Asawari Pagare

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Education

University of North Carolina at Chapel Hill — Chapel Hill, NC
Ph.D. in Chemistry, Advisor: Prof. Zhiyue Lu — 2021–01/2025 (Expected)

Indian Institute of Science (#1 ranked university in India) — Bangalore, India
B.S.(Research) - MSc in Chemistry — 2015–2020

Technical Skills

- **Coding:** Python, Julia, Bash scripting. (Python libraries: PyTorch, PyTorch Geometric, Pandas, Numpy, Scipy, SciKit, Matplotlib)
- **Softwares:** Matlab, Mathematica, Autodock vina, KNIME, Blender
- **Applied mathematical skills:** Information theory, Probability theory, Stochastic thermodynamics, Statistical Mechanics, Calculus, Complex Analysis, Differential Equations (ODEs, PDEs, Markov models, etc), Linear Algebra, Machine learning, Deep learning.
- **Modeling and Simulation:** Langevin dynamics simulations, Markov systems, Maximum Likelihood Estimation, Data classification and clustering.
- **Relevant courses:** Mathematical Methods of Theoretical Physics, Introduction to Population PK/PD Analysis with Nonlinear Mixed Effects Models (NONMEM), Computational Medicinal Chemistry school, Computer-Aided Drug Design, Statistical Mechanics and Thermodynamics, Machine learning with Graphs.

Research and Teaching Experience

Graduate Research Assistant at the University of North Carolina at Chapel Hill
Lu Group, Department of Chemistry — 2020-Current

- **Using information theory and numerical simulations to elucidate enhanced performance in sensing concentration changes by multi-state receptors in nonequilibrium.**:
  - Demonstrated that a ligand-receptor sensor modeled as a multi-state Markov graph (target proteins) show enhanced performance in sensing a concentration increase if it has experienced another one before in combination with a subsequent critical resetting period of lower concentration (capturing drug concentrations between two doses). This effect was explained using eigen analysis of the transition rate matrix.
  - Sampling and machine learning was applied to establish a relationship between the Markovian graph and the observed effect shedding light on exposure-response relationships.

  Inspires tweaking the best drug efficacy in target best therapies by identifying the critical resetting period for the target.[1]

- **Stochastic distinguishability of Markovian trajectories.**:
  - Derived (using probability theory, Markov model and linear algebra) a computationally cheap formulation for the distinguishability of different temporal environments by an arbitrary sensor in nonequlibrium using KL divergence that circumvents sampling difficulties and relates it to individual transition events and their waiting time statistics.

  Novel insights into temporal pattern recognition by biological and artificial sensors. [2]

- **Elucidating multiplexing in biological receptors using theoretical modeling and simulations.**:

– Demonstrated (using Langevin dynamics simulations, probability and information theory) that a binary ligand-receptor sensor can multiplex – sense multiple environmental information (concentration, temperature, flow speed, etc) simultaneously.

– A theoretical upper bound of multiplexing was obtained and a mathematical technique called the rank-deficient maximum likelihood was proposed to obtain the upper bound for a receptor and identify it's accuracy and sensitivity in sensing different environmental variables.

Inspires pharmacological studies on controlling environmental factors in target-based therapies to enhance desired efficacy. [3]

Teaching Assistant at the University of North Carolina at Chapel Hill
Quantitative Lab II (102L) in Summer II 2024 and Spring 2022
Physical Chemistry lab (481L) in Fall 2021
– Mentored, managed and lead students to run experiments, analyze and interpret data

Selected Undergraduate Research Experiences

BS Thesis and MSc Thesis at the Indian Institute of Science Bangalore, India
Cherayil Group, Department of Inorganic and Physical Chemistry 2018-2020

- MSc Thesis – Stochastic thermodynamics of a polymer in linear mixed flow.
- BS Thesis – Stochastic thermodynamics of a harmonically trapped colloid in linear mixed flow.[4]

Summer Intern at the University at Buffalo Buffalo, USA
Errington Group, Department of Chemical and Biological Engineering Summer, 2018

- Monte Carlo and Molecular Dynamics simulations.

Selected Publications and Presentations

[1] **A. Pagare** and Z. Lu, "Information benchmark for biological sensors beyond steady states – mpemba-like sensory withdrawal effect", *arXiv:2406.04304, 2024*,

[2] **A. Pagare**, Z. Zhang, J. Zheng, and Z. Lu, "Stochastic distinguishability of markovian trajectories", *J Chem Phys.*, vol. 160, no. 171101, 2024.

[3] **A. Pagare**, S. H. Min, and Z. Lu, "Theoretical upper bound of multiplexing in biological sensory receptors", *Physical Review Research*, vol. 5, no. 2, p. 023 032, 2023.

[4] **A. Pagare** and B. J. Cherayil, "Stochastic thermodynamics of a harmonically trapped colloid in linear mixed flow", *Physical Review E*, vol. 100, no. 5, p. 052 124, 2019.

- Poster presentation on **Information theoretical study of ligand-receptors reveal the withdrawal effect and the design principles for efficient sensing** Oct 2024
  2024 Computational Medicinal Chemistry School, Cambridge, MA.
- Poster presentation on **Information theory classification of biological sensors** June 2024
  American Conference on Theoretical Chemistry 2024, Chapel Hill, NC.
- Poster presentation on **Theoretical upper bound of multiplexing in biological sensory receptors** May 2022
  The Workshop on Stochastic Thermodynamics III, WOST III 2022
- Oral presentation on **Can a single ligand-receptor sense multiple channels of information?**' March 2022
  APS March Meeting 2022, Chicago, Illinois.

Awards

- Graduate Student Transportation grant awarded by the College of Arts and Science at UNC Chapel Hill. 2024
- Kishore Vigyanik Prothsahan Yojana (KVPY) Fellowship 2015–2020
  Awarded by the Dept. of Science and Technology, Govt. of India. Awarded to the top 250 (less than 0.001%) students in India for demonstrated abilities in science and technology.