Shikha Mallick

mallickshikha@gmail.com | https://mshik.github.io/

RESEARCH INTERESTS

I am interested in analyzing large-scale networks using network analysis and graph learning models at scale.

EDUCATION

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

- GPA: 8.4/10
- Advisor: Dr. Sahely Bhadra
- Thesis: Graph Generative Network for Novel Protein-specific de novo Drug Generation

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

- Percentage: 78.4%
- Graduated First Class with Honors
- Final Year Project: Timetable Generation using Genetic Algorithms in Java

PUBLICATIONS

Book Chapters

1. Mallick, S., Bhadra, S. (2023). CDGCN: Conditional de novo Drug Generative Model Using Graph Convolution Networks. In: Tang, H. (eds) Research in Computational Molecular Biology. RECOMB 2023. Lecture Notes in Computer Science, vol 13976. Springer, Cham. https://doi.org/10.1007/978-3-031-29119-7_7

Conferences

1. Mallick, S., Bhadra, S. (2023). CDGCN: Conditional de novo Drug Generative Model Using Graph Convolution Networks. In: Tang, H. (eds) Research in Computational Molecular Biology. RECOMB 2023. Lecture Notes in Computer Science, vol 13976. Springer, Cham. https://doi.org/10.1007/978-3-031-29119-7_7
2. Mallick, S., Boioli, F., Aglave, R., Petris, P., Mas, P. (2023). Solubility prediction of industrial chemicals: Feeding Graph Neural Networks with physics-based simulations data. In: AIChE Annual Meeting 2023. 257a - Physics and Data-Informed Formulation Design and Development for Chemical Processes. https://www.researchgate.net/publication/370133485_Solubility_prediction_of_industrial_chemicals_Feeding_Graph_Neural_Networks_with_physics-based_simulations_data

PRESENTATIONS AND TALKS

1. " CDGCN: Conditional de novo Drug Generative Model Using Graph Convolution Networks ", 27th Annual International Conference on Research in Computational Molecular Biology, Istanbul, Turkey, 18th April 2023.
   (Conference Presentation Video Link)

RESEARCH EXPERIENCE

Research Scholar
Indian Institute of Technology (IIT) Palakkad, India Jul 2019 – Jul 2022

- Worked on conditional novel graph generation for novel target-specific drug molecules.

Junior Project Officer
Indian Institute of Technology (IIT) Kharagpur, India Jul 2018 – Apr 2019

- Worked on parallel algorithms for prime number factorization for cryptanalysis of RSA encryption algorithm.

INDUSTRY EXPERIENCE

Machine Learning Engineer
Siemens Industry Software, India Mar 2022 – Present

- Worked on 3D Shape Recognition using dynamic graphs on point clouds.
- Headed a project on Molecular Solubility Prediction using GNNs.
- Worked on an onsite project in Japan on Road Perception & Sensor Fusion using late fusion methods for Autonomous Driving.
- Worked on a project to densify sparse point clouds using 3D Gaussian Splatting for dynamic urban scenarios.

VOLUNTEER

Coordinator of Machine Learning Group (MLG)
Indian Institute of Technology (IIT) Palakkad, India Jul 2019 – Dec 2020

Lecturer at Data Analytics Club
Indian Institute of Technology (IIT) Palakkad, India Jul 2020 – Jun 2021

Co-Organizer and Host of Florence Nightingale Data Science Talk Series
MLG, Indian Institute of Technology (IIT) Palakkad, India Sep 2021

TEACHING

Teaching Assistantships

1. CS1020 (revised to ID1110): Introduction to Programming
   Indian Institute of Technology (IIT) Palakkad, India Jul 2019 – Sep 2019
   - Graduate Teaching Assistant for CS1020. Managed class discussions, graded homework assignments and helped with class projects (≈ 90 students).
2. DS5003: Data Engineering
   Indian Institute of Technology (IIT) Palakkad, India Jul 2020 – Sep 2020
   - Graduate Teaching Assistant for DS5003. Managed class discussions, graded homework assignments and helped with class projects (≈ 40 students).
3. CS5007 (revised to DS3040): Deep Learning
   Indian Institute of Technology (IIT) Palakkad, India Oct 2020 – Dec 2020
   - Graduate Teaching Assistant for CS5007. Managed class discussions, graded homework assignments and helped with class projects (≈ 60 students).
4. CS5512: Machine Learning
   Indian Institute of Technology (IIT) Palakkad, India Jan 2021 – Mar 2021
   - Graduate Teaching Assistant for CS5512. Managed class discussions, graded homework assignments and helped with class projects (≈ 60 students).

ACHIEVEMENTS

- Winner of the "AI in Healthcare Hackathon" sponsored by SINE IIT Bombay and Derbi Foundation. **(Project link)** Aug 2021
- Half-time Teaching/Research Assistantship (HTTA) by the Ministry of Human Resource Development (MHRD), India, for graduate studies. Jul 2019 – Dec 2021
- Among top 2% candidates in the Graduate Aptitude Test in Engineering (GATE) exam. Mar 2018
- Onsite Undergraduate Summer Internship in Asian Institute of Technology, Bangkok, Thailand. Jun 2016