

# Shreyas N. Samaga

Department of Computer Science

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**Research interests**   Topological Data Analysis, Multiparameter persistence, Graph Neural Networks, Topological Deep Learning, Category Theory for Machine Learning, Spatio-temporal learning on point clouds and graphs, LLMs.

**Education**   **Purdue University**   *West Lafayette, IN*  
PhD in Computer Science   *Aug 2021 – Present*  
Advisor: Prof. Tamal K. Dey

**Indian Institute of Science Education and Research Bhopal**   *Bhopal, INDIA*  
BS-MS Dual Degree majoring in Mathematics   *Aug 2015 – May 2020*  
MS Thesis Advisor: Dr. Dheeraj Kulkarni

**Appointments held**   **Research Intern, Lawrence Berkeley National Laboratory**  
Mentor: Dr. Dmitriy Morozov   *Jun 2023 – Aug 2023*  
Worked on topological analysis of Zeolites (microporous crystals) using multiparameter persistent homology to capture their structure  
Used gradient based tree learning for dimensionality reduction of the Persistence Images of Zeolites to reduce the redundancy in the captured topological information

**Visiting PhD Student, INRIA Saclay**  
Mentor: Prof. Steve Oudot   *May 2023 – Jun 2023*  
Proved that GRIL (Generalised Rank Invariant Landscape), 2-parameter persistence-based vectorization (see papers), is stratifiably smooth and computed the gradient w.r.t. input bifiltration functions. Used this to build learnable topological layer based on 2-parameter persistence - D-GRIL (see papers)

**Research Intern, Adobe Media and Data Science Research**  
Mentors: Piyush Gupta and Siddharth Ramesh   *May 2022 – Aug 2022*  
Used the topological information present in the self-attention maps of language models like BERT, when modelled as weighted graphs, to improve the performance on GLUE Benchmark tasks by about 3%  
Explored the idea of topological distillation for self-attention maps in a teacher-student learning framework

**Independent Researcher, Ethereum Foundation**  
Collaborator: Aditya Asgaonkar   *May 2021 – Aug 2021*

Identified critical network links that an adversarial attack could exploit to disrupt the network's functionality  
 Applied TDA techniques to Eth 2.0 network to strengthen the structural and health analysis of the network

### **Project Student, IIT Delhi**

Mentor: Dr. Ishaan Gupta

*May 2020 – Oct 2020*

Evaluated the effect of hypertension and diabetes on COVID-19 mortality in India using machine learning models. People with diabetes are 2.11 times more likely to have a fatal outcome (see papers)

Predicted the mortality of COVID-19 using machine learning models with an AUC-ROC of 0.92 based on noninvasive blood parameter data (see papers)

### **MS Thesis, Chennai Mathematical Institute**

Mentor: Dr. Priyavrat Deshpande

*Jan 2020 – May 2020*

Applied methods from Topological Data Analysis to a socio-economic dataset from India, as part of my MS thesis

### **DAAD WISE Fellow, Technische Universität Dresden**

Mentor: Prof. Dr. Andreas Thom & Dr. Martin Nietzsche

*May 2018 – Jul 2018*

Worked on application of Algebraic Topology to Social Choice Theory and wrote an expository article (see papers)

### **Charpak Fellow, University of Strasbourg**

Mentor: Prof. Athanase Papadopoulos

*May 2017 – Jul 2017*

Studied about homotopies and Poincaré groups of a topological space

### **Grants, awards and scholarships**

Purdue Graduate Student Travel Grant, Purdue University	2024
NSF Travel Grant, NSF	2023
Research Grant for Beacon Chain Network Topological Analysis, Ethereum Foundation	2021
Director's Gold Medal, IISER Bhopal	2020
Department Gold Medal, IISER Bhopal	2020
DAAD-WISE Fellowship, DAAD	2018
Charpak Summer Research Fellowship, Campus France	2017
CNR Rao Education Foundation Prize, IISER Bhopal	Aug 2016
CNR Rao Education Foundation Prize, IISER Bhopal	Jan 2016
INSPIRE Fellowship, Govt. of India	2015

### **Publications**

**2025**

Tamal K. Dey, **Shreyas N. Samaga** (author order acc. last name). [Quasi Zigzag Persistence: A Topological Framework for Analyzing Time-Varying Data](#), *arXiv preprint*, 2025.

## 2024

Mustafa Hajij, Mathilde Papillon, Florian Frantzen, Jens Agerberg, Ibrahim AlJabea, Rubén Ballester, Claudio Battiloro, Guillermo Bernárdez, Tolga Birdal, Aiden Brent, Peter Chin, Sergio Escalera, Simone Fiorellino, Odin Hoff Gardaa, Gurusankar Gopalakrishnan, Devendra Govil, Josef Hoppe, Maneel Reddy Karri, Jude Khouja, Manuel Lecha, Neal Livesay, Jan Meißner, Soham Mukherjee, Alexander Nikitin, Theodore Papamarkou, Jaro Prilepok, Karthikeyan Natesan Ramamurthy, Paul Rosen, Aldo Guzmán-Sáenz, Alessandro Salatiello, **Shreyas N. Samaga**, Simone Scardapane, Michael T. Schaub, Luca Scofano, Indro Spinelli, Lev Telyatnikov, Quang Truong, Robin Walters, Maosheng Yang, Olga Zaghien, Ghada Zamzmi, Ali Zia, Nina Miolane (author order acc. to last name after first three authors). [TopoX: A Suite of Python Packages for Machine Learning on Topological Domains](#). *Journal of Machine Learning Research*, 25(374), 1-8, 2024

Soham Mukherjee\*, **Shreyas N. Samaga**\*, Cheng Xin, Steve Oudot, Tamal K. Dey. [D-GRIL: End-to-End Topological Learning with 2-parameter Persistence](#). *arXiv preprint*, 2024.

Tamal K. Dey, Florian Russold, and **Shreyas N. Samaga** (author order acc. to last name). [Efficient Algorithms for Complexes of Persistence Modules with Applications..](#) *40th International Symposium on Computational Geometry (SoCG 2024)*. Schloss Dagstuhl–Leibniz-Zentrum für Informatik, 2024.

## 2023

Cheng Xin\*, Soham Mukherjee\*, **Shreyas N. Samaga**, Tamal K. Dey. [GRIL: A 2-parameter Persistence Based Vectorization for Machine Learning](#). *Proceedings of 2nd Annual Workshop on Topology, Algebra, and Geometry in Machine Learning (TAG-ML)*, in *Proceedings of Machine Learning Research* 221:313-333, 2023. **(Spotlight Oral)**

## 2022

Mustafa Hajij, Ghada Zamzmi, Theodore Papamarkou, Nina Miolane, Aldo Guzman-Saenz, Karthikeyan Natesan Ramamurthy, Tolga Birdal, Tamal K. Dey, Soham Mukherjee, **Shreyas N. Samaga**, Neal Livesay, Robin Walters, Paul Rosen, Michael T. Schaub. [Topological Deep Learning: Going Beyond Graph Data](#). *arXiv preprint*, 2022.

Samarth Bhatia, Yukti Makhija, Sneha Jayaswal, Shalendra Singh, Prabhat Singh Malik, Sri Krishna Venigalla, Pallavi Gupta, **Shreyas N. Samaga**, Rabi Narayan Hota, Ishaan Gupta. [Severity and mortality prediction models to triage Indian COVID-19 patients](#). *PLOS Digital Health*, 1(3):e0000020, 2022.

## 2021

Sneha Kumar Jayaswal, Shalendra Singh, Prabhat Singh Malik, Sri Krishna Venigalla, Pallavi Gupta, **Shreyas N. Samaga**, Rabi Narayan Hota, Surinder Singh Bhatia, Ishaan Gupta. [Detrimental effect of diabetes and hypertension on the severity and mortality of COVID-19 infection: A multi-center case-control study from India](#). *Diabetes & Metabolic Syndrome: Clinical Research & Reviews*, 15(5):102248, 2021.

Yukti Makhija, Samarth Bhatia, Shalendra Singh, Sneha Kumar Jayaswal, Prabhat Singh Malik, Pallavi Gupta, **Shreyas N. Samaga**, Shreya Johri, Sri Krishna Venigalla, Rabi Narayan Hota, Surinder Singh Bhatia, Ishaan Gupta. [Challenges in the application of a mortality prediction model for COVID-19 patients on an Indian cohort](#). *arXiv preprint, 2021*.

**2018**

**Shreyas Samaga**. [On the homotopy type of choice spaces](#). *arXiv preprint, 2018*.

## Research Projects

### Current Projects

Characterizing hallucination in LLMs using topological information.

### Past Projects

Proposed quasi zigzag persistence as a framework for analyzing topological information from spatiotemporal data. We vectorize this topological information using ZZ-GRIL and prove that it is stable. Further, we propose an algorithm to compute ZZ-GRIL by establishing the required theoretical results. We showed that this framework is applicable in various domains including sleep stage classification.

Developed and implemented algorithms for complexes of persistence modules. We extend the persistence algorithm to complexes of modules that are not free, which is a more general class of modules. We showed that these algorithms can be applied to compute persistent sheaf cohomology, which captures the information present in a family of sheaves over a simplicial complex.

GRIL: Generalized Rank Invariant Landscape, a vectorization scheme for 2-parameter persistence modules. GRIL does not need to reduce a 2-parameter persistence module to a family of 1-parameter persistence modules to vectorize it but vectorizes the entire 2-parameter persistence module at once. Experimentally, we showed that GRIL compares well with the existing multiparameter persistence vectorization methods.

Proved that GRIL is a stratifiably smooth map and computed an explicit formula for its gradient with respect to input bifiltration functions. Used this to build D-GRIL, an end-to-end learning layer based on 2-parameter persistence. This is one of the initial works on end-to-end learning using 2-parameter persistent homology. Showed that this can be used for bio-activity prediction in drug discovery, among other things.

Contributed to one of the foundational papers on Topological Deep Learning and [Topo-ModelX](#), a library for Topological Deep Learning.

## Teaching experience

### Purdue University

1/2 TA, CS 580: Algorithm Design, Analysis, and Implementation

*Spring 2025*

1/2 TA, CS 531: Computational Geometry

*Spring 2024*

TA, CS 177: Programming with Multimedia Objects

*Spring 2022*

TA, CS 177: Programming with Multimedia Objects

*Fall 2021*

**The Ohio State University**

TA, CSE 1222: Introduction to Computer Programming in C++  
for Engineers and Scientists

*Spring 2021*

**Service**

I review for ICLR, NeurIPS (top reviewer 2024), ICML and LoG conferences.

Was one of the local organisers of [ComPer Workshop 2023](#).