

# SURBHI KUMAR

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## PROFESSIONAL SUMMARY

Ph.D. Candidate in Mathematics specializing in Topological Data Analysis and Graph Representation Learning for biomedical applications, including brain network modeling and ligand-based virtual screening (LBVS) for drug discovery. Experienced in CUDA-enabled GPU programming and scalable model development on high-performance computing (HPC) clusters. Passionate about developing scalable, data-driven solutions through mathematical insights.

## EDUCATION

### The University of Texas at Dallas

Ph.D. in Mathematics | GPA: 3.75/4

Expected - May 2028

### The University of Texas at Dallas

M.S. in Mathematics (Data Science Specialization) | GPA: 3.75/4

Expected - Dec 2026

### National Institute of Technology, Rourkela

Master of Mathematics |GPA: 7.87/10

May 2017

### Guru Nanak Dev University

Bachelor of Science (Majors: Mathematics, Computer Science, Physics) | GPA: 7.9/10

June 2015

## TECHNICAL SKILLS

- Programming Languages:** Python, C, C++, Java, SQL, R, MATLAB, Mathematica
- Libraries & Frameworks:** PyTorch, PyTorch Geometric, DGL, TensorFlow, scikit-learn, NetworkX, RDKit, XGBoost, NumPy, SciPy, Gudhi, Ripser
- Tools & Platforms:** CUDA, Slurm (HPC), Linux, Neo4j, Git, Databricks, Jupyter Notebook, LaTeX, MS Office

## PROJECTS

- TopU-LBVS: A Realistic Multi-Target Benchmark for Ligand-Based Virtual Screening (In Progress):** Constructed the unbiased TopU95 multi-target dataset from CHEMBL35 and established a rigorous benchmarking protocol. Evaluated naïve models, classical machine learning baselines, deep learning graph models, and modern foundation models under a unified framework for fair and reproducible comparison. This debiasing strategy reduces artificial class separation and provides a realistic evaluation setting across diverse protein targets.
- Brain Network Graph Classification (Under Review, ICML 2026):** Analyzed how atlas choice affects downstream performance in brain network models and introduced edge-based quadratics to improve structural expressiveness, validated through multi-atlas baselines with consistent gains.
- Low-Shot Graph Learning with Topological and Spectral Embeddings (Accepted, LOG 2025):** Introduced a prototype-based low-shot graph learning model using Betti vectors and spectral DoS embeddings, outperforming GNN and Graph Transformer models under scarce supervision.

## EXPERIENCE

### Teaching Assistant

The University of Texas at Dallas

Aug 2023 – Present

- Conduct problem-solving sessions and oversee grading for multiple calculus courses; serving as Head TA for Calculus of Several Variables with responsibility for TA coordination and grading logistics.

### Subject Matter Expert - Advanced Mathematics

Ed-Tech Industry (Remote)

Jun 2017 - Jul 2023

- Developed advanced mathematics content for leading Ed-Tech platforms including Chegg and Meritnation.

## RESEARCH PUBLICATION

- Journal Publication:** Kumar, S., Saha Ray, S. Numerical treatment for Burgers–Fisher and generalized Burgers–Fisher equations. *Math Sci* 15, 21–28 (2021). <https://doi.org/10.1007/s40096-020-00356-3>