Adeesh **Kolluru**

PhD Student, Carnegie Mellon University

Personal Website | linkedin.com/in/adeesh-kolluru-5b7b66133 | github.com/adeeshkolluru | kolluru.adeesh@gmail.com

Interests : AI for Science and Climate Change, Graph Neural Networks, Transfer Learning, Molecular and Material Discovery

Education

Carnegie Mellon University 2020 - Present

PhD in Chemical Engineering

Deep Learning for Material Discovery, Advisor : *Dr. Zachary Ulissi*

Indian Institute of Technology Delhi 2016 - 2020

B. Tech in Chemical Engineering

Machine learning for bioprocess control, Advisor : *Dr. Anurag Rathore, IIT Delhi*
Machine learning for air quality sensor calibration, *Dr. V. Faye McNeill, Columbia University*
Machine learning for protein motif identification, *Dr. Duane Loh, National University of Singapore*

Industrial Internships

Meta AI Summer 2022

Research Intern (AI), Fundamental AI Research (FAIR) Accel Team

- Developing large graph neural networks that work across molecules, materials, proteins
- Scaling graph neural networks for applications in material discovery

Research Projects

Transfer Learning using Attentions across Atomic Systems with Graph Neural Networks (TAAG)

Carnegie Mellon University and Meta AI

- Demonstrated that transfer learning across 3D atomic systems from a catalyst to small molecule database and across tasks using graph neural networks is feasible.
- Demonstrated that transfer learning approaches outperforms models trained from scratch by 53% and 17% energy mean absolute error for *CO dataset and Open Catalyst 2020 dataset's adsorption energy prediction task respectively.
- Proposed an attention based transfer learning framework, TAAG, that outperforms the best transfer learning approach by prioritizing important embeddings or features across interaction layers.
- TAAG outperforms the non-pretraining approach by 6% at an average for out of domain data like MD17.

Transfer Learning | Graph Neural Networks | Molecules | Materials

Rotation Invariant Graph Neural Network using Spin Convolution

Carnegie Mellon University and Meta AI

- Worked on developing a novel Graph Neural Network that predicts energies and forces of molecules and catalyst systems
- This model captures 3D complex angular features in a novel way and is rotationally invariant
- Results are demonstrated on OC20, QM9, MD17 Datasets

Graph Neural Networks | Rotational symmetries

Fellowships, Awards & Recognition

2022 *Phillips and Huang Family Fellowship in Energy* from CMU College of Engineering
2020 *Merit Award* : For being in the **Top 7%** of Chemical Engineering batch of IIT Delhi
2018 *Distinctive Performance in Overall Activities* from Chemical Engineering Society, IIT Delhi
2018 *Colors Award* : For being a promising sportsperson of IIT Delhi
2016 *KVPY Fellowship* : Awarded by Govt. of India for being in the **Top 1%** in math and science across the country
2016 *National Science Talent Search Exam (NSTSE)* : Awarded Gold Medal, Tablet for securing **All India Rank 1**

Skills

Languages : Python (PyTorch, PyTorch Geometric, DGL, TensorFlow, Keras), C++ **Software :** Ansys, Fluent, Matlab, Gromacs

Relevant Coursework

Advanced ChemE : Advanced Process Control, Molecular Modeling and Simulations, Advanced Chemical Engineering Thermodynamics, Applications of Computational Fluid Dynamics, Advanced Bioprocesses and Bioseparations
CS & Math : Linear Algebra, Probability & Statistics, Machine Learning, Advanced Machine Learning, Historical Advances in Machine Learning, Crafting Software
Economics : Microeconomics & Game Theory, Macroeconomics & Economic Policies

Publications

[5] **The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysis**
R Tran*, J Lan*, M Shuaibi*, BM Wood*, S Goyal*, A Das, J Heras-Domingo, **A Kolluru**, A Rizvi, N Shoghi, A Sriram, Z Ulissi, CL Zitnick
arXiv preprint arXiv:2206.08917

[4] **Spherical Channels for Modeling Atomic Interactions**
CL Zitnick, A Das, **A Kolluru**, J Lan, M Shuaibi, A Sriram, ZW Ulissi, B Wood
arXiv preprint

[3] **Open Challenges in Developing Generalizable Large Scale Machine Learning Models for Catalyst Discovery**
A Kolluru*, M Shuaibi*, A Palizhati, N Shoghi, A Das, BM Wood, L Zitnick, JR Kitchin, ZW Ulissi
ACS Catalysis

[2] **Transfer Learning using Attentions across Atomic Systems with Graph Neural Networks (TAAG)**
A Kolluru, N Shoghi, M Shuaibi, S Goyal, A. Das, L. Zitnick, ZW Ulissi
The Journal of Chemical Physics

[1] **Rotation Invariant Graph Neural Network using Spin Convolution**
M.Shuaibi, **A. Kolluru**, A. Das, A. Grover, A. Sriram, Z. Ulissi, C.L. Zitnick
arXiv preprint arXiv:2106.09575

Professional Activities

- **Reviewer**
  NeurIPS 2022 Competition Track
- **Talks**
  Transfer Learning with Large Scale GNNs across Molecular Datasets ; *AIChE 2021*, *TRI Workshop 2022*
- **Summer Schools Participation**
  London Geometry and Machine Learning Summer School 2021 [LOGML]
  Machine Learning Summer School 2021 Taipei [MLSS]
- **Teaching Assistant**
  Mathematical Methods of Chemical Engineering - *Spring 2021*, *Spring 2022*
  Advanced Chemical Engineering Thermodynamics - *Fall 2021*
- **Challenge Organization**
  Open Catalyst Challenge - NeurIPS 2021 , NeurIPS 2022
- **Tutorial Organization**
  Open Catalyst Project Tutorial [Link] - Climate Change with ML workshop, NeurIPS 2021

Extracurricular Activities

Leadership
- Served as Sports Secretary of the Board for Sports Activities, IIT Delhi
- Captained the Aquatics and Water polo team in Intra-College competitions
- Conducted various National debating tournaments as Representative of Debating Club, IIT Delhi

Sports
- Represented IIT Delhi in Waterpolo and won Silver medal in 4x100 Medley Relay Aavhan Sports Meet 2018, IIT Bombay
- Won Best Waterpolo Player award twice consecutively in Intra-College competitions of IIT Delhi

Cultural
- Breaking Adjudicator, Intra-IIT Parliamentary Debate'18
- Breaking Speaker, Intra-IIT Parliamentary Debate'19

Voluntary work
- Mentored a group of students as a part of Student Mentorship Program
- Volunteered for Humanity Foundation that works for the welfare of visually impaired students