SHIVANGI GUPTA

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EDUCATION

Ph.D. in Computer Science (Jan 2020 - Present)
The University of Alabama in Huntsville, AL
Advisor - Dr. Vineetha Menon
Cumulative: 3.74/4.0

Master of Science in Computer Science (Aug 2017 - May 2019)
The University of Alabama in Huntsville, AL
Cumulative: 3.64/4.0

Bachelor of Technology in Computer Science (July 2012 - June 2016)
Jaypee Institute of Information Technology, India
Cumulative: 8.2/10.0

RESEARCH EXPERIENCE

Doctoral Dissertation, CS Department, UAH (Jan 2020 - Present)

- My dissertation research focuses on **studying drug-target interaction using novel big data techniques**.
- This research aims to create a machine learning framework to identify unique physio-chemical descriptors of a protein that can aid in maximizing the prediction rate of a potential protein molecular conformations.

Computing Graduate Intern, Lawrence Livermore National Laboratory (LLNL), CA (May 2023 - Present)

- Implementing a working version of Google's ProtENN model on LLNL supercomputer.
- Evaluating the model's performance on the LLNL generated synthetic protein sequence dataset.
- Designing and implementing inference algorithms to boost the predictive power of the model.

Graduate Research Assistant, CS Department, UAH (May 2022 - Present)

- **Artificial Intelligence - Accelerated Drug Discovery Project (AI-ADD)**
  - Responsible for investigating and implementing appropriate machine learning algorithms that can aid in identifying the optimum number of protein conformations that can be used in docking.
- **Transparent AI-driven Assistive Autonomous (AI/AA) Systems**
  - Responsible for investigating and implementing object detection models to identify target of interest in a combat search and rescue operations (CSAR).
  - Responsible for implementing Explainable AI (XAI) methods that communicates its outcomes of the implemented object detection models in a non-technical way so that every rescue member involved understands and trusts the system's thought and execution processes.

Graduate Teaching Assistant, CS Department, UAH (May 2020 - Apr 2022)

- Instructor for the course CS214 – Introduction to Discrete Structures.
- Responsible for preparing and teaching the course material, grading assignments, quizzes, tests and providing assistance to students during non-classroom times.

Graduate Teaching Assistant, CS Department, UAH (Dec 2019 - Apr 2020)

- Lab instructor for Computer Organization and Switching Theory (CS309), Introduction to Digital Computer Architecture (CS413) and Introduction to Computer Architecture (CS513).
- Responsible for managing the lab sessions along with conducting and grading quiz/exams.

Graduate Research Assistant, CS Department, UAH (Dec 2017 - May 2019)

- Worked in a team of 12 members on a NASA **funded research project VISAGE** (Visualization for Integrated Satellite, Airborne and Ground-based Data Exploration). The Goal of the project is to provide three-dimensional visualization and basic analytics capabilities for different environmental datasets in an interactive user interface.
- Designed and developed Python and IDL scripts to automate SIMBA (System for Integrating Multi-platform Data to Build the Atmospheric Column) both spatially and temporarily.
- Developed data readers in Python for generated SIMBA output data.
- Created S3 buckets for the SIMBA output data on Amazon Cloud.
- Responsible for managing the data in S3 buckets on Amazon Cloud.
- For more information on the project go to https://www.itsc.uah.edu/home/projects/visage-visualization-integrated-satellite-airborne-and-ground-based-data-exploration

Graduate Teaching Assistant, CS Department, UAH (Aug 2017 - Dec 2017)

- Worked as a TA for the course CS143 - Introduction to Technologies for Multimedia and Gaming. Evaluated coding assignments, tests, projects and proctored tests.

Research Assistant, Indian Space Research Organization (ISRO) (Aug 2016 - May 2017)

- Worked on a government funded research project to discriminate different mangrove species found in Sunderbans, West Bengal, India using hyperspectral data. The goal of the project is to explore Hyperion and AVIRIS-NG data sets using Spherical Angle Mapping (SAM) technique for their capability to discriminate mangrove species.
- Pre-processed AVIRIS-NG and Hyperion data sets in Python and developed a mangrove species spectral library in ENVI.
- Successfully applied SAM technique to the pre-processed datasets for classification using python and MATLAB. ENVI and ArcGIS were used for the visualization of the original and classified data.
- Designed and developed a Graphical User Interface in MATLAB for time series generation of SCATSAT-1 (microwave data) data products at 2 km spatial resolution in order to study the temporal variation of backscatter value over Sunderbans.
- From the research, it was concluded that fine resolution AVIRIS-NG hyperspectral data is capable of discriminating against fifteen mangrove species. Classification results of AVIRIS-NG data are significantly better as compared to Hyperion data. 15 mangrove species classified by AVIRIS-NG data with ±5m accuracy using SAM classification.
- For more information on the project go to github.com/shivangi-gupta/Mangrove-species-classification-report

PUBLICATIONS

Peer-reviewed Journal Articles

- ***Published***
  - **S. Gupta**, J. Baudry and V. Menon, *"Using Big Data Analytics to "back engineer" conformational selection mechanisms"*, Molecules. 2022; 27(8):2509. https://doi.org/10.3390/molecules27082509
  - **S. Gupta**, J. Baudry and V. Menon, *"Big Data Analytics for Improved Prediction of Ligand Binding and Conformational Selection"*, Frontiers, 2022. https://doi.org/10.3389/fmolb.2022.953984

Peer-reviewed Conference Articles

- ***Published***
  - **S. Gupta**, V. Menon and J. Baudry, *"Wavelet-based Spectral Analysis For Protein Conformation Selection and Prediction Using AI in Drug Discovery Applications", in Proceedings of IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* 2022.

TECHNICAL SKILLS

Programming: Python, Unix, R, C#, IDL, SQL
Libraries: Numpy, Pandas, Scikit-Learn, Tensorflow, Pytorch
Data Visualization: Matplotlib, Seaborn
Machine learning: Neural networks, dimensionality reduction, regression, classification techniques - logistic regression, Decision tree, Naive Bayes, clustering K-means
Operating systems: Windows, Linux
Version control: Git
Other: HPC, AWS, Oracle VM, ENVI, ArcGIS

COMMITTEE SERVICE & LEADERSHIP

Lead student volunteer | Supercomputing conference (SC23) (Nov 2023)
Student volunteer | IEEE BIBM 2022 (Dec 2022)
Student volunteer |Supercomputing conference (SC22) (Nov 2022)
Treasurer | UAH Circle K International (CKI) (Apr 2020 - Mar 2021)
Fundraising Chair | UAH Circle K International (CKI) (Mar 2018 - Apr 2019)
Student Ambassador | UAH Office of Diversity, Equity and Inclusion (Aug 2018 - Apr 2019)