M. VIGNESH VENKATARAMAN

Email: mvenkataraman@ph.iitr.ac.in
Github: VIGNESHinZONE

EDUCATION

Indian Institute of Technology , Roorkee *2017 - Present*
Integrated Master of Science , Physics
Department of Physics

National Center For Excellence , Bangalore *2014 - 2016*
Computer Science Stream
Central Board of Secondary Education (CBSE) Overall Percentage: 92.4

AREA OF INTREST

Machine Learning, Deep Learning, Software Devlopment

RELEVANT EXPERIENCE

NLP Intern at CRIS Lab, Columbia University Oct 2020 - Present, Remote
Collaborated with Prof. Venkat's group, on developing new Drug Discovery methods using existing Molecular Scaffolds that already follow the underlying chemistry. So far have we have been researching the existing RL-based approach and Molecular Transformer to combine different groups of scaffolds as a Reaction Prediction task. Conduct weekly meetings, discussing the progress and potential research ideas.We are currently working with both graph and string representation of Molecules, SMILES.

Undergraduate Researcher at Sathpathi Lab, IIT Roorkee Nov 2019 - Nov 2020, Roorkee
- Built an ensemble ML model to predict potential inhibitors of the SARS coronavirus protease molecule. The ensemble was built on models trained using Graph Neural Networks, Neural Networks, Tree and Boosting methods. Was able to achieve an average AUC-score - 0.76 and an average PRC-AUC - 0.301 on 5 folds. Were able to predict 12 potential drugs after docking.

- Applying deep learning techniques on pharmacore fingerprints for Alzheimer's disease with Biomolecules from PubChem dataset and drugs from the Drugbank dataset. Had to work with a highly imbalanced dataset and applied focal loss function. Obtained a 0.89 F1 score on Test data and predicted 107 potential drugs for further testing.

OPEN SOURCE CONTRIBUTIONS

DeepChem
The DeepChem project is an open-source python library that provides tools for drug discovery, materials science, quantum chemistry, and biology. I had implemented the Crystal graph model for Adsorption Datasets following, "Lattice Convolutional Neural Network Modeling of Adsorbate Coverage Effects" by Lym et al.
[COMMITS]

DGL-Lifesci
The DGL-Lifesci is an open-source python library for deep learning on graphs with models specific for Molecular and Biological graphs. I implemented a model which benchmarks on the MOLNET dataset, "Path-Augmented Graph Transformer Network" by Chen et al.
[COMMITS]

SKILLS

Programming Languages	C , C++ , Python , Fortran , Javascript , Latex
Frameworks	Pytorch , Tensorflow, React, Keras, Anaconda Distributions , Sklearn , Scipy
Software	Experience in NVDIA DGX systems , SLURM , Git
Language	English , Hindi , Tamil

RELEVANT COURSES

Coursework

Numerical Analysis Computational Physics, Linear Algebra, Ordinary Partial Differential Equations, Quantum Computing, Mathematical Modelling Simulation, Algorithms Data Structures, Advanced Mathematical Physics

Self-study

Machine Learning Deep Learning by DeepLearning.ai(Coursera), Computer Vision(CS-231), Deep Learning(NPTEL) by Prof. Khapra , Machine Learning(NPTEL) by Prof. Ravindran

NOTABLE ACHIEVEMENTS

INSPIRE SCHOLARSHIP by Department of Science and Technology , Government of India

Secured an **ALL INDIA RANK** -5791 in JEE MAIN.

Secured an **ALL INDIA RANK** -6868 in JEE Advanced.

Trinity GuildHall Award in Keyboard with Distinction in Level -1,2,3 from Trinity College London.

Trinity GuildHall Award in Theory of Music with Distinction in Level-1,2,3 from Trinity College London.

EXTRA-CURRICULARS

Member of Material Informatics and ML group in Sathpathi Lab 2019 - present

A meeting and discussion group with the team of Doctoral, graduate, and undergraduate students discussing and brainstorming various ideas in the fields of Material Science and Bio-materials.

Member of Cinematic Section 2017 - 2019

A group on campus promoting Film Making culture, having worked on various projects as a member under scriptwriting and Production verticals.

REFRENCES

Prof. Soumitra Satapathi

Assistant Professor
Department of Physics
Indian Institute of Technology Roorkee, India
Phone: +91-1332-284819
Email: ssphf.fph@iitr.ac.in