Shaswata Roy

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Background

Over 5 years of experience during a Ph.D. in physics, specializing in the interface of biophysics, mathematical modeling, and machine learning.

Education

Purdue University, West Lafayette, IN Aug 2019 – July 2025
Ph.D. in Physics *CGPA: 3.71/4*
Advisor: Dr. Jing Liu

Indian Institute of Technology Madras Aug 2014 – Jun 2019
BS (Hon.) + MS *CGPA: 8.57/10*

Publication

Roy S., Seitz C., Samaddar M., Ma H., Li Q. , Molina C.S., Liu J., "Inferring bursting kinetics of GBP5 using the Two State Model fed by single molecular imaging" *In preparation, 2025*

L Domingo, M Chehimi, S Banerjee, S He Yuxun, S Konakanchi, L Ogunfowora, **S Roy**, S Selvarajan, M Djukic, C Johnson, "A hybrid quantum-classical fusion neural network to improve protein-ligand binding affinity predictions for drug discovery" *IEEE International Conference on Quantum Computing and Engineering (QCE) 2024*

Ziegler KF, Joshi K, Wright CS, **Roy S**, Caruso W, Biswas RR, Iyer-Biswas , "Scaling of stochastic growth and division dynamics: A comparative study of individual rod-shaped cells in the Mother Machine and SChemostat platforms" *Mol Biol Cell, 2024*

Joshi, K., Ziegler, K.F., **Roy, S.**, Wright, C.S., Gandhi, R., Stonecipher, J., Biswas, R.R., Iyer-Biswas, S. , "Non-Markovian memory in a bacterium" *biorxiv, 2023*

Joshi, K., **Roy, S.**, Biswas, R.R., Iyer-Biswas, S., "Cellular dynamics under time-varying conditions" *biorxiv, 2023*

Conferences

Roy S., Seitz C., Liu J., "Transcriptional bursting kinetics provide insights into the mechanisms governing Interferon-mediated transcriptional memory" *(Oral) American Physical Society , 2025*

Research Experience

Purdue University - Liu Lab Jan 2024 - Present
Advisor: Dr. Jing Liu

- **Spatial Transcriptomics** Designed a pipeline for extracting spots data from smFISH and Xenium Experiments (Repository)
- **Gene Regulatory Network** Developed a model to study the effects of the JAK-STAT signaling pathway on target genes and the consequent effect on transcriptional memory
- **Plant Cell Metabolites Pathway** Developed a computational model for the signaling pathway associated with floral volatiles to test the effect of benzaledhyde on the volatile compounds and the effect of circadian rhythm

Purdue University - Iyer-Biswas Lab Aug 2019 - Dec 2023
Advisor: Dr. Srividya Iyer Biswas

- **Image Analysis Pipeline** Designed a pipeline from scratch to analyze phase contrast imaging data.
- **Stochastic Modeling of Cellular Processes** Developed models for understanding emergent phenomena in cells relating to growth, division, and homeostasis.

Indian Institute of Technology Madras Aug 2017 - Jun 2019
Advisor: Dr. Neelima Gupte

- Worked on self-assembly and pattern formation in active rods
- Simulated nonlinear systems to test the effect of noise on chaotic regimes in high-dimensional systems.

Work Experience

Graduate Teaching Assistant Aug 2019 – Present
Purdue University, West Lafayette, IN

- Designed and taught a Data Mine course to undergrads to get them familiar with data science methodologies
- Have been consistently given a high student evaluation (4 out of 5) during my time teaching

Graduate Data Science Researcher - Ingenii Aug 2022–Jul 2023
Hybrid Quantum Neural Network for predicting drug interaction

- Developed a hybrid quantum-classical deep learning model that combines 3D and spatial graph convolutional neural networks for improved protein-ligand binding affinity prediction, resulting in a 6% increase in accuracy over classical approaches. (Repository)

Graduate Data Science Researcher - Merck Aug 2023–Dec 2023
Generative Molecular Modeling

- Worked with Merck to research and implement several molecular generation models to improve the properties of a candidate drug molecule. (Repository)

Technical Skills

Languages: Python, C/C++, R, Julia, Bash
Machine Learning: PyTorch, Scikit-Learn, Tensorflow
Data Analysis: NumPy, Pandas, Matplotlib
Bioinformatics Tools: Biopython, BLAST, Ensembl, snakemake, KEGG
Other: High Performance Computing (SLURM), Git, AWS, Docker

Research Internship

IAS Fellowship May 2017 – Aug 2017
Indian Institute of Science

Award and Recognition

- INSPIRE Scholar 2014-2019
- Summer Research Grant 2021-2024
- Xplore Access 2024