

EESHAAN JAIN

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EDUCATION

École Polytechnique Fédérale de Lausanne

PhD in Computer Science under *Prof. Charlotte Bunne, AI in Molecular Medicine Lab*
Semester Exchange in Computer Science

Lausanne, Switzerland

Sep '24 – Ongoing

Sep '22 – Feb '23

Indian Institute of Technology Bombay

Dual Degree: B.Tech in Electrical Engineering and M.Tech in Artificial Intelligence (Grade: **9.73/10.0**)

Mumbai, India

Jul '19 – Jun '24

PUBLICATIONS

1. **Eeshaan Jain** et al. "**Graph Edit Distance with General Costs Using Neural Set Divergence**", at [NeurIPS 2024](#).
2. **Eeshaan Jain** et al. "**Efficient Data Subset Selection to Generalize Training Across Models: Transductive and Inductive Networks**", at [NeurIPS 2023](#).
3. **Eeshaan Jain** et al. "**Graph Edit Distance Evaluation Datasets: Pitfalls and Mitigation**", under review.
4. **Eeshaan Jain** et al. "**Solving Graph Combinatorial Problems via Differentiable Permutation Functions**", under review.

SCHOLASTIC ACHIEVEMENTS

- 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)
- **Department Rank 1** out of 79 students in the Dual Degree Programme, Electrical Engineering (2020 – 2022)
- Awarded the **AP Grade** for **outstanding performance** in Partial Differential Equations and Quantum Chemistry (2021)
- Secured an **All India Rank of 355** in JEE Advanced among 0.25 million candidates (2019)
- Secured an **All India Rank of 120** in JEE Mains (Engineering) among 1.3 million candidates (2019)
- Ranked **top 300 across India** and appeared in the Indian National Chemistry and Astronomy Olympiads (2019)

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)

Montreal, Canada (Jun'24)

Hackathon Winner: *Kinase Selectivity Challenge - Predict interactions between proteins and molecules*

INDUSTRY EXPERIENCE

Efficient Data Subset Selection to Generalize Training Across Models

May '22 – May '23

Google Research, Bachelor's Thesis-I with *Prof. Abir De, Prof. Rishabh Iyer (UT Dallas)*

Remote, IIT Bombay

- Introduced a **GNN** and **attention-based** model encoder for crude **approximation** of outputs over a set of architectures
- Relaxed the **combinatorial optimization** objective for subset selection on the novel trainable & differentiable selectors
- Demonstrated that our approach constantly **outperformed** other methods in terms of **accuracy, subset selection time** and **memory consumption** and in **AutoML** tasks such as Neural Architecture Search and Hyperparameter Optimization

Scalable Inference on Low-Power Devices via Hardware Optimization

May '22 - Jul '22

AWL, Inc. Japan: Core Artificial Intelligence Team along with Sony Japan

Sapporo, Japan

- Surveyed optimization frameworks based around **model compression, quantized training** and **inference speed-up**
- Implemented novel **hardware-optimized operations** and routines on CPUs using **Apache TVM** to bring down single image and graph inference times on low-power devices by **8x** without hurting the metrics of the outputs
- Utilized GPU-based **TensorRT** and **DLA** frameworks with CPU fallbacks to speed up batched inference on Jetson GPUs

RESEARCH EXPERIENCE

End-to-end Differentiable Approaches for Combinatorial Optimization on Graphs

Jul '23 - Jun '24

Dual Degree Project, Guide: *Prof. Abir De, Prof. Soumen Chakrabarti*

IIT Bombay

- Designed end-to-end differential approaches to APX-Hard **combinatorial optimization** problems on graphs
- Released **new** and **unbiased** datasets for learning **reasoning algorithms** on graphs via distant supervision

Generalization Bounds and Explainability of Graph Neural Networks

May '23 - Aug '23

Research Assistant, Guide: *Prof. Vikas Garg, Amauri H. Souza*

Aalto University

- Derived stronger and tighter **generalization bounds** for different subclasses of message-passing networks
- Connected notions of **robustness, generalizability** and **faithfulness** of explanations with extensions to temporal graphs

Fairness Audits of Black Box Neural Networks

Jan '23 - May '23

Bachelor's Thesis-II, Guide: Prof. Abir De

IIT Bombay

- Approximated fairness of blackbox models through **near-optimal querying** of data points under budget constraints
- Devised an **RL-based algorithm** to sample points through a VAE coupled with a **Gaussian Process** surrogate model
- Introduced a new fairness metric called **Disparity** bridging group and individual fairness notions, and formulated a disparity-minimization-based **greedy optimization** problem to **minimize post-audit manipulation**

TECHNICAL PROJECTS

Post-Hoc Out-of-Distribution Detection

Mar '22 - May '22

Guide: Prof. Sunita Sarawagi (CS 726: Advanced Machine Learning)

IIT Bombay

- Introduced a scoring function based on the assumption of a **Dirichlet distribution** on the DNN's softmax-ed logits for OOD detection and showed that it could be asymptotically interpreted as an **ensemble** of two positive scoring functions
- Showed that the score already **outperformed** other OOD methods on multiple datasets using **FPR95, AUROC** and **AUPR**
- **Reduced** the number of hyperparameters to tune by demonstrating the **efficacy** of marginless loss functions for the task

Efficient Matroid-constraint-based Submodular Maximization

Mar '22 - May '22

Guide: Prof. Ganesh Ramakrishnan (CS 769: Optimization for Machine Learning)

IIT Bombay

- Implemented the efficient **Continuous-Greedy** and **Accelerated Continuous-Greedy** algorithms in SUBMODLIB to maximize submodular functions under a matroid constraint with $(1 - 1/e - \epsilon)$ guarantees
- Modified the **Pipage-Rounding** subroutine for **efficient translation** of fractional solutions to discrete subsets
- Implemented the **Submodular Welfare Problem** and, **Separable** and **Generalized Assignment Problem**

Sparse Estimation of Epidemic State using Graph Neural Networks

Sep '21 - Nov '21

Guide: Prof. Abir De (CS768: Learning with Graphs)

IIT Bombay

- Generated random and **small-world networks** using the Erdős-Rényi, Watts-Strogatz, and Barabási-Albert models
- Implemented the **SIR** contagion model, treating the epidemic as a CTMC, on our graphs to get a **spatio-temporal** dataset
- Performed **node classification** (S/I/R) using **GCNs** by monitoring only a **small subset** of nodes (15% - 25%)

TECHNICAL SKILLS

Programming Languages: Python, C++, Scala, Julia

Machine Learning: PyTorch, PyTorch-Geometric, NLTK, Scikit-Learn, OpenCV, TVM, TensorRT

KEY COURSEWORK

Machine Learning: Programming for Data Science, Introduction to Machine Learning, Learning with Graphs, Foundations of Intelligent Learning Agents, Advanced Machine Learning, Optimization for Machine Learning, Natural Language Processing[†]

Electrical Engineering and Computer Science: Probability and Random Processes, Signal Processing, Microprocessors, Communication Systems, Digital Signal Processing, Image Processing, Markov Chains, Operating Systems, Information Theory and Coding[†], Automatic Speech Processing[†], Functional Programming[†], Advanced Concentration Inequalities ([†] taken at EPFL)

Mathematics and Physics: Calculus, Linear Algebra, Partial Differential Equations, Complex Analysis, Quantum Physics

POSITIONS OF RESPONSIBILITY

Student Mentor

May '23 - Ongoing

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

IIT Bombay

- **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:** CS 769: Optimization for Machine Learning, CS 768: Learning with Graphs, CS 419: Machine Learning
- **Math and Sciences:** MA 207: Partial Differential Equations, MA 108: Differential Equations, CH 107: Quantum Chemistry

EXTRA CURRICULAR ACTIVITIES AND OTHER ACHIEVEMENTS

Achievements	<ul style="list-style-type: none">• Represented IIT Bombay at Chemenigma hosted by IISc Bangalore, and stood first overall• Completed all six levels of Speed Arithmetic under IPA, and stood 2nd in their national-level competition• Winner of the 2020 Poker tournament hosted at IIT Bombay
Volunteering	<ul style="list-style-type: none">• 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	<ul style="list-style-type: none">• 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