Abhay Kshirsagar | Curriculum Vitae

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Education

Indian Institute of Science Education and Research, Kolkata — **Kolkata, India**
Dept. Biological Sciences, Minor in Computer Science — *2019 – Present*
GPA – 8.59/10

Interests and Hobbies

Research Int.: I am mainly interested in understanding Bio-molecular phenomena and protein design using machine learning and molecular dynamics. Specifically interested in designing small molecule drugs and biological nano-materials for therapeutic and industrial applications.

Hobbies: Origami, Drumming

Publications

Conformational Ensemble of the NSP1 CTD in SARS-CoV2: Perspectives from the Free Energy Landscape
*Pallab Dutta, **Abhay Kshirsagar**, Parth Bibekar, and Neelanjana Sengupta* — *Feb 2023*
In this Study we investigate the conformational ensemble of NSP1-CTD of SARS-CoV-2 virus by leveraging Enhanced Sampling Method like Replica Exchange Molecular Dynamics and gain insights on its conformational landscape by using methods such as Expectation Maximized Molecular Dynamics. **DOI**: 10.1016/j.bpj.2023.02.010

Projects and Experience

Master's Thesis Project
Prof. Deva U. Priyakumar, IIIT Hyderabad, India — *Jun 2023 – Present*

- Currently building Machine Learning models that can Predict Amyloidogenic Hotspot regions in Protein Sequences.
- Exploring how Physical and Chemical properties can be incorporated in LLMs to improve the prediction accuracy.
- Learned about LLMs and how they can be used for Protein Sequence Encoding

Exploring the the Free Energy Landscape of IDPs
Prof. Neelanjana Sengupta, IISER Kolkata, India — *Nov 2021 – Dec 2022*

- Studied the Conformational Landscape of C-Terminal Region of NSP1 Protein from SARS-CoV-2
- Learned about Replica Exchange Molecular Dynamics, Molecular Dynamics Simulations, Expectation Maximized Molecular Dynamics, Gaussian Mixture Models, Parallel programming and HPC (High Performance Computing)

NLP Researcher
At Wavel.ai — *Jun 2022 – Aug 2022*

- Worked in the core team to learn, explore, and build state-of-the-art TTS models for multilingual and multispeaker voice cloning.
- Implemented a tokenizers for Malayalam and Telugu languages and improved performance compared to previous tokenizers.
- Learned about Transformers, Diffusion and various Generative Networks like Denoising Diffusion, Normalizing Flows and implemented them.

Predicting Global Horizonal Irradiance [Code ,Certificate]
Hackathon Submission — *Nov 2021 – Dec 2021*

- Implemented Long Short Term Memory Networks on previous GHI and could cover data of a solar farm.
- Learned about Data Augmentation and Time Series Analysis
- Qualified To be Finalist Teams among 30 Teams

Wind Farm Layout Optimization [Code]
Hackathon Submission — *Oct 2020 – Nov 2020*

- Implemented Particle Swarm Optimization Algorithm (PSO) in Python.
- The algorithm finds the optimal wind turbine farm layout using PSO and Wind Data of a particular region.
- Learned about genetic algorithms and various optimization models

Summer Project [Report]
Prof. Jayasri Das Sarma — *Jun 2020 – Nov 2020*

- Studied the parallels between m-CoV and SARS-CoV-2 and how is can be used as a model organism for studying SARS-CoV-2 in mice.

Welearn Bot [Code]
Team Project — *Feb 2020 – Jun 2020*

- A cli application for interacting with Welearn IISER-Kolkata for downloading files getting assignment deadlines
- Implemented the cache file system for the downloaded files and calendar event creation
- Implemented the google calendar integration for adding assignment and examination deadlines as an event on google calendar for those productivity.

Achievements

HPC Hackathon
Funding for Research *Dec 2021*

- Our Team won the HPC Hackathon organized by DST-India and Powered by Amazon Web Services
- We received a prize of $10,000 (USD) in compute credits by AWS for our project proposal.

KVPY SB Scholar
Scholarship *Jun 2020*

- Qualified for a scholarship program for students interested in pursuing science after appearing in a highly competitive exam and interview process.
- Ranked 56 amongst 20,000 students participating in the fellowship exam.

INSPIRE Scholar
Scholarship *Jun 2019*

- Qualified for a scholarship program for students interested in pursuing science and showing merit in Higher Secondary Education.

Relevant Courses

Biology

Theory : Protein Structure Function and Engineering, Biochemistry, Evolutionary Biology, Genetics, Biophysics, Molecular Genetics, Immunology, Gene Regulation, Cancer Biology, Developmental Biology
Lab : Biochemistry laboratory, Ecology, Evolutionary biology, Developmental Biology Lab

Computational and Data Sciences

Theory : Programming and Data Structures 1 and 2, Machine Learning and Network Analysis, Natural Language Processing, Artificial Intelligence: Search Methods

Online Certifications

- Machine Learning by Andrew Ng - [Certificate]
- Introduction Neural Networks - [Certificate]
- Convolutional Neural Networks - [Certificate]
- Improving Deep Neural Networks: Hyperparameter Tuning, Regularization and Optimization - [Certificate]

Skills

Languages: Python, C/C++, MATLAB, Dart

Frameworks: Keras, PyTorch

Web Dev: HTML/CSS, JavaScript

Android Dev: Flutter

Extra Curriculars

SlashDot Club, The Coding and Designing Club
Office Bearer. Post: Convener *Aug 2021*

- I was the convener of SlashDot Club which is the Coding Club of IISER Kolkata
- During my period I have taken Workshops on Web Development where I taught HTML, CSS and JavaScript.
- I was also an active member of Code Chef College chapter of IISER Kolkata

Campus Radio
Web Development Team *Jan 2021*

- I headed the Web Development Team at Campus Radio and created website with a database Back-end
- For the Website I used tools like Firebase for storing Images, And personal Data
- I also created an app which connects to the Fire-base with CRUD functions that allows user to Modify the Data seamlessly through the GUI