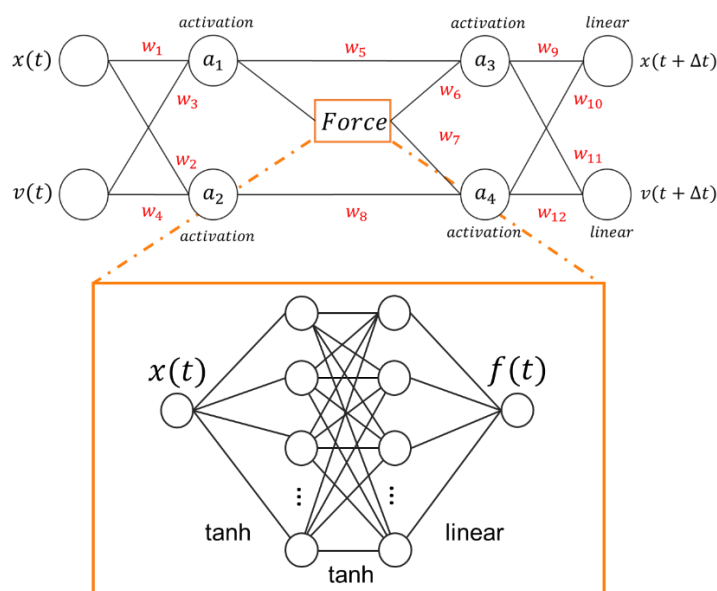


Figure 2: Generic neural network used as the starting point to find the parsimonious neural network as the network that explains the data in the simplest manner possible. The force sub-network is highlighted in orange and is fed into the generic neural network as a pre-trained model, whose weights are subsequently kept fixed throughout

Since the starting neural network represents a highly non-linear mapping from input positions and velocities to output positions and velocities, finding the PNN model reduces to the finding the

simplest function describing the relation between the inputs and outputs, an optimization problem in the function space spanned by the possible activations and weights of the network. We consider four possible activation functions: linear, rectified linear unit (‘relu’), hyperbolic tangent (‘tanh’) and exponential linear unit (‘elu’). The weights connecting the artificial neurons can be either *fixed* or *trainable*, with the fixed category allowing the following values: 0, ½ and 1. This is motivated by the fact that physical laws are often governed by integer or simple fractional coefficients. Future work will consider other common values found in physical laws, including additional fractional numbers and irrational numbers such as π and e . Our network has twelve weights (each with four possible settings) and four activation functions to optimize, see Figure 2 (top panel). A brute force approach to finding a PNN model would require training approximately 4 billion neural networks, a highly computationally intensive task, even for the relatively small network proposed here. We thus resort to evolutionary optimization, using a genetic algorithm to find the most parsimonious network consistent with our data.

The genetic algorithm is designed to find the most parsimonious description of our data, and thus favors: i) linear activation functions over non-linear ones, and ii) non-trainable weights with simple integers or fractions (0, ½, and 1 in our first attempt) over optimizable weights. To achieve this, we define the fitness for each individual network in our population to be a combination of its accuracy in reproducing the testing data and its parsimony:

$$F = f_1(E_{test}) + \sum_{i=1}^4 w_i^2 + \sum_{j=1}^{12} f_2(w_j)$$

Where $-F$ is the fitness ascribed to each individual, E_{test} represents the mean squared error on the testing set and the function f_1 is a logarithmic function that converts the wide range errors that can result from the NN training into a scale comparable to the other terms, see Supplementary Material. The second term runs over the four neurons, i , of the network and is designed to favor simple activation functions. The *linear*, *relu*, *tanh* and *elu* activation functions are assigned scores of $w_i = 0, 1, 2$ and 3 respectively. The third term runs over the network weights and favors fixed, simple weights over trainable ones. A fixed weight value of 0 is assigned a score of 0, while fixed weight values of ½ and 1 are assigned the score 1, and a trainable weight is assigned a score of 2. Evolutionary optimization to obtain PNNs based on the fitness above is performed using the DEAP package [37]. For each generation, individual networks are trained to reproduce the data above using the Keras functional API. We start with a population of 200 individuals and evolve them for

50 generations, additional details of the genetic algorithm are included in the Supplementary Material.

Quite interestingly, the resulting PNNs reproduce the training, validation and testing data more accurately than the architecturally complex NNs described before. Figure 3(a) compares the RMSE for position and velocity obtained from the three PNNs with highest fitness and the feedforward NN. More importantly, the PNNs result in excellent long-term stability and time reversibility, evaluated using the same procedure as before. Figures 3(b) and 3(c) compare the performance of the fittest PNN (denoted PNN 1) when used to predict the particle trajectory to that of the Verlet integrator in terms of conservation of total energy and time reversibility. Unlike a physics-agnostic feedforward NN, PNN 1 *learns* time-reversibility and that energy is a constant of motion, where more naïve models like a first order Euler integration would not satisfy these requirements. This long-term energy conservation and time reversibility can be further improved via a “chained” model, where the PNN is chained together multiple times, with the outputs from one link in the chain supplied as inputs to the next link and all links sharing the same weights, see Supplementary Material for details. The chained model trains the PNN to take a long series of steps accurately and while the improvements in our case are marginal, this approach is a simple example of using transfer learning techniques to improve model performance.

Having established that PNN 1 *learns* time reversibility and that energy is a constant of motion, we now explore whether they are interpretable, i.e. whether it could *teach* us what it learned. The resulting PNNs are simple models, with most weights (11 out of 12 weights) taking fixed values (with as many as three being zero) and all activation functions taking the simplest possible alternative (linear functions). As an example, the parameters of PNN 1 are shown in Figure 3(d) and other PNNs with high fitness are shown in the Supplementary Material. This allows us to trivially obtain equations to predict the new position and velocity given the position and velocity at the previous time and the force evaluation. Equations (1-3) describe the top three PNNs discovered from the data.

$$\begin{aligned}
 x(t + \Delta t) &= x(t) + v(t) * \Delta t + \frac{1}{2} f \left(x(t) + v(t) \frac{\Delta t}{2} \right) \frac{\Delta t^2}{1.0005m} \\
 v(t + \Delta t) &= v(t) + f \left(x(t) + v(t) \frac{\Delta t}{2} \right) \frac{\Delta t}{1.0005m}
 \end{aligned}
 \tag{1}$$

$$\begin{aligned}
x(t + \Delta t) &= x(t) + 1.00005 v(t) * \Delta t + \frac{1}{2} f \left(X_t + V_t \frac{\Delta t}{2} \right) \frac{\Delta t^2}{1.0005m} \\
v(t + \Delta t) &= 1.0001 v(t) + f \left(x(t) + v(t) \frac{\Delta t}{2} \right) \frac{\Delta t}{1.0005m}
\end{aligned} \tag{2}$$

$$\begin{aligned}
x(t + \Delta t) &= x(t) + 1.00035 v(t) * \Delta t + \frac{1}{2} f \left(x(t) + 1.0007 v(t) \frac{\Delta t}{2} \right) \frac{\Delta t^2}{1.0005m} \\
v(t + \Delta t) &= 0.99995 v(t) + f \left(x(t) + 1.0007 v(t) \frac{\Delta t}{2} \right) \frac{\Delta t}{1.0005m}
\end{aligned} \tag{3}$$

Inspecting PNN 1, we find the following. The first layer advances the position by half a timestep, the second layer computes the force at this half-step position, carrying forward the unmodified velocity. The third and final layer advances the position by a second half-step, using the velocity computed from the second layer. This is indeed the position Verlet algorithm except that the NN training makes a 5 in 10,000 error in mass. This algorithm is both reversible and symplectic, i.e. it conserves volume in phase space. We note that other algorithms like the Runge-Kutta family (with the Euler method as the first order member) are not symplectic nor time reversible. Interestingly, while Verlet-style integrators have been long known, a justification of the position Verlet algorithm using Trotter's theorem was only proposed in 1992 [28].

PNN 2 and 3 are similarly interpretable. We note that PNN 2 evaluates the force at the half step and PNN 3 only $0.0007\Delta t$ from it; this central force evaluation is critical for time reversibility. The main additional difference between these networks and PNN 1 is that a few additional parameters remain adjustable and the NN training converges the weights to nearly, but not exactly, the ideal value.

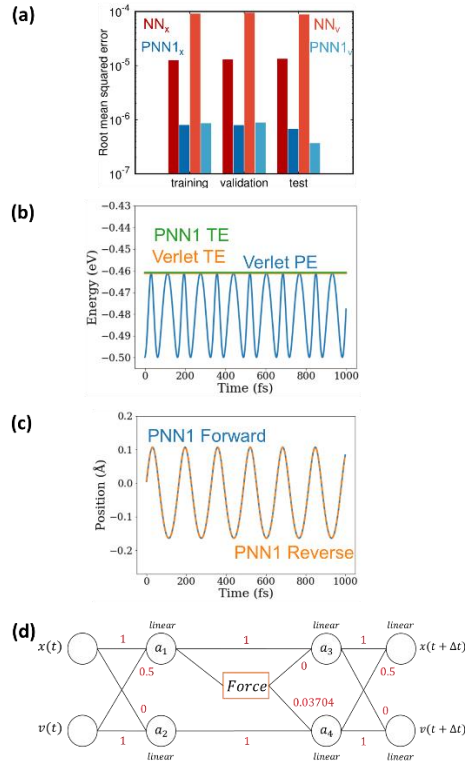


Figure 3: (a) PNN model 1 RMSEs on the training/validation/test sets compared to the feed forward network (b) We see that energy conservation between PNN1 and the verlet integrator is comparable (c) Forward and reverse trajectories generated by PNN1 show good reversibility (d) A visualization of PNN model 1 found by the genetic algorithm, attempting to predict positions and velocities one step ahead

In summary, parsimonious neural networks are capable of learning interpretable models from data and extract underlying symmetries in the problem at hand. Specifically, we feed data describing the classical evolution of a particle in an external potential and the PNN produces integration schemes that are accurate, conserve energy and satisfy time reversibility. Furthermore, they can be easily interpretable as discrete versions of Newton's equations of motion. Quite interestingly, the PNNs learn the non-trivial need to evaluate the force at the half step for time reversibility. The optimization could have predicted the first order algorithm, which is not reversible, but it favored central-difference based integrators. We note that other high-order integrators, e.g. members of the Runge-Kutta family, are not compatible with our initial network. These can easily be incorporated by starting with a more complex network; in this first effort on PNNs we decided to keep the computational complexity relatively low. The resulting networks would not come as a surprise to

experts in molecular dynamics simulations as this community has developed, over decades, accurate algorithms to integrate Newton's equations of motion. The fact that such knowledge and algorithms can be extracted automatically from observational data has, however, deep implications. While our PNNs could have discovered an Euler integration scheme, they favored the Verlet algorithm due to its higher accuracy. The Runge Kutta algorithm is incompatible with our relatively small network.

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