Speeding up MACE

Description

MACE [1] is a new type of graph neural network that can be trained on datasets of energies and forces. MACE has been shown to provide outstanding generalization performance across many different problems [2] and can be used to obtain very accurate molecular dynamic simulations [3]. However, the computational cost of MACE can be very high.

In this project, we aim to speed up MACE in two ways.

First, we will consider using model distillation [4] to obtain a smaller version of mace with similar predictive performance at a low compute cost.

Second, we will implement and train MACE at low precision. While low precision can hurt performance, we will use specific training algorithms [5] to mitigate this. The project will investigate the best way to introduce low-precision arithmetic into MACE, maximizing the trade-off between speed and quality of the resulting MACE simulations.

References

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[3] Moore, J. Harry, Daniel J. Cole, and Gabor Csanyi. "Computing hydration free energies of small molecules with first principles accuracy." arXiv preprint arXiv:2405.18171 (2024).

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