

Amirtha Varshini A S

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EDUCATION

- **Georgia Institute of Technology**, Atlanta, GA Aug. 2021 - May 2023
Master of Science in Computer Science (ML Concentration) **GPA: 4.0/4.0**
- **National Institute of Technology Tiruchirappalli**, India Jul. 2014 - May 2018
Bachelor of Technology in Electronics and Communication Engineering **GPA: 8.90/10**

TECHNICAL SKILLS

- **Languages:** Python, C++, C, SQL, Bash
- **Machine Learning & Frameworks:** PyTorch, TensorFlow, Scikit-learn, HuggingFace, DeepChem, Chemprop, CUDA, W&B, MLflow
- **Cheminformatics & Modeling:** RDKit, CReM, docking (AutoDock, Glide), OpenMM, structural alerts filtering, molecular property calculators
- **Data & Systems:** AWS, GCP, Redun, DuckDB, Linux
- **Graduate Coursework:** Machine Learning with Limited Supervision, Deep Reinforcement Learning, Computer Vision, Graduate Algorithms, Advanced Machine Learning, Deep Learning Specialization (Coursera)

EXPERIENCE

- **Montai Therapeutics**, Cambridge, MA - *Machine Learning Scientist II* Jul 2023 – Present
 - **Developed SynFlowNet**, a reaction-based GFlowNet model that generates synthesizable molecules from chemical reactions and building blocks. Trained models with the **Boltz-2 reward function** and bioactivity model scores, enabling probabilistic sampling of high-quality compounds with favorable physicochemical properties; multiple candidates were **validated by synthesis**.
 - **Designed fragment-based de novo workflows** with the CReM framework, generating chemically valid and synthetically accessible structures by design. Implemented **multi-objective optimization** with ADME property filters, bioactivity predictions, and reward conditioning to balance potency, novelty, and drug-likeness; contributed to the **open-source CReM library**.
 - **Built predictive ML models** for molecular property and SAR potency prediction (Spearman >0.8). Improved in-house enrichment factor by **28%** through large-scale pretraining (MolData) and delivered an additional **30% gain** in collaboration with Pfizer using PubMed-derived biochemical datasets.
 - **Advanced deep learning approaches:** integrated graph neural networks, transformers, Chemprop, and MegaMolBART embeddings with cheminformatics descriptors. Applied hybrid modeling with uncertainty quantification for robust compound nomination (**AUC ~0.8 across diverse targets**).
 - **Built interpretability frameworks** for GNNs and Transformers, applying Monte Carlo Tree Search and counterfactual generation to extract mechanistic substructure rationales. Developed **Streamlit dashboards** with RDKit visualization and SMARTS-based filters to display activity rationales, model predictions, and flagged structural alerts, directly supporting medicinal chemistry design decisions.
 - **Engineered scalable ML pipelines** on AWS for generative and predictive modeling, integrating cheminformatics modules (RDKit filters, property calculators, docking scores) with MLflow, Redun, DuckDB, and Weights & Biases. Enabled reproducible, distributed execution of large-scale de novo design and SAR modeling workflows.
 - **Contributed to scientific dissemination:** accepted poster at NeurIPS WiML workshop and open-source code contributions; regularly presented research outcomes to cross-functional teams.
- **Amazon Robotics**, Westborough, MA - *Software Development Engineer Intern* May 2022 - Aug. 2022
 - Performed object tracking on packages in a warehouse by integrating with segmented shipping labels returned by AR-ID, an ML, and CV-based solution. Successfully enabled AR-ID, an AI and computer vision-based barcode scanner, to process multiple packages using this tracking.
 - Developed an app using Augmented Reality(AR) in Microsoft Hololens 2 to identify the current package picked or stowed, based on the collision of the tracked package's hologram with a spatially anchored hologram mesh.
- **Qualcomm**, Bengaluru, India - *Software Engineer* Jul. 2018 - Aug. 2021
 - **ADAS team** -Designed Minidump feature on a QNX Real-time operating system to capture a snapshot of a system post-crash. Brought down the download time by **70%** and the size from **12GB to 300 MB**, enabling faster analysis
 - Developed a GDB-based Python and C parser to extract debug information from the collected kernel dump.
 - Built FastRPC framework to offload high-compute tasks from CPU to Digital Signal Processors, improving performance
 - Implemented tools to monitor system metrics such as watchdog timer, heartbeat, power consumption, and memory usage
 - Worked on bring-up of an SoC with ARM Architecture and developed tools for power, temperature & memory metrics

- **Interpreting GFlowNets for Drug Discovery** — NeurIPS WiML Workshop (Poster) Aug. 2025 – Current
 - Designed the first **interpretability framework for hierarchical GFlowNets** in molecular design, advancing transparency of deep generative models for drug discovery.
 - Engineered **gradient-based saliency maps** and **SMARTS-driven counterfactuals** to produce atom-level attributions with causal evidence of substructure importance, accelerating molecular optimization.
 - Applied **sparse autoencoders and linear probes** to SynFlowNet embeddings, disentangling drug-likeness (QED) into interpretable latent factors such as size, polarity, and lipophilicity.
 - Demonstrated recovery of chemically meaningful motifs (functional groups, rings, halogens) from embeddings, bridging ML representations with medicinal chemistry reasoning.
 - Recognition: Ranked in the **top 15% of reviewers** for NeurIPS WiML Workshop, highlighting research quality and contribution to the community.
 - **Resources:** OpenReview Link | GitHub Code
- **Explainability for Graph Neural Networks in Proactive Robot Assistance** — Georgia Tech (Advisor: Prof. Soeren Edelkamp)
 - Developed explainability methods for a **dynamic spatio-temporal GNN** performing real-time object tracking and future movement prediction in home environments.
 - Implemented **GNNExplainer** and novel counterfactual approaches to generate edge- and time-based explanations, producing **human-aligned, intuitive outputs**.
 - Created new evaluation metrics (**Edge-Time F1, Time Recall**) and validated across real-world activity datasets (HOMER).
 - Conducted ablation studies with saliency, attention weights, and temporal perturbations to assess explanation faithfulness.
 - Contributed to **PyTorch Geometric** explainer modules through metric design and code reviews. **GitHub: Link**
- **Text-to-video generation using Latent Diffusion** Aug. 2022 - Dec. 2022
 - Trained a transformer to generate future video frame embeddings on top of the Stable Diffusion encoder. **Link**
 - Outperformed the TGANv2 baseline by **26%** improvement in Frechet Video Distance score by using a novel combination of loss functions and video interpolation components.
- **Deep Reinforcement Learning (RL) based autonomous driving** Jan. 2022 - May 2022
 - Built TQC (Truncated Quantile Critics) algorithm with experience replay and increased rewards by **17%** for navigation in a self-driving simulator Donkeycar. Improved rewards by **42%** by training a Variational Autoencoder to compress inputs.
 - Generated a semantic segmentation mask using a pretrained autoencoder to visualize the model for interpretability. **Link**
- **Semantic Similarity and Toxicity Detection of Questions in Quora** Sep. 2021 - Dec. 2021
 - Using PyTorch, compared the results of BERT, Bi-LSTM, Bi-RNN, and Bi-GRU models with NLP word-embedding techniques TF-IDF Vectorization and Word2Vec to predict intent similarity and toxicity of questions on Quora. **Link**
 - Achieved F1-score of **0.7** by fine-tuning BERT to predict question sincerity and accuracy **0.89** for questions' similarities.
- **Computer Vision Tools for Non-verbal Communication in Interviews** Aug. 2021 - Dec. 2021
 - Devised a K-Nearest Neighbours(KNN) model to estimate head pose in videos with accuracy **83%**. Obtained features as the difference in minima and maxima of first-order pitch differences, from OpenFace Keypoints output on AMI corpus. **Link**
 - **Runner-up** at Innovation Competition 2022, an Entrepreneurial challenge of VentureLabs, Georgia Tech.
- **Low-cost intelligent vision in automotive (LIVA)** Jun. 2019 - Oct. 2019
 - Collected dataset of depth images using Kinect V2 mounted on a moving car. Achieved object detection accuracy **85%** in real-time to recognize pedestrians and vehicles by fine-tuning YOLO V3 model with depth images and COCO dataset.
 - Converted model to DLC and ran inference on Linux Vehicle platform using SNPE (Snapdragon Neural Processing Engine)
 - Top 6 finalists out of the 230+ applicants in Maker's Challenge of QBuzz 2019, Qualcomm's annual tech conference.
- **Real-Time Hand Gesture Recognition system** Jan. 2018 - May 2018
 - Fine-tuned Inception V3 Architecture on ASL dataset to detect gestures with **98%** accuracy and controlled a custom-built robotic arm. Published a paper as the **first author:** Amirtha Varshini, A.S. and et.al, "Real-time Hand Gesture Recognition for Robotic Arm and Home Automation", (**ISEEIE 2021**) **Link**
 - Best Final Year Project Award by Sonata and Centre for Entrepreneurship Development and Incubation, NIT Trichy.

ACHIEVEMENTS

- Granted scholarship to represent College of Computing, Georgia Tech at **Grace Hoppers Conference, 2022**
- Runner-up at **Innovation Competition 2022**, an Entrepreneurial challenge of VentureLabs, Georgia Tech.
- Recipient of **K. C. Mahindra Scholarship** for Post Graduate Studies Abroad, 2021
- Top 6 finalists out of the 230+ applicants in Maker's Challenge of QBuzz 2019, Qualcomm's annual tech conference.
- Recipient of **AIEEE Merit Scholarship for Rank 1448 (Top 0.1% amongst 1,350,000 candidates)** in JEE Main'14
- Received **two Qualstar recognitions** for innovation and excellent delivery of results.
- Poster on 'Automated Bug Triage with ML' selected for Qualcomm ML Summit'19