

# Shreyas Bhat

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## EDUCATION

University of North Carolina at Chapel Hill

PhD, Computer Science

Advisor: **Prof. Junier Oliva**

Chapel Hill, NC

Aug. 2024 – Present

Birla Institute of Technology and Science, Pilani

B.E. Electronics, M.Sc. Biology, Minor in Data Science

Goa, India

Aug. 2019 – 2024

## RESEARCH INTEREST

Multi-agent systems, Interactive ML, Language Processing, Generative Models for Structure Data and Sets, Intelligent Agents, Reinforcement Learning, Active Learning, AI for Health, and Medical Imaging.

## EXPERIENCE

LUPA Lab, UNC Chapel Hill

Graduate Research Assistant

Aug. 2024 – Present

Chapel Hill, United States

- Developed a universal, permutation-invariant set-based foundational model with semantic grounding to enable cross-dataset reasoning; achieved **71% improvement in average F1** and **24% reduction in RMSE** across 6 benchmark datasets.
- Developed an interactive agent framework that dynamically selects cost-effective features and display options for black-box decision-makers (LLMs); **outperformed baselines in 17/17 environments**, increasing decision accuracy by up to **18% under budget constraints**.
- Supervisor: **Prof. Junier Oliva**

QTIM, Harvard University, MIT and MGH

Research Intern

Jan. 2023 – June 2024

Boston, United States

- Led development of a multimodal deep learning system for non-invasive molecular profiling of brain metastases; achieved **state-of-the-art 72% F1** on CDK and TMB biomarker prediction from MR imaging. (**RSNA 2023, ISBI workshops 2024**)
- Assisted in designing predictive models integrating MRI with clinical data to forecast immune checkpoint inhibitor (ICI) efficacy, **improving patient stratification accuracy by 15%** for treatment response. (**MICCAI workshop 2024**).
- Supervisor: **Prof. Jayashree Kalpathy-Cramer, Prof. Bruce Rosen, Prof. Christopher Bridge, Prof. Albert Kim**

APPCAIR AI Labs, BITS Pilani

Undergrad Student Researcher

Jan 2022 – May 2023

Goa, India

- Proposed and developed a self-refining LLM framework with logical feedback for target-specific molecule generation; **reduced docking energies by 15–25% compared to baselines** on JAK2 and DRD2 targets (**AAAI 2024**).
- Devised a reliable model compression method via iterative knowledge distillation with calibration-sensitive adjustments, **compressing models by 80% with less than 2% accuracy loss**, while preserving calibration (**ICIP 2023**).
- Built molecular property predictors using enhanced Graph and Message Passing Neural Networks, achieving **7–10% lower MAE** and improved performance on the QM9 benchmark.
- Supervisor: **Prof. Ashwin Srinivasan**

## SELECTED PUBLICATIONS

- “Generating Novel Leads for Drug Discovery Using LLMs for Logical Feedback” - **Shreyas Bhat Brahmavar**, Ashwin Srinivasan, Tirtharaj Dash, Lovekesh Vig, Arijit Roy, Sowmya Krishnan, Raviprasad Aduri. *Accepted at AAAI 2024 main track full-paper*.[\[Link\]](#)
- “IKD+: Reliable Low Complexity Deep Models for Retinopathy Classification” - **Shreyas Bhat Brahmavar**, Rohit Rajesh, Tirtharaj Dash, Lovekesh Vig, Tanmay Tulsidas Verlekar, Md Mahmudul Hasan, Tariq Khan, Erik Meijering, Ashwin Srinivasan. *Accepted at IEEE International Conference on Image Processing 2023 short paper*.[\[Link\]](#)

## SELECTED PREPRINTS AND WORKSHOP PAPERS

- “Towards Universal Neural Inference” - **Shreyas Bhat Brahmavar**, Yang Li, Junier Oliva. *Under Review* [\[Preprint\]](#)
- “Dynamic Information Sub-Selection for Decision Support” - Hung-Tien Huang, Maxwell Lennon, **Shreyas Bhat Brahmavar**, Sean Sylvia, Junier B Oliva. *Under Review* [\[Preprint\]](#)

3. “Multimodal Deep Learning-Based Prediction of Immune Checkpoint Inhibitor Efficacy in Brain Metastases” - Tobias R. Bodenmann, Nelson Gil, Felix J. Dorfner, Mason C. Cleveland, Jay B. Patel, **Shreyas Bhat Brahnavar**, Melisa S. Guelen, Dagoberto Pulido-Arias, Jayashree Kalpathy-Cramer, Jean-Philippe Thiran, Bruce R. Rosen, Elizabeth Gerstner, Albert E. Kim & Christopher P. Bridge, *Accepted at CaPTion workshop, MICCAI 2024*. [[Link](#)]
4. “Deep Learning-based Non-Invasive Molecular Profiling of Brain Metastases from MR Imaging” - **Shreyas Bhat Brahnavar\***, Tiago Goncalves\*, Tobias R. Bodenmann, Syed Rakin Ahmed, Jay B. Patel, Praveer Singh, Katharina V. Hoebel, Mason C. Cleveland, Felix Dorfner, Dagoberto Pulido-Arias, Bruce R. Rosen, Jaime S. Cardoso, Jayashree Kalpathy-Cramer, Elizabeth Gerstner, Albert E. Kim, Christopher P. Bridge. *Accepted at ISBI 2024 abstract*
5. “Efficient Integration of Molecular Representation and Message-Passing Neural Networks for Predicting Small Molecule Drug-like Properties” - **Shreyas Bhat Brahnavar**, Mrunmay Mohan Shelar, Revanth Harinarthini, Hemanth Bandaru, Nahush Harihar Kumta, Ojas Wadhwani, and Raviprasad Aduri, *Accepted at International Conference on Drug Discovery 2022 abstract* [[Poster](#)][[Link](#)]

\* - Equal contribution.

## PROJECTS

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### Neural Tangent Kernel | [[GitHub](#)]

- Implemented and reproduced results from the NTK paper and extended it to the momentum optimiser, and derived the math behind.

### Game-theoretic Multi-Agent system

- Proposed and developed MAS-Zero-GT, a hybrid multi-agent framework combining LLM-driven reasoning with game-theoretic guarantees to ensure stable and coherent coordination for a variety of problems like the iterated prisoner’s dilemma.

### Code-Soup: Adversarial Learning Library | [[GitHub](#)]

- Contributed to the code base of code-soup, which is the python code for the book “Adversarial Deep Learning” written by Dr. Di Jin, Dr. Yifang Yin, Yaman Kumar, and Dr. Rajiv Ratn Shah, and its tutorials. You can use this in conjunction with a course on Adversarial Deep Learning or for study on your own.

### Learning paradigms on STL10 | [[GitHub](#)]

- Analyzed and compared different learning methods such as pseudo-labelling for semi-supervised, SimCLR Contrastive Learning for self-supervised on STL10 dataset. Additionally, used AutoAugment as an augmentation strategy for contrastive learning.

## TALKS / PRESENTATIONS

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1. “Using Deep Learning for Non-Invasive Molecular Profiling of Brain Metastases from MR Imaging” at **Martinos Center**, Boston, MA.
2. “Efficient Integration of Molecular Representation and Message-Passing Neural Networks for Predicting Small Molecule Drug-like Properties” was recognized as the **best poster** at ICDD 2022, the AI/ML for drug discovery track.

## OTHER ROLES

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### Reviewing and Teaching

- Reviewer at ICLR 2025, 2026 & AAAI 2026
- First Degree Teaching Assistant **BITS F464 - Machine Learning**: Conducted labs and tutorials on Linear Regression, Bayes Nets, SVMs, Neural Nets, Decision Trees and clustering for 150 cross-disciplinary students.
- Led the **Society for Artificial Intelligence and Deep Learning**, BITS-Goa AI society to promote research and open source projects among the undergraduate students.
- Lead Instructor for “Introduction to Machine Learning and Deep Learning” course: Delivered comprehensive lectures on ML/DL fundamentals to diverse student groups
- Co-Author of **Concepts of Deep Learning** website: Maintained an educational platform covering Python basics to advanced computer vision concepts.

## RELEVANT COURSES

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Theoretical Machine Learning, Reinforcement Learning, Optimization for Machine Learning, Foundation of Data Science, Applied Statistics and Methods, Optimization, Artificial Intelligence, Multimodal AI, LLMs for software engineering, Control Systems.