Ayan Chatterjee

Short Bio

I am currently a fourth-year Ph.D. student at the Network Science Institute (NetSI) of Northeastern University, Boston. My research interests primarily lie in the field of graph machine learning, with a specific focus on areas such as link prediction, graph embeddings, and the application of network science in the context of biological networks. Prior to my time at NetSI, I gained valuable experience while working at NVIDIA Graphics, where I contributed to the development of various GPU architectures, including Turing, Ampere, and Hopper. These advancements in GPU technology have played a significant role in fueling the ongoing revolution in artificial intelligence.

Contact Information

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Education

Northeastern University (2019 - Present)
Ph.D. Student, Network Science Institute
Advisor: Prof. Tina Eliassi-Rad
Research Interests: Graph Machine Learning, Link Prediction, Interpretability, XAI, and Network Science.

Publications

Ayan Chatterjee, Robin Walters, Giulia Menichetti, Tina Eliassi-Rad. 2023. Disentangling Node Attributes from Graph Topology for Improved Generalizability in Link Prediction. Under review to NeurIPS 2023. Pre-print: https://arxiv.org/abs/2307.08877.

Ayan Chatterjee, Robin Walters, Zohair Shafi, Omair Shafi Ahmed, Michael Sebek, Deisy Gysi, Rose Yu, Tina Eliassi-Rad, Albert-László Barabási, Giulia Menichetti. 2021. Improving the generalizability of protein-ligand binding predictions with AI-Bind. Nat Commun 14, 1989 (2023). https://doi.org/10.1038/s41467-023-37572-z.

Zohair Shafi, **Ayan Chatterjee**, Tina Eliassi-Rad. 2023. Explaining Node Embeddings. In preparation for Applied Network Science.

Ayan Chatterjee, Qingtao Cao, Amirhossein Sajadi, Babak Ravandi. Deterministic random walk model in NetLogo and the identification of asymmetric saturation time in random graph. Appl Netw Sci 8, 33 (2023). https://doi.org/10.1007/s41109-023-00559-2.

Tünde Pacza, Mayara L. Martins, Maha Rockaya, Katalin Müller, **Ayan Chatterjee**, Albert-László Barabási & József Baranyi. MilkyBase, a database of human milk composition as a function of maternal-, infant- and measurement conditions. Sci Data 9, 557 (2022). https://doi.org/10.1038/s41597-022-01663-1.

Google Scholar: here.

Book Chapter	**Ayan Chatterjee**, Debayan Das, Amitava Mukherjee, Mrinal Kanti Naskar, Design of structural controllability for complex network architecture, in the book 'Advanced Methods for Complex Network Analysis, IGI Global Publishers, 2016. https://doi.org/10.4018/978-1-4666-9964-9.ch004.

Invited Talks

2022   Identifying interactions between novel protein targets and ligands: AI-Bind and AI-assisted molecular docking. Khoury College of Computer Sciences, Northeastern University, Boston. [Slides]

2022   Channing Methods Meeting on identifying interactions between novel protein targets and ligands: AI-Bind and AI-assisted molecular docking . Harvard T.H. Chan School of Public Health, Harvard University, Boston. [Slides]

Work Experience

Alexion AstraZeneca Rare Disease - *Summer Intern*   May 2023 - Aug 2023
Inductive link prediction on protein-protein interaction network for rare-disease centric target identification.

NVIDIA - *Computer Architect*   Aug 2017 - Aug 2019
Designing GPU architecture for AI acceleration and ray tracing.

Reviewer

Journal of Machine Learning Research

Workshop on Graph Learning Benchmarks

Learning on Graphs Conference

Transactions on Knowledge Discovery from Data