

Ayan Chatterjee

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Research Interests

Graph Machine Learning, Link Prediction, Drug Discovery, Artificial General Intelligence, Biological Networks, Social Networks, Generalizability

Education

Ph.D. in Network Science (with Computer Science specialization), 2019-Present

Network Science Institute, Northeastern University, Boston, MA.

Advisor: Prof. Tina Eliassi-Rad, President Joseph E. Aoun Professor, Khoury College of Computer Sciences and Network Science Institute, Northeastern University, Boston, MA.

Dissertation: Advances in Graph Machine Learning through Network Science with Applications in Drug Discovery, Expected Fall 2024

Committee: Tina Eliassi-Rad, Samuel Scarpino, Olga Vitek, and John Palowitch

Master of Technology (M.Tech) in Electronic Systems Engineering, 2015-2017

Indian Institute of Science, Bangalore, India

Thesis Topic: Multipacket Reception in Wireless Networks

Advisor: Dr. Chandramani Singh and Dr. T. V. Prabhakar

Bachelor of Electronics Telecommunication Engineering, 2011-2015

Jadavpur University, Kolkata, India

Thesis Topic: FPGA-based VGA Controller Design for CRTs and Graphics Processor Design

Advisor: Prof. M. K. Naskar

Professional Experience and Internships

Research Assistant, Network Science Institute, Northeastern University, Boston, Fall 2019 - Present

Topic: Generalizability in Graph Machine Learning

Advisor: Prof. Tina Eliassi-Rad

Internship at Google Research, Fall 2023 - Spring 2024

Topic: Foundation Model for Temporal Link Prediction

Mentor: John Plaowitch, Google

Internship at Alexion AstraZeneca Rare Disease, Summer 2023
Topic: Protein-protein interaction prediction using graph machine learning
Mentor: Babak Ravandi

Computer Architect at NVIDIA, 2017-2019
Topic: Designing low-power GPU architecture
Manager: Raghavendra H. Bhat

Internship at IBM Global Remote Monitoring Program, August 2015 - February 2015
Topic: Control of complex networks
Advisor: Dr. Amitava Mukherjee

Internship at Indian Statistical Institute, Kolkata, India. May 2014 - July 2014
Topic: Software implementation of several state-of-the-art stream ciphers
Advisor: Prof. Subhamoy Maitra

Peer-reviewed Publications

Inductive Link Prediction in Static and Temporal Graphs for Isolated Nodes. A. Chatterjee, R. Walters, G. Menichetti, T. Eliassi-Rad. Temporal Graph Learning Workshop @ NeurIPS 2023.

Improving the generalizability of protein-ligand binding predictions with AI-Bind. A. Chatterjee, R. Walters, Z. Shafi et al. Nat Commun 14, 1989 (2023).
<https://doi.org/10.1038/s41467-023-37572-z>

Deterministic random walk model in NetLogo and the identification of asymmetric saturation time in random graphs. A. Chatterjee, Q. Cao, A. Sajadi, et al. Appl Netw Sci 8, 33 (2023). <https://doi.org/10.1007/s41109-023-00559-2>

GRASP: Accelerating Shortest Path Attacks via Graph Attention. Zohair Shafi, Benjamin A Miller, Ayan Chatterjee, Tina Eliassi-Rad, Rajmonda S. Caceres. Deep Learning on Graphs Workshop @ KDD 2023.

MilkyBase, a database of human milk composition as a function of maternal-, infant- and measurement conditions. Pacza, T., Martins, M.L., Rockaya, M. et al. Sci Data 9, 557 (2022). <https://doi.org/10.1038/s41597-022-01663-1>

SCENIC: An Area and Energy-Efficient CNN-based Hardware Accelerator for Discernable

Classification of Brain Pathologies using MRI. B. S. T. Naidu et al. 2022 35th International Conference on VLSI Design and 2022 21st International Conference on Embedded Systems (VLSID), Bangalore, India, 2022, pp. 168-173, doi: 10.1109/VLSID2022.2022.00042

Snickometer edge detection by feature extraction in TF plane and wavelet domain. A Ghosh, A Chatterjee, A Roy, A Mukherjee, M.K. Naskar. 2018 IEEE Applied Signal Processing Conference (ASPCON), 143-148.

Non-autonomous dynamic network model involving growth and decay. A Chatterjee, A Chakraborty, S Pal, A Mukherjee, M.K. Naskar. 016 IEEE International Conference on Advanced Networks and Telecommunications Systems (ANTS), Bangalore, India, 2016, pp. 1-6, doi: 10.1109/ANTS.2016.7947793.

O (N²) Heuristic for the Estimation of Driver Nodes for the Controllability of Directed Complex Networks. A. Bhattacharya, A. Chatterjee, D. Das, A. Mukherjee, M.K. Naskar. LARGE SCALE COMPLEX NETWORK ANALYSIS: LSCNA2015, 32

AS 802.15. 4: A modified IEEE 802.15. 4 standard for more reliable communication and utilization of inactive period using optimized sleep period. B. Bandyopadhyay, S.J. Ahmed, D. Das, A. Chatterjee. 2014 Annual IEEE India Conference (INDICON), 1-6

Characterizing behavior of Complex networks against perturbations and generation of Pseudo-random networks. D. Das, A. Chatterjee, B. Bandyopadhyay, S.J. Ahmed. 2014 Annual IEEE India Conference (INDICON), 1-6

Markov chain-based analysis of IEEE 802.15. 6 mac protocol in real life scenario. B. Bandyopadhyay, D. Das, A. Chatterjee, S.J. Ahmed, A. Mukherjee. Proceedings of the 9th international conference on body area networks, 331-337

A Degree-first Greedy Search Algorithm for the Evaluation of Structural Controllability of Real World Directed Complex Networks. D. Das, A. Chatterjee, N. Pal, A. Mukherjee, M.K. Naskar. Netw. Protoc. Algorithms 6 (1), 1-18

Heuristic for maximum matching in directed complex networks. A. Chatterjee, D. Das, M. K. Naskar, N. Pal and A. Mukherjee. 2013 International Conference on Advances in

Computing, Communications and Informatics (ICACCI), Mysore, India, 2013, pp. 1146-1151, doi: 10.1109/ICACCI.2013.6637339

Book Chapters

Design of Structural Controllability for Complex Network Architecture. A. Mukherjee, A. Chatterjee, et al. Advanced Methods for Complex Network Analysis, edited by Natarajan Meghanathan, IGI Global, 2016, pp. 98-124.
<https://doi.org/10.4018/978-1-4666-9964-9.ch004>

Pre-prints

Topology-Driven Negative Sampling Enhances Generalizability in Protein-Protein Interaction Prediction. A. Chatterjee, B. Ravandi, ..., T. Eliassi-Rad. arXiv preprint
<https://www.biorxiv.org/content/10.1101/2024.04.27.591478v1>

Disentangling Node Attributes from Graph Topology for Improved Generalizability in Link Prediction. A. Chatterjee, R. Walters, G. Menichetti, T. Eliassi-Rad. arXiv preprint
<https://arxiv.org/abs/2307.08877>

Link Capacity Distributions and Optimal Capacities for Competent Network Performance. S. Pal, A. Chatterjee, D. Bakshi, A. Mukherjee. arXiv preprint
<https://arxiv.org/abs/2002.02522>

Talks and Conference Presentations

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

Presented "Non-Autonomous Dynamic Network Model Involving Growth And Decay" at the IEEE International Conference on Advanced Networks and Telecommunications Systems between 6-9 November 2016 in Bangalore, India.

Teaching and Mentoring

Teaching assistant for Fall 2023: NETS 7332 -- Machine Learning with Graphs (CRN 19900) <https://eliassi.org/fa23nets.html>

Mentored 6 undergraduate and Master's students at Northeastern University in 4 different research projects.

Mentored 1 intern and 1 new hire at NVIDIA, Bangalore, India.

Academic Service

Peer reviewer for the Journal of Machine Learning Research, Workshop on Graph Learning Benchmarks @ KDD 2023, Learning on Graphs Conference 2022/2023, Transactions on Knowledge Discovery from Data, Temporal Graph Learning Workshop @ NeurIPS 2023, Nature Communications.

Undergraduate Student Representative at Jadavpur University, India. 2011-2015.

Other Academic Achievements and Special Laurels

Pharmacy Golden Jubilee Best Student of the Year award for the student who scored the highest percentage of marks in the UG Final Examination 2015.

University Medal for standing first in merit at the Bachelor of Electronics & Telecommunication Engineering (BETCE) Final Examination 2015.

J. P. Saha Memorial Gold-Centered Silver Medal for securing the highest total marks in the theoretical papers at the Bachelor of Electronics & Telecommunication Engineering (BETCE) Final Examination 2015.

Pran Kumar Bhattacharya Memorial Gold Medal for standing First in order of merit at the Bachelor of Electronics & Telecommunication Engineering (BETCE) Final Examination 2015.

Prof. Sudhanshu Deb Memorial Gold-Centered Silver Medal for securing the highest aggregate marks in IC Technology and Design and VLSI Design at BETCE Final Examination 2015.

Dr. B. C. Roy Memorial Gold-Centered Silver Medal for securing the highest aggregate score in all courses at the Bachelor of Engineering Examination 2015.

Sourav Banerjee Memorial Gold-Centered Silver Medal for standing First in order of merit at the Bachelor of Electronics & Telecommunication Engineering (BETCE) Final Examination 2015.

Prof. Debidas Mukhopadhyay Memorial Gold-Centered Silver Medal for securing the highest aggregate marks in Electron Devices 1&2 at the Bachelor of Electronics & Telecommunication Engineering (BETCE) Final Examination 2015.

DAAD-WISE Scholarship in 2014 for summer research internship at RWTH Aachen

University, Germany.

Summer Research Fellowship organized by the Indian Academy of Sciences in 2014.

Rank in West Bengal in Higher Secondary Examination (+2) among ~ 7,00,000 students in 2011.

54th Rank in the West Bengal Joint Entrance Examination (Engineering) among ~ 1,10,000 students in 2011.

7th Rank in the Secondary Examination (10) among ~ 9,00,000 students in 2009.

Mamraj Agarwal Rashtriya Puraskar for obtaining 93.25% in the Secondary Examination 2009 held under the West Bengal Board of Secondary Education.

Outreach

YouTube Channel for teaching Network Science and Graph Machine Learning to a broad audience: <https://www.youtube.com/@NetworksAndGraphs>

Extracurricular Activities and Hobbies

Coordinator and Instructor at the Science Camp in May 2013 organized by the Matrix Publishers, Kolkata, India.

Guitarist in college band. Participated in various competitions representing Jadavpur University, India.

Guitar instructor at Forte Piano School of Music, Bangalore, India between 2016-2018.