Madhurima Mondal, PhD

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Final year Ph.D. candidate with expertise in Deep Learning, Graph Neural Networks, and Generative AI for bioinformatics applications. Looking for full-time, co-op, or internship roles in AI/ML or Software Engineering starting in Spring 2025; open to relocation within the USA.

EDUCATION

AUG 2025	**Ph.D., Electrical & Computer Engineering**, Texas A&M University, TX, USA Focus: Deep Learning, Graph Neural Network, Large Language Models
AUG 2021	**M.Tech, Electronics & Electrical Comm. Engineering**, Indian Institute of Technology (IIT) Kharagpur Specialization:Visual Information Processing and Embedded Systems
AUG 2021	**B.Tech, Electronics & Electrical Comm. Engineering**, Indian Institute of Technology (IIT) Kharagpur

EXPERIENCE

MAY 2023 – AUG 2023	**NSF funded Research Engineer Intern**, Sumaq Life LLC, USA Worked in building models for drug repurposing in cancer treatments, using analytical approaches.
MAY 2020 – JUN 2020	**Machine Learning Engineer Intern**, Samsung R&D Institute, India Built deep learning frameworks for music generation using generative adversarial networks (GAN).
MAY 2019 – JUL 2019	**Visiting Exchange Student**, University of Illinois at Urbana Champaign, USA Researched data-driven techniques for disease classification from bacterial and human genome data.

RESEARCH WORK

MAY 2021 – present **Graduate Research Assistant**, Texas A&M University, USA
Working towards developing advance computational frameworks for drug repurposing through Drug-Target Interaction (DTI).

- **Diffusion Graph VAE: Anticancer drug efficacy prediction** A Graph Variational Autoencoder (VAE) incorporating diffusion convolution is designed for regression-based drug efficacy prediction. By transforming SMILES strings into 2D graph representation, the model encodes topological properties of drug molecules. This graph-diffusion message passing model outperforms SMILES-based baselines by 45% and conventional VAEs by 5% in predictive performance. [GitHub]
- **SAM-DTI: A Spatial Attention Model for DTI Prediction** Designed a spatial attention-based framework that models fine-grained spatial correlations between SMILES-derived drug representations and protein sequences. By learning pairwise interaction, the model captures residue level interactions that improve prediction accuracy. The model achieved improvements in AUROC, and AUPRC over state-of-the-art baselines. [GitHub]
- **LinkDTI: Heterogeneous Message Passing for DTI** A heterogeneous graph neural network-based message passing framework for accurately predict links among diverse biomedical entities in a knowledge graph. By integrating multi-hop message passing with tailored negative sampling, we frame drug-target interaction as a link prediction task within the graph. Our model achieves consistently superior performance, with up to 3.8% higher AUROC compared to baselines under different sampling ratios [GitHub]
- **DTIFormer: An LLM-based DTI Prediction Model** Working on a multi-modal framework combining 2D image-based topological features, and language-based sequential features of drug and protein sequences to predict DTI via attention-based fusion. [GitHub]
- **Fine tuning LLM and its applications using Reinforcement Learning** Proposing a generative AI framework for literature summarization using RLAIF, comparing zero, one, and few-shot prompt strategies to guide model behavior. The model will explore RLHF-based fine-tuning for reduced hallucinations to PubMed-based knowledge graph.[GitHub]
- **Drug repurposing using Boolean Network** We develop a data-independent Boolean Network model to simulate binary message passing over nodes representing interacting genes to evaluate combination treatment effectiveness in endometrial cancer. This directed acyclic graphical framework is particularly suited for under-studied cancers with sparse data. Simulating 16,740 treatment combinations, we suggest an average 80% improvement in efficacy in immunotherapy treatment predictions compared to conventional regimens. [GitHub]

TECHNICAL SKILLS

Languages	Python, C/C++, R, JAVA, MATLAB
Tools	Google Cloud Platform, VS Code, PyCharm, Google Colab, AWS, Azure, Vision Control (Git), Linux Shell
Libraries	DGL, PyG, PyTorch, Pandas, NumPy, Matplotlib, Tensorflow
Courses	Machine Learning, Deep Learning, Generative AI with LLM, Graph Representation Learning
Gen AI	BERT and T5 variants, GPT-style models, prompt-based feature extraction, RAG
Competencies	AI/ML, Analytical Skills, Research, Communication

PUBLICATIONS

Google Scholar	Contributed to a range of journal articles and conference papers, both individually and in collaboration with other researchers. An up-to-date list of publications can be found on the Google Scholar profile.

AWARDS

2024	Selected for departmental **poster presentation award**, Texas A&M University.
2017	Selected as **Secretary of Technology** at Mother Teresa Hall of Residence, IIT Kharagpur.
2017	Selected as **Captain** in Inter Hall Maths Olympiad team, IIT Kharagpur.
2016	Won **Broze medal** in Annunal National Service Scheme Campaign, IIT Kharagpur.
2016	Selected for B.Stat. (Hons.) in **Indian Statistical Institute** (ISI), among 70 students nationwide.
2016	Selected for UG admission in **Indian Institute of Science (IISc)**, among 300 students across India.
2015	Awarded **Kishore Vaigyanik Protsahan Yojana (KVPY)** fellowship among top 1000 students in India.
2015	Completed Sony Global Math Challenge with **World Rank 1071**, **India Rank 44**, and **State Rank 1**.
2014	Cleared **Regional Mathematics Olympiad** (RMO) with **Rank 2** (**1st among girls**) conducted by Homi Bhabha Centre for Science Education (HBCSE), India.
2013	Cleared **Regional Mathematics Olympiad (RMO)** conducted by HBCSE, India.
2012	Selected for **National Talent Search Examination** (NTSE) with Stage I **Rank 2** (**1st among girls**) among top 1000 students in India.

EXTRA CURRICULAR ACTIVITIES

MAY 2016 – MAY 2018	**Student Volunteer**, National Service Scheme, India Bagged bronze medal in Annual NSS Camp 2016 among more than 10 teams, taught more than 60 village kids weekly, and made roads in the village.
AUG 2017 – MAY 2018	**Secretary of Technology**, Mother Teresa Hall of Residence, IIT Kgarahpur Organized more than 80 sophomores for events in the MT Hall of Residence. and supervised technology General Championship (GC) events like Product Design, Maths Olympiad in MT Hall of Residence.
MAY 2016 – MAY 2018	**Captain of Maths Olympiad team**, Mother Teresa Hall of Residence, IIT Kgarahpur Led a 4-member team of MT Hall of Residence for the general championship, and participated in the GC competition as a candidate in consecutive three years of undergraduate studies.