Yogesh Todarwal

Roslagstullsbacken 5, room-1305, 11421, Stockholm
+46 0734860589 todarwl@kth.se yogesh-todarwal github.com personal-webpage

About Me

With a strong background in programming, mathematical modeling, simulations, and machine learning, I am excited to transition into the corporate world. I am quick to learn and open to acquiring new skills necessary to tackle complex challenges in areas such as predictive modeling, AI-driven decision-making, and deep learning. My scientific approach allows me to leverage my quantitative skills to deliver innovative AI solutions that contribute to business success.

Education

KTH Royal Institute of Technology **Dec. 2018 – Jan. 2024**
Ph.D. in Computational Science *Stockholm, Sweden*

Indian Institute of Technology Bombay **Jul. 2013 – May 2018**
5-year Integrated B.Sc–M.Sc. in Chemistry *Bombay, India*

Work Experience

Multiscale Simulation Enhancements (Ph.D. Researcher) **Dec. 2018 – Jan. 2024**
–Python, Bash, HPC *Stockholm, Sweden*

- Refined force field parameters for molecular dynamics simulations, ensuring less than 1 kcal/mol error in potential energy calculations.
- Automated the process of force field parameterization using a Python-based pipeline, resulting in a 20% reduction in time-to-completion for simulation setups.
- Performed and analyzed large-scale simulation data (3M+ atoms) to predict binding affinities, achieving a high correlation with experimental results, which aided in early Alzheimer's detection research.
- Developed Bash scripts for efficient job management on HPC servers, optimizing resource usage and simulation throughput.
- Implemented data visualization techniques with Python to interpret simulation outcomes, enhancing the clarity of presentations

Machine Learning for Chemical Analysis (Research Assistant) **Mar. 2018 – Aug. 2018**
–Neural Networks, Feature Selection, Hyperparameter Optimization, Random Forest, Data Analysis *Mumbai, India*

- Performed data preprocessing by compiling and cleaning datasets sourced from published experimental results and in silico optimized molecular structures.
- Developed machine learning models to predict diastereoselectivity in oxazole catalyzed asymmetric reactions.
- Enhanced model performance by incorporating feature selection via the random forest algorithm to identify crucial chemical parameters influencing reaction outcomes.
- Applied neural networks and conducted 5-fold cross-validation to ensure the reliability and accuracy of the predictive models

Quantitative Analysis and Predictive Modeling (Research Intern) **May 2016 – Jul. 2016**
–Autodock, Data preprocessing, Feature Engineering, Machine Learning *Nijmegen, Netherlands*

- Analyzed conformations and allosteric modulations in a double-cage porphyrin systems using Monte Carlo algorithm and semi-empirical optimization techniques to maximize computational efficiency.
- Developed a QSPR model with linear regression to predict binding affinities within host-guest systems, demonstrating a significant correlation with molecular properties.

Certificates

- **Cognizant** Artificial Intelligence Job Simulation on Forage — Jun. 2024
- **MLOps**: Model Development and Integration from LinkedIn Learning — Feb. 2024
- **SQL** Essential Learning from LinkedIn Learning — Feb. 2024
- Kaggle: Introduction to **Machine Learning** — Aug. 2022
- PDC Summer School on Introduction to **High Performance Computing** — Aug. 2019

Skills

Languages : Python, Bash, C++, SQL
Operating Systems: Linux, Windows, MacOS
Software/Library : Pandas, NumPy, Matplotlib, Keras, Scipy, scikit-learn, Github/Gitlab, PyTorch

Publications

While pursuing my Ph.D. under the guidance of Prof. Patrick Norman, I contributed to nine research projects, each culminating in publications in international peer-reviewed journals. For a detailed overview of my research activities and outputs, please visit my research portfolio.

Relevant Coursework

- Linear Algebra
- Data Analysis
- Differential Equations
- Calculus
- Advance Quantum Chemistry
- Computer Programming and Utilization (C++ and bash)
- Programming in Python
- Introduction to High-Performance Computing.

Selected Presentation Opportunities

- Poster presentation in a multiscale molecular dynamics workshop at the EPFL, Switzerland. 2022
- Research presentation to Master students taking the course BB2280 (Molecular modeling). 2021
- Poster presentation in Computing π-Conjugated Compounds conference. 2021
- ITN-COSINE workshop at the Trieste, Italy. 2019
- Wavefunction based methods workshop at Heidelberg University, Germany. 2019
- Ph.D. secondment at the SDU, Denmark. 2019

Position of Responsibility

Assistant Manager of 50th inter-IIT sports Meet 2014 **Aug. 2014 – Dec. 2014**
Food and Beverage department

- Leadership: Administrated the allocation and execution of a refreshment budget of INR 1.5 million
- Planning: Formulated tendering process for messing facility to be provided for 1700 participants and 200 officials

Coordinator, MOOD INDIGO 2014 **Apr. 2014 – Dec. 2014**
Asia's largest cultural festival, Food and Beverages Department

- Cooperation: Worked in a team of 15 members
- Negotiation: Involved in helping the Core Group Members in fixing deals with various food vendors
- Management: Responsible for the food court set up on the campus during the festival

Phonathon volunteer conducted by Student Alumni Relations Cell (SARC) **Jun. 2014**
IIT Bombay Representation and Networking

- Networking: Represented IIT Bombay to establish strong relations with IITB Alumni
- Communication: Called 100+ IIT Bombay alumni for their reunion and alumni-student mentorship program

Scholastic Achievements and Awards

- A research article published with 1st author was highlighted by CBH school news within KTH (Link). 2021
- Undergraduate Research Award (URA 01) for outstanding contribution to academic research in the year 2016-2017 2017
- INSPIRE SCHOLARSHIP by the Department of Science and Technology, Govt. of India. This fellowship with the worth of INR 320,000 has been awarded to the top 1% of the Indian students pursuing basic sciences. 2013
- Ranked in the top 1% of the country in the Joint Entrance Exam (JEE) taken by about 900,000 students. 2013

Personal Interest

My days often begin with enriching my mind through inspiring podcasts and self-help books. As evening approaches, I switch gears to physical activities for a healthy balance. In the evenings, you'll often find me doing Zumba, out running to catch my breath, or relaxing with some comedy movies. Trekking, hiking, and camping? Count me in for all those outdoor adventures!