ME 697 - Project Check Point 1

Due Date: 2/2/2025

Project Objective

The project aims to replicate the process of writing a paper/report in scientific machine learning. In summary, you will have to conduct a literature review, select a paper to replicate, implement the code of the paper following best practices, and write a six-page report.

Project Timeline

The project timeline is as follows:

- **Project Checkpoint 1 (this assignment). Due 2/2/2025.** You must identify a specific paper from the list below to read in detail, identify your weaknesses on the topic covered, and start building your background knowledge to understand its material. More details below.
- **Project Checkpoint 2. Due 3/2/2025.** By this time, you should have read your chosen paper in detail and understood the mathematics of the paper. More details on the assignment will follow.
- **Project Checkpoint 3. Due 4/6/2025.** By this time, you should have implemented the first version of the code and solved a synthetic verification example. More details on the assignment will follow.
- **Project Report. Due 5/10.** By this time, you should have replicated the examples of the paper. It doesn't matter if you have successfully replicated everything. You don't have to be 100% successful in replicating the paper to get the full grade. More details on the assignment will follow.

Paper Selection

You must pick **one of the following papers** to replicate:

- **Surrogate modeling**
    - Sun et al., 2020, Surrogate modeling for fluid flows based on physics-constrained deep learning without simulation data, Computer Methods in Applied Mechanics and Engineering, https://doi.org/10.1016/j.cma.2019.112732
    - Batzner et al., 2022, E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials, Nature Communications, https://www.nature.com/articles/s41467-022-29939-5

    - Kontolati et al., 2023, On the influence of over-parameterization in manifold-based surrogates and deep neural operators, Journal of Computational Physics, https://doi.org/10.1016/j.jcp.2023.112008
- **Inverse problems**
    - Alberts et al., 2023, Physics-informed information field theory for modeling physical systems with uncertainty quantification, Journal of Computational Physics, https://doi.org/10.1016/j.jcp.2023.112100
    - Karnakov et al., 2024, Solving inverse problems in physics by optimizing a discrete loss: Fast and accurate learning without neural networks, Proceedings of the National Academy of Science, https://doi.org/10.1093/pnasnexus/pgae005
- **Dynamical systems**
    - Brunton et al., 2016, Discovering governing equations from data by sparse identification of nonlinear dynamical systems, Proceedings of the National Academy of Science, https://www.pnas.org/doi/abs/10.1073/pnas.1517384113
    - Cenedese et al., 2022, Data-driven modeling and prediction of non-linearizable dynamics via spectral submanifolds, Nature Communications, https://www.nature.com/articles/s41467-022-28518-y
    - Kontolati et al., 2024, Learning nonlinear operators in latent spaces for real-time predictions of complex dynamics in physical systems, Nature Communications, https://www.nature.com/articles/s41467-024-49411-w

Project Check Point 1

Write this page and submit it on gradescope.

Name: Shaunak Mukherjee
Date: 02/02/2025
Did you use generative AI? Which one did you use? How did you use it?
You can use generative AI to help you edit your text. But you will be responsible for correcting your write-up.
Yes.
I used Chat-GPT.
After composing/writing each answers by **myself,** I used chatGTPT to make the texts sound more cohesive and cogent. Gen-AI definitely writes better English sentences than me.

Understand what the suggested papers are about

- Read the abstracts and skim through all suggested papers.
- Google the authors' names and/or paper titles and try to find if they have codes that replicate their papers or a lecture video explaining the paper. Both of these will help you understand the paper faster. Feel free to discuss your findings with others on the discussion forums.

Nothing to report.

Read more carefully the papers you find more interesting

Pick two papers that you find interesting and dedicate about one or two hours to each one of them to dig a little deeper. You can read them a bit more carefully. You can watch the YouTube videos you found, etc. Your goal is to learn more so that you can make an informed choice moving forward.

Two papers I read
1. Learning nonlinear operators in latent spaces for real-time predictions of complex dynamics in physical systems by Kontolati et al Nat. Comm 2023.
And a few associated videos-
1. https://www.youtube.com/watch?v=qtIdH7Koo7I
2. https://www.youtube.com/watch?v=-VENSFxJstU
3. https://www.youtube.com/watch?v=9fQkLQZe3u8

2. Next, I read E(3)-equivariant graph neural networks by Batzner et al Nat. Comm. 2022.
1. https://www.youtube.com/watch?v=oePOO8bN7Co
2. https://www.youtube.com/watch?v=ZR1NTBPBDOo
3. https://www.youtube.com/watch?v=JwYPVP-vm6A
4. other reading materials
https://projects.volkamerlab.org/teachopencadd/talktorials/T036_e3_equivariant_gnn.html
5. https://www.nature.com/articles/s41467-023-38468-8
6. https://proceedings.mlr.press/v139/satorras21a/satorras21a.pdf

What is the paper you picked?

E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials by Batzner et al. Nat. Comm. 2022, 13, 2453

What is the big problem/need addressed by the paper?

At a very high level, the paper addresses a fundamental challenge in molecular dynamics simulations, i.e. the need for accurate and computationally efficient interatomic potentials. Traditional quantum mechanical methods, like density functional theory (DFT), provide high accuracy but are computationally expensive, limiting simulations to short time scales and small atomic systems. On the other hand, classical interatomic potentials are computationally efficient but lack the accuracy required for reliable predictions.

As a feasible solution, researchers have explored machine learning (ML) and deep learning (DL) techniques & models- ML-IPs, NN-IPs, GNN-IPs, DimeNet, and GemNet etc. While these models improve efficiency and precision over classical potentials, they require large training datasets, which are often difficult to obtain due to the limited availability of experimentally validated ab initio data.

This is where Neural Equivariant Interatomic Potentials (NequIP) comes in. NequIP is a novel E(3)-equivariant graph neural network that directly incorporates rotational and reflection symmetries into its architecture. NequIP significantly improves data efficiency requiring up to three orders of magnitude fewer training data than existing ML-IPs while achieving state-of-the-art accuracy across a wide range of molecules and materials. So it possible to simulate complex physical phenomena over longer time scales and larger atomic systems. This breakthrough allows researchers to perform high-fidelity molecular dynamics DFT IP simulations with unprecedented accuracy and efficiency, overcoming the limitations of both classical potentials and traditional quantum mechanical calculations.

What is the specific objective of the paper?

Your answer here.

High level objective is to introduce Neural Equivariant Interatomic Potentials (NequIP)- a new deep learning method for simulations and estimation of interatomic potentials from ab-initio calculations more accurately with limited training dataset. The key aspects of this objective are:

First, Novelty of the model, E(3)-equivariant neural network architecture: NequIP employs E(3)-equivariant convolutions which is type of graph neutral network for

interactions of geometric tensors, which is a significant departure from most contemporary symmetry-aware models listed as GNN-Ips etc. that use invariant convolutions acting only on scalars. The method outlined here uses relative position vectors rather than simply dis-
tances (scalars) together with higher-order geometric tensors. This approach results in a more information-rich and faithful representation of atomic environments.

Second training data and accuracy, using the novel NequIP technique: The authors aim to achieve state-of-the-art accuracy on a diverse set of molecules and materials (e.g. water in different phases, chemical reaction at a solid/gas interface, an amorphous Lithium Phosphate, and a Lithium superionic conductor) while demonstrating remarkable data efficiency. They challenge the common belief that deep neural networks require massive training sets by showing that NequIP can outperform existing models with up to three orders of magnitude fewer training data.

Third, Enabling high-fidelity molecular dynamics simulations: The high data efficiency of NequIP allows for the construction of accurate potentials using high-order quantum chemical levels of theory as reference. This enables high-fidelity molecular dynamics simulations over long time scales, which is crucial for studying complex physical phenomena beyond the current limitations of first-principles methods. They address the fundamental trade-off between obtaining high computational efficiency and predicting faithful dynamics in molecular simulations. This opens door for acceptance of ML/DL techniques in MD simulations for scientific community.

What are the gaps in your background knowledge you would have to cover to understand the paper fully?

Identify your knowledge gaps. Do you understand the mathematical terminology? Is there a reference to a specific mathematical topic you are unfamiliar with? It is okay if you are unfamiliar with the topic which will be covered in class. However, it is also okay if an unfamiliar topic is not covered in class. Push yourself a little bit. You will not be penalized for selecting a difficult topic. Your answer here.

My knowledge gaps can be categorized into two main areas:

Molecular Dynamics & Ab-initio Calculations

I have a decent foundation in concepts of atomic potentials, advanced quantum mechanics, and group theory. However, my background is primarily experimental, and I have limited experience with computational methods such as Density Functional Theory

(DFT) for interatomic potential (IP) calculations. I am also unfamiliar with Potential Energy Surface (PES) modeling, though I have a keen interest in learning how these concepts are applied in MD simulations.

Graph Neural Networks & Mathematical Concepts

I have experience with Convolutional Neural Networks (CNNs) but am not familiar with Graph Neural Networks (GNNs) at all, particularly in the context of graph theory. While I understand mathematical notation and concepts used in this paper, I am less familiar with how they are applied to simulations and GNNs in this paper.

Additionally, there are a few mathematical topics that I need to explore further:
- E(3)-equivariance, with respect to group transformations in 3D.
- Rotational, reflectional, and translational symmetry operations used here
- Polynomial envelope functions and their role in neural network computations.
- While I am familiar with Bessel functions and spherical harmonics from solving Schrödinger's equation for hydrogen atoms and simple molecules, I need to deepen my understanding of their application in this context.