Eeshaan Jain

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Education

École Polytechnique Fédérale de Lausanne — Lausanne, Switzerland
*1st year PhD in Computer Science @ AI in Molecular Medicine Lab (GPA: **6/6**)* — *Sep '24 – Ongoing*
Advisor: Prof. Charlotte Bunne
Semester Exchange in Computer Science — *Sep '22 – Feb '23*

Indian Institute of Technology Bombay — Mumbai, India
*Dual Degree: B.Tech in Electrical Engineering and M.Tech in Artificial Intelligence (GPA: **9.73/10.0**)* — *Jul '19 – Jun '24*
Advisors: Prof. Abir De, Prof. Soumen Chakrabarti
*Institute **Silver Medalist**, Department **Rank 1***

Research Interests

Agentic Systems, Reinforcement Learning, AI for Biology, Learning on Graphs, Submodular Optimization

Publications

[1] **Eeshaan Jain***, Kiril Vasilev*, Alexandre Misrahi*, Phil F Cheng, Petros Liakopoulos, Olivier Michielin, Michael Moor, Charlotte Bunne. *MTBBench: A Multimodal Sequential Clinical Decision-Making Benchmark in Oncology*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2025.

[2] **Eeshaan Jain**, Johann Wenckstern, Benedikt von Querfurth, Charlotte Bunne. *Test-Time View Selection for Multi-Modal Decision Making*. *In Submission*, 2025.
◇ Oral Presentation at *Machine Learning for Genomics Explorations Workshop*, *ICLR* 2025.
◇ *Generative and Experimental Perspectives for Biomolecular Design Workshop*, *ICLR* 2025.

[3] Indradyumna Roy*, Saswat Meher* **Eeshaan Jain**, Soumen Chakrabarti, Abir De. *Graph Matching Systems Deserve Better Benchmarks*. *International Conference on Machine Learning (ICML)*, 2025.

[4] **Eeshaan Jain***, Johann Wenckstern*, Kiril Vasilev, Matteo Pariset, Andreas Wicki, Gabriele Gut, Charlotte Bunne. *AI-powered virtual tissues from spatial proteomics for clinical diagnostics and biomedical discovery*. *In Submission (arXiv:2501.06039)*, 2025.
◇ Best Paper Award at *Machine Learning for Genomics Explorations Workshop*, *ICLR* 2025.

[5] **Eeshaan Jain***, Indradyumna Roy*, Soumen Chakrabarti, Abir De. *Clique Number Estimation via Differentiable Functions of Adjacency Matrix Permutations*. *International Conference on Learning Representations (ICLR)*, 2025.

[6] **Eeshaan Jain**, Indradyumna Roy, Saswat Meher, Soumen Chakrabarti, Abir De. Graph Edit Distance Evaluation Datasets: Pitfalls and Mitigation. *Learning on Graphs Conference (LOG)* (Extended Abstract), 2024.

[7] **Eeshaan Jain***, Indradyumna Roy*, Saswat Meher, Soumen Chakrabarti, Abir De. *Graph Edit Distance with General Costs Using Neural Set Divergence*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2024.
◇ Also presented at *Learning on Graphs Conference (LOG)* (Extended Abstract), 2024.

[8] **Eeshaan Jain**, Tushar Nandy, Gaurav Aggarwal, Ashish Tendulkar, Rishabh Iyer, Abir De. *Efficient Data Subset Selection to Generalize Training Across Models: Transductive and Inductive Networks*. *Advances in Neural Information Processing Systems (NeurIPS)*, 2023.

* *denotes equal contribution.*

Fellowships and Awards

- Outstanding research in first year of PhD by **EPFL (600$)** (*2025*)
- Awarded research and travel grant by **Broad Institute of MIT and Harvard (3500$)** for attending ICLR (*2025*)
- Awarded the **Best Poster Award** at Easter European ML Summer School in Novi Sad, Serbia (*2024*)
- Awarded the **Institute Silver Medal** at IIT Bombay for outstanding academic performance (#2 rank) (*2024*)
- Awarded the **Undergraduate Research Award** for the most outstanding Bachelor's Thesis in Electrical Engineering (*2023*)
- Awarded **Google Conference Scholarship (3000$)** and **NeurIPS Scholar Award** for attending NeurIPS (*2023*)
- Awarded the **Institute Academic Prize** for being the top 2 ranks in Electrical Engineering (*2021 & 2022*)

Industry Experience

Google Research *May '22 – May '23*

Bachelor's Thesis-I with Gaurav Aggarwal, Prof. Abir De, Prof. Rishabh Iyer (UT Dallas) *Remote*

- Associated papers: [8] (NeurIPS 2023)
- Introduced SubSelNet: A GNN and attention-based model encoder for efficient approximation of outputs across architectures, with trainable, differentiable selectors that relax the combinatorial optimization objective for subset selection. Demonstrated consistent outperformance in accuracy, selection time, and memory efficiency in AutoML tasks, including Neural Architecture Search and Hyperparameter Optimization.

AWL, Inc. Japan, Sony Japan *May '22 - Jul '22*

Core AI Team: Scalable Inference on Low-Power Devices via Hardware Optimization *Japan*

- Conducted an extensive survey of frameworks for model compression, quantized training, and inference acceleration. Engineered novel CPU-optimized operations with Apache TVM, achieving up to $8\times$ reduction in inference latency on low-power devices without degrading output fidelity. Integrated GPU-accelerated TensorRT and DLA pipelines with seamless CPU fallbacks to enhance batched inference efficiency on Jetson platforms.

Research Experience

End-to-end Differentiable Approaches for Combinatorial Optimization on Graphs *Jul '23 - Jun '24*

Master's Thesis, Advisor: Prof. Abir De, Prof. Soumen Chakrabarti *IIT Bombay*

- Associated papers: [7] (NeurIPS 2024 + LoG 2024), [6] (LoG 2024), [5] (ICLR 2025), [3] (In submission 2025)
- Developed end-to-end differentiable methods for APX-Hard combinatorial optimization on graphs and released novel, unbiased datasets for training reasoning algorithms through distant supervision.

Generalization Bounds and Explainability of Graph Neural Networks *May '23 - Aug '23*

Research Assistant, Advisor: Prof. Vikas Garg, Amauri H. Souza *Aalto University*

- Derived tighter Rademacher generalization bounds for subclasses of message-passing networks, extending the analysis to temporal GNNs. Established connections between robustness, generalizability, and faithfulness of explanations in dynamic graph settings.

Fairness Audits of Black Box Neural Networks *Jan '23 - May '23*

Bachelor's Thesis-II, Advisor: Prof. Abir De *IIT Bombay*

- Developed a comprehensive framework for auditing fairness in black-box models through near-optimal querying under budget constraints. Designed an RL-driven sampling strategy combining a VAE and Gaussian Process surrogate to efficiently explore the input space. Introduced *Disparity*, a novel fairness metric that unifies group and individual fairness, and formulated a disparity-minimization greedy optimization algorithm to mitigate post-audit manipulation effectively.

Technical Projects

Post-Hoc Out-of-Distribution Detection *Mar '22 - May '22*

Advisor: Prof. Sunita Sarawagi (CS 726: Advanced Machine Learning) *IIT Bombay*

- Developed a novel OOD detection scoring function based on a Dirichlet distribution assumption over DNN softmax logits, asymptotically interpreted as an ensemble of two positive scoring functions. Demonstrated consistent outperformance across multiple datasets using FPR95, AUROC, and AUPR metrics, while reducing hyperparameter tuning complexity by showcasing the effectiveness of marginless loss functions.

Efficient Matroid-constraint-based Submodular Maximization *Mar '22 - May '22*

Advisor: Prof. Ganesh Ramakrishnan (CS 769: Optimization for Machine Learning) *IIT Bombay*

- Extended SUBMODLIB by implementing Continuous-Greedy and Accelerated Continuous-Greedy algorithms for maximizing submodular functions under matroid constraints with $(1 - 1/e - \epsilon)$ guarantees. Further, enhanced solution translation through a modified Pipage-Rounding subroutine for efficient conversion of fractional solutions to discrete subsets, and incorporated formulations for the Submodular Welfare Problem, as well as Separable and Generalized Assignment Problems.

Sparse Estimation of Epidemic State using Graph Neural Networks *Sep '21 – Nov '21*

Advisor: Prof. Abir De (CS768: Learning with Graphs) *IIT Bombay*

- Generated random and small-world networks using Erdös–Rényi, Watts-Strogatz, and Barabási–Albert models, and simulated epidemic spread with the SIR contagion model, treated as a CTMC, to construct a spatio-temporal dataset. Applied GCNs for node classification (S/I/R), achieving effective monitoring by observing only (15%–25%) of nodes.

Summer Schools

Eastern European Machine Learning Summer School (Google Deepmind) *Novi Sad, Serbia (Jul'24)*
Best Poster Award: Efficient Data Subset Selection to Generalize Training Across Models: Transductive and Inductive Networks

Machine Learning for Drug Discovery Summer School (Recursion Pharma) *Montreal, Canada (Jun'24)*
Hackhaton Winner: Kinase Selectivity Chalenge - Predict interactions between proteins and molecules

Scholastic Achievements

- **Department Rank 1** out of 79 students in the Dual Degree Programme, Electrical Engineering (*2020 – 2022*)
- Achieved **All India Rank 120** in JEE Mains (1.3M candidates) and **Rank 355** in JEE Advanced (0.25M candidates) (*2019*)
- Ranked **top 300 across India** and appeared in the Indian National Chemistry and Astronomy Olympiads (*2019*)
- Secured an **All India Rank of 100** and received the **KVPY Fellowship** by Department of Science and Technology (*2018*)

Professional Activities, Leadership, and Service

Workshop Organizer

Assisted in organization of workshops at conferences

- **Learning Meaningful Representations of Life (LMRL):** An ICLR 2025 workshop on multi-scale and multi-modal representation learning from biological data

Student Mentor

Student Mentorship Program: Selected based on a rigorous process of interviews, SOP, and peer reviews

- **Institute Student Mentor:** Responsible for guiding **12 freshmen** through their first year in the institute
- **Department Academic Mentor:** Mentoring a group of **6 junior undergraduates** with their academics and research

Teaching Assistantships | IIT Bombay

Facilitating smooth course organization, grading papers, mentoring students, conducting tutorials and help sessions

- **Computer Science:** Optimization for Machine Learning, Learning with Graphs, Machine Learning, Intro to CS
- **Math and Sciences:** Partial Differential Equations, Ordinary, Differential Equations, Quantum Chemistry

Teaching Assistantships | EPFL

Facilitating smooth course organization, grading papers, mentoring students, conducting tutorials and help sessions

- **Computer Science:** Introduction to Computing, Foundation Models & Generative AI

Extra Curricular Activities and Other Achievements

Achievements	• First place, winning PC setup (~ 5000\$) at **Jump Trading** Speed Math competition, ICLR 2025 • First place, winning 10000\$ GPU Credits at **Jump Trading** Speed Math competition, NeurIPS 2024 • Completed all six levels of **Speed Arithmetic** under IPA, and **2nd** in their national-level competition • Winner of the 2020 **Poker** tournament hosted at IIT Bombay
Volunteering	• Acted as the **Lead Convener** of the Chemistry Club at IIT Bombay promoting the use of **AI in chemistry** • Took **Python** sessions for **1000+** undergraduates and graduates at IIT Bombay over the summer
Others	• Co-founded **AISRG** – the first student reading group on Artificial Intelligence at IIT Bombay • Elected **Class Representative** for the Electrical Engineering department for three consecutive years • Successfully completed an year-long training in **Chess** under **National Sports Organization**