Md Hasan Jawad Chowdhury

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Postdoctoral Research Associate
Data NanoAnalytics Group
Center for Nanophase Materials Science
Oak Ridge National Laboratory

Interests & Expertise

Machine Learning, Causal Discovery, Causal Inference, Explainable AI, Data Science, Predictive Modeling, Domain Generalization, Physics-Informed Neural Networks, ML in Computational Chemistry

Education

Ph.D. in Computer Science and Engineering (CGPA: 4.00) Aug 2019 - Dec 2024
University of North Carolina at Charlotte

- Thesis: Leveraging Domain Knowledge for Enhanced Causal Structure Learning and Out-of-Distribution Generalization in Observational Data
- Supervisor: Dr. Gabriel Terejanu

Bachelor of Computer Science and Engineering (CGPA: 3.31) Feb 2011 - Aug 2016
Bangladesh University of Engineering and Technology (BUET)

- Thesis: Image Retrieval with Relevance Feedback
- Supervisor: Dr. Md Monirul Islam

Work Experience

Postdoctoral Research Associate Feb 2025 - Present
Center for Nanophase Materials Science, Oak Ridge National Laboratory

- Responsibilities: Developing AI/ML algorithms for autonomous and human-in-the-loop experimental workflows to optimize scientific discovery and experimental efficiency. Designing models to enhance automation on scientific instruments while ensuring adaptability to unseen data. Modularizing and documenting code for research partners, supporting ORNL's mission of integrity, teamwork, and inclusive collaboration.

Graduate Research Assistant Aug 2019 - Dec 2024
Department of Computer Science, CCI, UNC Charlotte

- Responsibilities: Designed and developed interactive causal discovery models to incorporate domain knowledge and enhance causal structure learning. Focused on concept-driven causal learning for high-dimensional vector-valued data. Collaborated with chemical engineers on interdisciplinary research to develop invariant molecular representations for predicting adsorption energies using machine learning models.

Machine Learning, Summer Intern May 2023 - Aug 2023
Toyota Racing Development (TRD)

- Responsibilities: Developed surrogate models for TRD's Tire Model to effectively capture tire states, coefficients, and scaling parameters for accurate tire force and moment prediction. Employed a multi-task learning approach to build an invariant surface model that consistently aligns with both SOVA (sandpaper) and WFT (Wheel Force Transducer) tire data, reducing manual labor and streamlining the tire scaling process.

Data Science, Graduate Intern Jul 2022 - Aug 2022
Lowe's Technology

- Responsibilities: Conducted exploratory data analysis on supply chain metrics to identify key trends and insights. Developed descriptive, predictive, and prescriptive models for RDC traffic and labor analytics to simulate interventions and enhance operational efficiency.

Software Engineer Jul 2018 - Jul 2019
Misfit Technologies Ltd.

- Responsibilities: Led the development of *Lily*, an AI-powered chatbot providing pregnancy support and advice to millions of women. Designed and implemented backend features, including onboarding interactions, daily subscription texts, and AI-driven automated responses. Mentored junior developers, ensuring efficient feature deployment and compliance with project requirements.

Junior Software Engineer Aug 2016 - Feb 2018
Field Information Solution Ltd.

- Responsibilities: Developed software modules aligned with client requirements and technical specifications. Assisted in project maintenance, focusing on client support, analytics-based report generation, and bug fixes to ensure optimal system performance.

Publications

- **Chowdhury, J.** and Terejanu, G. (2025). CGLearn: Consistent Gradient-Based Learning for Out-of-Distribution Generalization. In *Proceedings of the 14th International Conference on Pattern Recognition Applications and Methods*, ISBN 978-989-758-730-6, ISSN 2184-4313, pages 103-112. DOI: 10.5220/0013260400003905

- **Chowdhury, J.**, Fricke, C., Bamidele, O., Bello, M., Yang, W., Heyden, A., & Terejanu, G. (2024). Invariant Molecular Representations for Heterogeneous Catalysis. Journal of Chemical Information and Modeling. https://doi.org/10.1021/acs.jcim.3c00594

- **Chowdhury, J.**, & Terejanu, G. (2023). CD-NOTEARS: Concept Driven Causal Structure Learning using NOTEARS. In 2023 IEEE International Conference on Machine Learning and Applications (ICMLA). https://doi.org/10.1109/ICMLA58977.2023.00118

- Rashid, R., **Chowdhury, J.**, & Terejanu, G. (2023). Causal Feature Selection: Methods and a Novel Causal Metric Evaluation Framework. In 2023 IEEE 10th International Conference on Data Science and Advanced Analytics (DSAA) (pp. 1-9). IEEE.

- Fricke, C. H., Bamidele, O. H., Bello, M., **Chowdhury, J.**, Terejanu, G., & Heyden, A. (2023). Modeling the Effect of Surface Platinum–Tin Alloys on Propane Dehydrogenation on Platinum–Tin Catalysts. ACS Catalysis, 13(16), 10627-10640.

- **Chowdhury, J.**; Rashid, R. and Terejanu, G. (2023). Evaluation of Induced Expert Knowledge in Causal Structure Learning by NOTEARS. In Proceedings of the 12th International Conference on Pattern Recognition Applications and Methods - ICPRAM, ISBN 978-989-758-626-2; ISSN 2184-4313, SciTePress, pages 136-146. DOI: 10.5220/0011716000003411

- Shen, J.; **Chowdhury, J.**; Banerjee, S. and Terejanu, G. (2023). Machine Fault Classification Using Hamiltonian Neural Networks. In Proceedings of the 12th International Conference on Pattern Recognition Applications and Methods - ICPRAM, ISBN 978-989-758-626-2; ISSN 2184-4313, SciTePress, pages 474-480. DOI: 10.5220/0011746800003411

- Rashid, R., **Chowdhury, J.**, & Terejanu, G. (2022, December). From Causal Pairs to Causal Graphs. In 2022 21st IEEE International Conference on Machine Learning and Applications (ICMLA) (pp. 802-807). IEEE.

- Terejanu, G., **Chowdhury, J.**, Rashid, R. and Chowdhury, A., 2020. Explainable Deep Modeling of Tabular Data using TableGraphNet. arXiv preprint arXiv:2002.05205

Highlighted Project

Curiosity-Based Learning – AI/ML for Autonomous Scientific Discovery Feb 2025 – Present

- Responsibilities: Developing AI/ML algorithms for active learning to optimize experiments and accelerate scientific discovery. Designing models to identify optimal conditions, reducing experimental costs while ensuring generalization to unseen data. Working with scanning probe microscopy to enhance autonomous scientific exploration.

CGLearn – Consistent Gradient-Based Learning for OOD Generalization Jun 2023 – Jan 2025

- Responsibilities: Developed AI/ML models to enhance out-of-distribution generalization by leveraging gradient agreement for invariant feature learning. Led implementation and open-source release, achieving state-of-the-art performance in diverse tasks.

Quantification of Affective Polarization – A framework leveraging LLMs Aug 2024 – Dec 2024

- Responsibilities: Developed a framework using LLaMA to quantify affective polarization in tweets on X (formerly Twitter). Designed mechanisms to analyze discussions on major events like climate change, leveraging LLMs for stance detection and sentiment analysis.

IMR - Invariant Molecular Representations for Heterogeneous Catalysis Sep 2022 – Dec 2023

- Responsibilities: Developed a Siamese neural network-based ML model for predicting adsorption energies using Invariant Molecular Representations (IMRs), achieving superior predictive accuracy by leveraging invariant relations across multiple environments.

ML-Based Tire Scaling - Optimizing tire performance through ML models Mar 2023 – Aug 2023

- Responsibilities: Collaborated as a UNCC team member in the UNCC-TRD project to optimize tire parameters and reduce manual labor. Designed a surrogate model to accurately process tire states, coefficients, and scaling parameters for precise force and moment determination, and developed an inverted model to align tire coefficients with multiple surface data, improving performance analysis.

Untangle - Modeling the 'Why' in supply chain performance Oct 2021 - Nov 2022

- Responsibilities: Developed a generalized modeling framework for identifying and understanding causal factors impacting supply chain performance. Designed causally driven models to provide counterfactual reasoning and interventional mechanisms for generating predictive insights under different what-if scenarios.

CausalBias - Evaluating the impact of domain knowledge on causal models Jun 2020 - Jul 2022

- Responsibilities: Designed and implemented optimization schemes for incorporating direct and indirect causal knowledge in structure learning. Developed 'Concept-Driven Causal Models' to enhance causal discovery using concept-level prior knowledge, demonstrating effectiveness across multiple use cases.

Lily - Easy-to-use tool for women to support health issues Aug 2018 - Jul 2019

- Responsibilities: Developed an AI-powered automated bot that provided information, advice, and support on pregnancy-related health issues. Worked on backend development, including onboarding interactions, daily subscription features, and AI-driven automated responses.

WinWin - Digital sales management system May 2017 - Feb 2018

- Responsibilities: Served as the core backend developer for a sales monitoring system, contributing to client order management, product inventory management, transaction processing, and payment system features.

RIDF - Remote monitoring and management tool Nov 2016 - May 2017

- Responsibilities: Led backend development for a remote monitoring system, building project management, progress reporting, and visualization features for infrastructure monitoring.

Skills

- Causal Discovery, Machine Learning, Predictive Analytics, Causal Inference, Statistics, Data Visualization, Data Analytics, Deep Neural Networks (DNN), Convolutional Neural Networks (CNN), Autoencoders (AE, VAE), Vision Models, Natural Language Processing (NLP), Large

Language Models (LLMs), Retrieval-Augmented Generation (RAG), Generative AI, Computer Vision, Pattern Recognition, Active Learning, Amazon Web Services (AWS), Software Development, Hugging Face, Singularity/Docker.

- Python, R, C/C++, Java, MATLAB, JavaScript, SQL, Django, LaTeX, Git.
- PyTorch, TensorFlow, Keras, Transformer.

Talks

- Prediction of Adsorption Energies using Invariant Molecular Representations (IMRs), Annual ECO-CBET Seminar, USC, May 2024
- AI with Domain Knowledge, Graduate Research Seminar, UNC Charlotte, September 2021
- Causal Analysis: Discovery, Validation & Inference, Inaugural Seminar for Lowe's-UNC Charlotte Collaboration, UNC Charlotte, August 2021
- Affective Polarization on Social Networks, Inaugural Seminar for UQ-NASCL Lab Collaboration, UNC Charlotte, Summer 2020

Services

- **Reviewer -** AISTATS 2022, AISTATS 2023 (Top 10% reviewers), ICMLA 2023
- **Volunteer –** BUET System Analysis Design and Development Group, 2011-2012

Travel Grants & Fellowships

- **2025** Travel Grant to attend & present at ICPRAM 2025 by UNC Charlotte.
- **2023** Graduate School Summer Fellowship, UNC Charlotte.
- **2023** Travel Grant to attend & present at ICMLA 2023 by UNC Charlotte.
- **2023** Travel Grant to attend & present ICPRAM 2023 by UNC Charlotte.
- **2019** Bangladesh-Sweden Trust Fund.