



Adeesh KOLLURU

PhD Student, Carnegie Mellon University

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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 foundational graph neural networks 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	<i>Phillips and Huang Family Fellowship in Energy</i> from CMU College of Engineering
2020	<i>Merit Award</i> : For being in the Top 7% of Chemical Engineering batch of IIT Delhi
2018	<i>Distinctive Performance in Overall Activities</i> from Chemical Engineering Society, IIT Delhi
2018	<i>Colors Award</i> : For being a promising sportsperson of IIT Delhi
2016	<i>KVPY Fellowship</i> : Awarded by Govt. of India for being in the Top 1% in math and science across the country
2016	<i>National Science Talent Search Exam (NSTSE)</i> : 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

- [4] **Spherical Channels for Modeling Atomic Interactions**
CL Zitnick, A Das, **A Kolluru**, J Lan, M Shuaibi, A Sriram, ZW Ulissi, B Wood
(Submitted)
- [3] **Open Challenges in Developing Generalizable Large Scale Machine Learning Models for Catalyst Discovery**
A Kolluru*, M Shuaibi*, A Palizhati, N Shoghi, A Das, B Wood, L Zitnick, JR Kitchin, ZW Ulissi
(Submitted)
- [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, TRI Symposium 2022
Transfer Learning with Large Scale GNNs across Molecular Datasets, AIChE 2021
- > **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 2022, Spring 2021*
Advanced Chemical Engineering Thermodynamics - *Fall 2021*
- > **Challenge Organization**
Open Catalyst Challenge - NeurIPS 2021 Competition Track [Link]
- > **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