SHIKHA MALLICK

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https://mshik.github.io/

EDUCATION

Ph.D. in Computer Science Sep 2025 – Present
University of Victoria BC, Canada

- **Coursework**: Data Mining • Algorithms and Data Models • Research Skills.
- **Research Area**: Bias in Social Networks • Graph Machine Learning • Generative Models • Reinforcement Learning.
- **Teaching Assistant**: CSC105 - Computers & Information Processing.
  Conducted labs, office hours for course content discussions, exam invigilation, and grading lab assignments.
- **Teaching Assistant Training**: Completed “New Employee Orientation - Privacy, Information Security, and Records Management".

Master of Science (Research) in Computer Science and Engineering Jul 2019 – Jul 2022
Indian Institute of Technology (IIT) Palakkad, India

- **CGPA**: 8.4/10 (Distinction).
- **Thesis**: Graph Generative Network for Novel Protein-Specific De Novo Drug Generation.
- **Coursework**: Deep Learning • Machine Learning • Linear Algebra • Probability Models • Graph Theory.
- **Research Area**: AI in Drug Discovery • Graph Machine Learning • Graph Generative Models • Bioinformatics.
- **Teaching Assistant**: C Programming lab • Data Engineering lab • Machine Learning lab • Deep Learning lab.
- **Positions of Responsibility**: Coordinator of Machine Learning Group, IIT Palakkad • Lecturer at Data Analytics Club, IIT Palakkad.

Bachelor of Technology in Computer Science and Engineering Aug 2013 – Jun 2017
Dr. A.P.J. Abdul Kalam Technical University Lucknow, India

- **CGPA**: 8.6/10 (Distinction).
- **Project**: Timetable Generator using Genetic Algorithms in Java.
- **Coursework**: Computer System and Programming in C • Data Structures Using C • Discrete Structures and Graph Theory • Design and Analysis of Algorithms • Artificial Intelligence.

PUBLICATIONS

CDGCN: Conditional de novo Drug generative model using Graph Convolution Networks Apr 2023
27th Annual International Conference on Research in Computational Molecular Biology Istanbul, Turkey

- Developed a novel graph neural network-based conditional deep generative model for the generation of de novo drugs for novel protein targets. This work was done as part of thesis work for Master of Science (Research) in the Department of Computer Science and Engineering at IIT Palakkad. Link to the paper: https://link.springer.com/chapter/10.1007/978-3-031-29119-7_7

Solubility prediction of industrial chemicals: Feeding GNNs with physics-based simulations data Apr 2023
AICHE Spring meeting 2023 Houston, US

- Developed a novel graph neural network-based deep predictive model for the prediction of Hansen solubility parameters of small molecules. This work was done as part of industry research in Siemens DISW and accepted for presentation. This work helped garner prospects for collaborations in the field of materials science. Link to the presentation: https://www.researchgate.net/publication/370133485_Solubility_prediction_of_industrial_chemicals_Feeding_Graph_Neural_Networks_with_physics-based_simulations_data

INDUSTRY EXPERIENCE

Engineering Services Engineer January 2023 – July 2025
Siemens Digital Industries Software Pune, India

- Developed a large-scale autonomous driving perception toolchain for road and lane involving image processing of camera sensor images with ROS (Robot Operating System) and C++ in an undisclosed project. Optimised the inference for road and lane using TensorRT.
- Developed a Gaussian splatting-based method for aiding annotators to annotate images from annotated LiDAR point clouds for autonomous driving applications in an undisclosed project.

Associate Engineering Services Engineer March 2022 – December 2022
Siemens Digital Industries Software Pune, India

- Developed a multi-modal model for detecting parts in a 3D CAD assembly involving a multi-view convolution neural network-based model for learning on vehicle parts using Pytorch Lightning and ONNX in an undisclosed project.
- Developed a graph neural network-based model for predicting Hansen solubility parameters of small molecules, which was accepted for presentation in the AIChE Spring meeting 2023.

MINI PROJECTS

XGB-EVM: Ensemble Deep Model for Disease Classification from FUNDUS Retina Images Aug 2021

Indian Institute of Technology (IIT) Palakkad, India

- Developed an ensemble deep learning model for the automatic detection of eye diseases (eg, glaucoma) from FUNDUS retina images, which won the first prize in the *AI for Healthcare Hackathon* sponsored by Derbi Foundation and SINE IIT Bombay. Link to the project: https://github.com/mshik/XGB-EVM.

xDet: Accurate On-the-Fly Covid19 Detector from X-ray Images Apr – Jul 2020

Indian Institute of Technology (IIT) Palakkad, India

- Developed a light-weight deep learning model for the automatic detection of chest diseases (eg, COVID-19) from chest x-ray images in significantly less time with comparable accuracy as compared to previous models. Link to the web app: https://creds.iitpkd.ac.in/xdet/.

ACHIEVEMENTS

- **First** prize for developing a winning solution for automatic detection of eye diseases in the *AI for Healthcare Hackathon* sponsored by SINE IIT Bombay and Derbi Foundation. Link to the project: https://github.com/mshik/XGB-EVM.

SKILLS

- **Programming Languages**: Python • C++.
- **Areas of Interest**: Social Networks • Graph Machine Learning • Generative Models • AI in Drug Discovery • Computer Vision • Bioinformatics
- **Toolkits**: PyTorch • MXNet • Tensorflow • TensorRT • ONNXRuntime • NumPy • Pandas • RDKit • Scikit Learn • PyMOL • Jupyter Notebook