STRIDERNETwith base Equivariant Graph Neural Network

To evaluate STRIDERNETapproach using an equivariant graph neural network, we implement Neural Equivariant Interatomic Potentials (NequIP) GNN following the architecture of (Batzner et al., 2022) with the final layer replaced to predict displacement vector for each node instead of energy. The basic configuration of hyperparameters is tabulated in Table 1.

Hyper-parameters	
PARAMETER	VALUE
Input node features	One hot node type, Node potential energy, Mean neighborhood energy, Sum neighborhood energy
Input edge features	Edge distance vector
Hidden Irreps	128x0e + 64x1e +4x2e
Spherical harmonic Irreps	1x3e + 1x0e
Radial MLP non-linearity	Swish
Radial MLP hidden layers	32
Radial MLP layers	1
Nequip convolution layers	2
No. of Bessel basis functions	8
Trajectory length(T)	10
Gradient accumulation steps	2
Graphs training batch size	2
Gradient clipping	0.5

Table 1. Hyper-parameters of Equivariant STRIDERNET

In figure 1 and 2 we show the performance of the model on the training and the validation data during the course of training. In both figures, we observe that the model is unable to reduce the energy of the system. Despite the best efforts, we observe that the model is not converging.

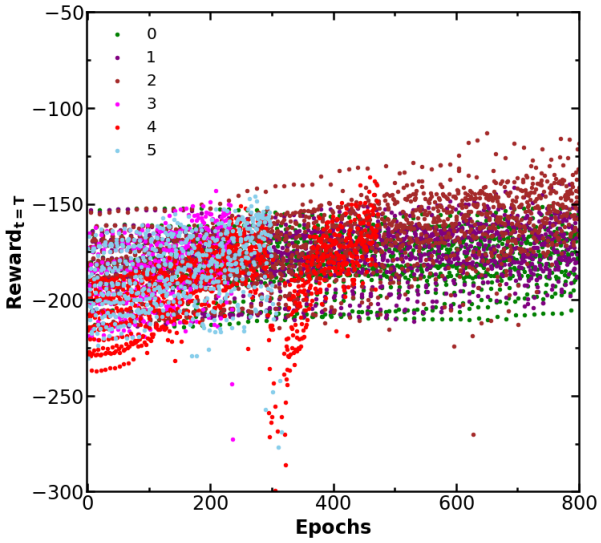

Figure 1. Reward curves of STRIDERNET with equivariant GNN on binary LJ system with 100 atoms. The labels[0-3] corresponds to same basic configuration as Table 1 with different learning rates of 5×10^{-3},1×10^{-2},2×10^{-2} and 5×10^{-2} respectively. The labels [4&5] corresponds to learning rate of 5×10^{-2} and increased batch size of 3 and 4 respectively.

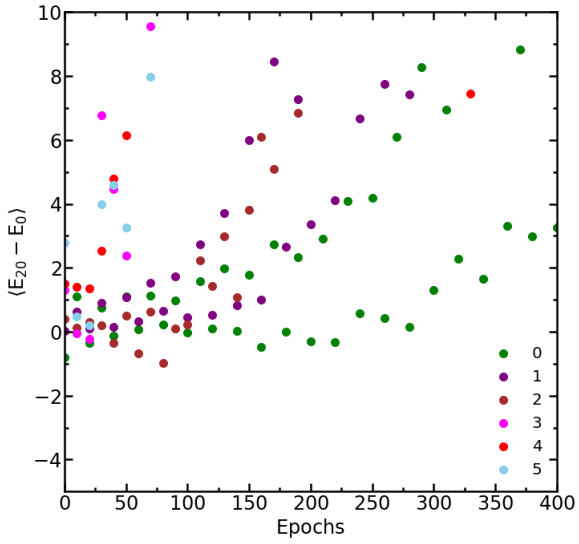

Figure 2. Validation curves of STRIDERNET with equivariant GNN on binary LJ system with 100 atoms. The labels[0-3] corresponds to same basic configuration as Table 1 with different learning rates of 5×10^{-3},1×10^{-2},2×10^{-2} and 5×10^{-2} respectively. The labels [4&5] corresponds to learning rate of 5×10^{-2} and increased batch size of 3 and 4 respectively.

References

Batzner, S., Musaelian, A., Sun, L., Geiger, M., Mailoa, J. P., Kornbluth, M., Molinari, N., Smidt, T. E., and Kozinsky, B. E (3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials. *Nature communications*, 13 (1):2453, 2022.