

Madhurima Mondal, PhD

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Final year PhD student, seeking for a Deep Learning, Software Engineering or related role for Spring 25/full-time. I am well-versed in Machine Learning, Deep Learning, Graph Neural Networks, and Large Language Models. I am willing to relocate within the USA.

EDUCATION

Texas A&M University	USA
<i>Doctor of Philosophy, Electrical and Computer Engineering</i>	<i>Aug. 21 – present</i>
Indian Institute of Technology (IIT) Kharagpur	India
<i>Dual Degree (B. Tech & M. Tech), Electronics and Electrical Communication Engineering</i>	<i>Aug. 2016 – May 2021</i>

INTERNSHIP EXPERIENCE

- NSF funded Research Engineer, **Sumaq Life LLC, MI , USA** May 2023 – Aug. 2023
- Developed AI-driven models for drug repurposing in cancer treatments, applying analytical skills and data science methods.
- Deep Learning Engineer, **Samsung R&D Institute, India** May 2020 – Jun. 2020
- Built proof-of-concept models for music generation using generative adversarial networks (GAN), leveraging Python and TensorFlow to automate experimental workflows.
- Visiting Exchange Student, **University of Illinois at Urbana Champaign, USA** May 2019 – Jul. 2019
- Researched AI-driven techniques for disease classification from bacterial and human genome data, integrating data science approaches to explore innovative solutions.

TECHNICAL SKILLS

Programming Languages: Python, C/C++, R, JAVA, MATLAB
Developer 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
Core Competencies: AI/ML, Data Science, Analytical Skills

RESEARCH WORK

Diffusion Graph VAE for Anti-cancer Drug Efficacy Prediction Jan. '24 – May '24
Texas A&M University, USA

- Developed a cutting-edge Graph Variational Autoencoder (VAE) model that integrates diffusion CNN to predict drug efficacies by processing graph representations of drugs and Cancer Cell Line Encyclopedia (CCLE). It demonstrated a notable performance advantage, outpacing character tokenization of SMILES strings by ~ 45%, and showing a ~ 5% improvement over conventional VAE approaches.

SAM-DTI: A Spatial Attention Model for DTI prediction May '24 – Aug. '24
Texas A&M University, USA

- Developed an advanced Pairwise interaction model leveraging spatial attention for drug and protein features from SMILES strings and protein sequence respectively. This approach aims to enhance Drug Target Interaction (DTI) prediction by combining molecular and sequence information within an interaction map framework with the potential to surpass conventional sequence-based methods.

LinkDTI: Drug-Target interaction prediction using heterogeneous message passing Jul. '24 – Dec. '24
Texas A&M University, USA

- Developed a novel heterogeneous graph-based negative sampling approach for Drug Target Interaction (DTI) prediction. This method incorporates heterogeneous message passing along with a link prediction task, effectively leveraging the diverse interactions between drugs, targets, diseases, and side effects to enhance predictive accuracy.

- Demonstrated the potential of this approach to significantly improve DTI prediction by capturing complex relational structures within the heterogeneous graph. The negative sampling technique ensures a more representative and informative sampling process, paving the way for more precise and reliable predictions in drug discovery applications.

DTIFormer: A LLM-DTI prediction model from dual representations

Jan '25 – present

Texas A&M University, USA

- Proposed an LLM based framework that dynamically integrates image-based topological features from molecular graphs with sequence embeddings from pretrained chemical language models, enhancing drug-target interaction.

Music Generation using GAN

May '20 – Jun. '20

Samsung R&D Institute, India

- Designed a Python-based model for generating refined music from raw MIDI files, employing a deep learning approach known as Generative Adversarial Network (GAN) with a LSTM based generator and discriminator. Utilized a substantial dataset sourced from Maestro, comprising raw MIDI files.

Fine tuning LLM and its applications using Reinforcement Learning

Aug. '23 – Jan. '24

Texas A&M University, USA

- Engaged in the application of generative AI for dialogue summarization using RLAI, conducting a comprehensive comparison of zero-shot, one-shot, and few-shot instances in prompt engineering to guide task direction. Evaluated the performance of PEFT and fine-tuned a FLAN-T5 model to generate less toxic content and explored applications of transfer learning in the reward model.

Drug repurposing using Boolean Network

Aug. '21 – Dec. '23

Texas A&M University, USA

- Created a boolean model designed to identify the optimal combination of drugs and supplements for treating endometrial cancer. The model leveraged a thorough analysis of existing FDA-approved drugs and dietary supplements commonly employed in endometrial cancer treatment. Developed using MATLAB, Python, and Multisim, the model evaluated 16,740 robust combinations, revealing an average efficacy increase of 80% compared to current treatment approaches. Predicted that incorporating immunotherapy in combination with dietary supplements may enhance the results over conventional combinations of drugs.

PUBLICATION

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

AWARDS

National Talent Search Examination(NTSE) : Stage 1 rank 2, 1st place among girls '12
Regional Mathematics Olympiad (HBCSE): '13, '14- Rank 2, 1st place among girls
Selected for National Mathematics Olympiad Training Camp at ISI Kolkata '14, '15
Sony Global Maths Olympiad : State rank 1 '15

LEADERSHIP SKILLS

Student Volunteer

May '16 – May '18

National Service Scheme, India

IIT Kharagpur, 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.

Secretary of Technology

Aug. '17 – May '18

Mother Teresa Hall of Residence

IIT Kharagpur, India

- Organized more than 80 sophomores in the Illumination event in the MT Hall of Residence.
- Supervised technology General Championship (GC) events like Product Design, Maths Olympiad in MT Hall of Residence.

Captain of Maths Olympiad team

Aug. '17 – May '18

Mother Teresa Hall of Residence

IIT Kharagpur, India

- Led a 4-member team of MT Hall of Residence for the general championship.
- Participated in the GC competition as a candidate in consecutive three years of undergraduate studies.