Adeesh KOLLURU

PhD Student at Carnegie Mellon University

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Interests : Graph Neural Networks, Transfer Learning, Computational Catalysis, Molecular Discovery

Education

2020-2025 *PhD in Chemical Engineering*, **Carnegie Mellon University**; Advisor : Zachary Ulissi
2016-2020 *B. Tech in Chemical Engineering*, **Indian Institute of Technology Delhi**

Projects

Rotation Invariant Graph Neural Network using Spin Convolution

Carnegie Mellon University and Facebook AI Research

- 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

Accelerating Geometry Optimization with Graph Neural Networks

Carnegie Mellon University and Facebook AI Research

- Developed a baseline for direct prediction of optimized geometry with Graph Neural Networks
- Analyzed and showed relative importance of various important metrics across conventional and recent methods

Geometric Optimization | Graph Neural Networks | Catalysts

Transfer Learning for catalytic/molecular predictions using OC20

Carnegie Mellon University and Facebook AI Research

- Conducted fine tuning experiments with pre-trained models on OC20 dataset to get upto to 50% improvement in performance on other small scale catalyst as well as 5-6% on small molecule databases.

Transfer Learning | Graph Neural Networks | Catalysts | Small Molecules

Delta Learning for Large Scale Catalyst Dataset

Dec '20 - Feb '21

Carnegie Mellon University

- Calculated and compared results for delta learning methods with multiple tight binding potentials (xTB, DFTB) for OC20 dataset that improves 7-8% model accuracies. Explored various referencing and normalization schemes for energy targets .

Machine Learning potentials | Delta Learning | Graph Neural Networks

Machine Learning based control of aeration rate for mammalian cells in a bioreactor

August 2019 - May 2020

B.Tech Thesis, Indian Institute of Technology Delhi | Advisor : Prof. Anurag Rathore

- Developed a machine learning based control model to optimize aeration rate for mammalian cell in a stirred tank reactor.
- It predicts Viable Cell Concentration (VCC) through a random forest model and the mass transfer coefficient from theoretical approach and combined them to determine the optimal aeration rate.

Machine Learning | Process Control | Reactor Modeling

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
CS & Math : Linear Algebra, Probability & Statistics, Machine Learning, Advanced Machine Learning, Historical Advances in Machine Learning, Crafting Software
Economics : Microeconomics & Game Theory, Macroeconomics and Economic Policies

Publications

[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
ACS Catalysis (*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 on Catalyst 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