Structure preserving neural networks and applications to optimal control problems

Zhen Zhang, Division of Applied Mathematics, Brown University

Pengzhan Jin, School of Mathematical Sciences, Peking University

George Em Karniadakis, Division of Applied Mathematics, Brown University

In this talk, we introduce the machine learning tools, Symplectic Networks for learning many-body Hamiltonian systems from data [1]. Our primary goal is to develop data-driven models that can accurately predict the next states of such systems given their current states while preserving their symmetries. To achieve this, we embed symplecticity into fully connected neural networks and graph neural networks, which allows us to incorporate intrinsic symmetries of such systems directly into the models.

In recent years, various neural network-based models have been proposed to identify Hamiltonian systems from data [2, 3, 4]. These models have been utilized in a wide range of applications, including image prediction [3], generative modeling [5], and continuous control [6]. The construction of these learning models primarily relies on the structure of standard numerical time-stepping methods. A noteworthy model specific to Hamiltonian systems is the Hamiltonian neural network (HNN) proposed in [3]. Unlike traditional approaches that approximate the total vector field, HNNs leverage a standard neural network to approximate the Hamiltonian. In this framework, the input consists of both the phase points and their derivatives. If the available data only consists of time-dependent discrete phase points, a numerical integrator must be applied to construct the loss. In comparison, symplectic networks enable the use of phase points directly as data without any discretization procedure.

In computational terms, we would like to build a parameterized family of functions ϕ, such that $x(t_i) \approx \phi(x(t_i - dt))$ and satisfies properties including conservation of energy, volume preservation in the phase space and permutation equivariance. The first two properties can be guaranteed by symplecticity, which inspires us to develop a model that is intrinsically symplectic while being able to approximate arbitrary symplectic maps (universal approximation). Inspired by fully connected neural networks which are composed of linear and activation functions, we propose symplectic networks which are composed of symplectic linear modules and symplectic activation modules. Both modules are easily parameterizable lower/upper triangular matrix-like maps. The permutation equivariance can be ensured by additional graph structure on these basic modules.

As a specific example, we consider the motion of Lennard-Jones argon particles in the NVE ensemble. We first run molecular dynamics simulations to obtain a ground truth trajectory $\{p(t_i), q(t_i)\}_{i=1}^{n}$, where p and q corresponds to the momentums and positions of particles. Then we downsample the data every k steps to get $\{p(t_{i+k}), q(t_{i+k})\}_{i=1}^{\frac{n}{k}}$. The input to the neural network will be $\{p(t_{i+k}), q(t_{i+k})\}_{i=1}^{\frac{n}{k}-1}$ while the output will be $\{p(t_{i+k}), q(t_{i+k})\}_{i=2}^{\frac{n}{k}}$. That is, we try to learn the time $k\Delta t$ map of the phase flow. This corresponds to a more realistic setting and can justify the use of neural network models as surrogate models in order to accelerate molecular dynamics simulation.

We evaluate the performance of these models through theoretical analysis, experimentally using valid prediction time (VPT) metrics [7], and by comparing the deviation of the total energy from the ground truth in high-dimensional conservative systems. Our simulation results demonstrate that even small-sized symplectic networks can generalize well and handle long-term prediction, making them effective tools for learning complex dynamical systems. Furthermore, we demonstrate the applicability of symplectic networks to more realistic settings, such as modeling high-dimensional path-planning problems of multiple agents [8].

References

* indicates equal contribution or alphabetical order.

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