Topological Deep Learning Challenge 2025: Expanding the Data Landscape

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Abstract

This paper describes the 2025 edition of the *Topological Deep Learning Challenge: Expanding the Data Landscape*, hosted at the first Topology, Algebra, and Geometry in Data Science (TAG-DS) Conference. This year's challenge aimed to address the data bottleneck in the field by systematically expanding the ecosystem of Topological Deep Learning (TDL). Powered by `TopoBench`, the challenge was organized into two primary missions: enriching the data landscape with diverse datasets, and advancing core data infrastructure. In particular, participants were invited to contribute to the open-source platform by implementing new dataset loaders, designing new benchmark tasks, or engineering robust, scalable data pipelines. The initiative successfully yielded 44 qualifying submissions. This paper outlines the scope of the competition and summarizes the key results and findings, highlighting the new resources now available to the TDL community.

1 Introduction

Many physical systems—from molecules to galaxies—are driven by interactions among their components: chemical interactions between atoms, functional connectivity between brain regions, or gravitational forces between stars. Conventionally, these physical relations are modeled with graphs, allowing Graph Neural Networks (GNNs) [Scarselli et al., 2008] to extract key insights [Kipf and Welling, 2017, Santoro et al., 2017, Zhang and Chen, 2018, Schlichtkrull et al., 2018, Zhang et al., 2020]. However, these systems also involve richer interactions of varying strengths that extend beyond the pairwise relations typically modeled by graphs. For example, while graphs capture atoms as nodes and bonds as edges, they overlook higher-order structures, such as carbon rings and functional groups [Zang et al., 2023]. Ignoring these interactions leaves an incomplete picture of the underlying dynamics.

Topological Neural Networks (TNNs) have recently emerged to address this limitation by accounting for such higher-order interactions [Hajij et al., 2022, Bodnar, 2022, Papillon et al., 2023c]. As part

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Proceedings of the 1st Conference on Topology, Algebra, and Geometry in Data Science(TAG-DS 2025).

of the broader field of Topological Deep Learning (TDL), these methods extend GNNs to naturally process relations between two or more elements using concepts from algebraic topology [Bick et al., 2023, Barbarossa and Sardellitti, 2020]. TDL is already postulated to become a relevant tool across many research areas, from complex physical systems [Battiston et al., 2021] and signal processing [Barbarossa and Sardellitti, 2020] to molecular analysis [Bodnar et al., 2021], computer networks [Bernárdez et al., 2023, 2025], neuroscience [Lecha et al., 2025], and cosmology [Lee and Villaescusa-Navarro, 2025]. However, for TDL to realize its full potential, the data landscape must evolve [Papamarkou et al., 2024]; the current reliance on a small subset of benchmarks creates a bottleneck for both innovation and rigorous evaluation.

To propel the field forward and build upon the success of the first two editions [Papillon et al., 2023b, Bernárdez et al., 2024], the *Topological Deep Learning Challenge 2025* focused on expanding the foundational benchmarks of TDL. This meant adapting diverse datasets from the GNN community and beyond, as well as building infrastructure for large-scale datasets. Central to this effort was `TopoBench`, the premier open-source platform for developing and benchmarking TDL models [Telyatnikov et al., 2025a]. `TopoBench` provides a unified interface for datasets, loaders, and tasks across topological domains, enabling reproducible comparisons and accelerating model development.

The challenge concluded with substantial international participation, with 44 valid submissions from 30 teams across more than 20 distinct institutions worldwide. These contributions have significantly enriched the TDL ecosystem by integrating diverse datasets—ranging from particle physics to neuroscience—and by establishing robust, scalable data pipelines capable of handling large-scale TDL. This paper details the challenge setup and submission requirements, as well as highlights the winning contributions that set new standards for the field.

2 Setup of the Challenge

The challenge[2] was hosted at the first Topology, Algebra, and Geometry in Data Science (TAG-DS) Conference and sponsored by Arlequin AI. Participants were asked to contribute to the `TopoBench` library in one of two missions or tracks: *(i))* implementing new dataset loaders and *(ii))* developing data infrastructure for large-scale or new benchmark tasks.

2.1 Guidelines

Participation was free and open to everyone. To enroll in the challenge, participants had to:

- Open a Pull Request (PR) on `TopoBench` and fill out the Registration Google Form with PR and team information.
- Ensure the PR passes all tests and meets the submission requirements before the deadline.

Teams were accepted with a maximum of 2 members, though larger teams were possible upon approval. A single team was permitted to submit multiple PRs, both within and among the different challenge categories proposed.

Consistent with the aims of an open environment for sharing participation, this activity was completely voluntary. However, due to legal restrictions, individuals affiliated with institutions on the Restricted Foreign Research Institutions list were not eligible for reward outcomes, including co-authorship on this white paper.

2.2 Submission Requirements

A submission consisted of a Pull Request (PR) to the `TopoBench` repository. To be valid, the PR had to pass all tests, including linting and formatting. Each PR could contain at most one dataset loader, although a loader could support multiple datasets via configuration files.

Mission A: Expanding the Data Landscape

This Mission focused on contributing new dataset loaders. It was divided into two categories, A.1 and A.2. For submissions in Mission A, participants were required to:

[2] Challenge Repository: `https://github.com/geometric-intelligence/TopoBench`

1. Implement a dataset loader class inheriting from `AbstractLoader` in the appropriate domain directory.
2. Ensure that the dataset is hosted on an open-source platform.
3. Include comprehensive unit tests that satisfy the `TopoBench` CI/CD pipeline requirements.
4. Include a pipeline test demonstrating that an existing model in `TopoBench` can successfully train on the contributed dataset.

Mission B: Advancing the Data Infrastructure

This Mission centered on developing a novel data infrastructure. It was also divided into two categories, B.1 and B.2. Although requirements in this Mission were more flexible due to the complexity of the tasks, they included these constraints:

1. Maintain code quality standards by passing the existing `TopoBench` CI/CD workflow.
2. Include at least one pipeline test demonstrating that a model can train on the contributed dataset/task (e.g., using small slices of data for large-scale datasets to keep runtime reasonable).

Crucially, participants in Mission B needed to address both inductive learning, where models must generalize to unseen nodes and graph structures, and transductive learning, which operates within a fixed graph structure. To handle these large-scale settings, teams engineered robust pipelines using `OnDiskDataset` loaders to bypass memory bottlenecks.

2.3 Award Categories

The challenge was organized into two primary missions designed to systematically expand the TDL ecosystem.

Mission A - Expanding the Data Landscape:

- **Category A.1:** Broadening Benchmarks with Graphs & Point Clouds (Difficulty: Easy/Medium). Implementation of well-established graph or point cloud datasets to bridge the gap between TDL and mainstream GNN research.
- **Category A.2:** Curating Natively Higher-Order Datasets (Difficulty: Medium). Integration of datasets where higher-order structures (e.g., simplicial complexes, hypergraphs) are a native feature of the data.

Mission B - Advancing the Data Infrastructure:

- **Category B.1:** Developing Large-Scale Inductive Data Infrastructure (Difficulty: Hard). Implementation of a robust `OnDiskDataset` loader to bypass memory bottlenecks during "lifting" operations. A bonus "Survival" difficulty was available for tackling large-scale transductive learning.
- **Category B.2:** Pioneering New TDL Benchmark Tasks (Difficulty: Varies). Introduction of novel benchmark tasks beyond standard node-level classification (e.g., link prediction in hypergraphs).

2.4 Prizes

With great thanks to our sponsor Arlequin AI, this year's edition of the challenge offered cash prizes for each category winner: $200 USD for each A category and $800 USD for each of the more challenging B categories. Furthermore, selected teams were invited for research internships at the Geometric Intelligence Lab (University of California Santa Barbara) or the Intelligent Maintenance and Operations Systems Lab (École Polytechnique Fédérale de Lausanne, Switzerland).

2.5 Evaluation Method

To decide on the winners in each category, a panel of fifteen `TopoBench` maintainers and collaborators voted on their first and second choice submissions. The Condorcet method was used to rank the submissions. Reviewers were asked to base their rankings on the following criteria, which were visible to challenge participants:

- **Correctness:** Does the submission implement the dataset correctly? Is it reasonable and well-defined?
- **Code quality:** How readable and clean is the implementation? How well does the submission respect the requirements?
- **Documentation & tests:** Are docstrings clear? Are unit tests robust?

Note that these criteria did not reward final model performance on the dataset. Rather, the goal was to deliver well-written, usable datasets and infrastructure that enable further experimentation and insight in the field.

2.6 Software Practices

All submitted code had to comply with the challenge's GitHub Action workflow, successfully passing all tests, linting, and formatting (i.e., ruff). Moreover, to ensure consistency, we asked participants to use TopoNetX's [Hajij et al., 2024] classes to manage simplicial/cell/combinatorial complexes whenever these topological domains were the target of the data loading process.

3 Submissions and Winners

The challenge received a total of 44 submissions from 30 different teams, formed by a total of 45 individual participants; Tables 1, 2, 3 and 4 list all of the submissions and link to their corresponding PRs. The participation was distributed across the two missions as follows:

- **Mission A (Expanding the Data Landscape):** 34 submissions total, with 25 in Category A.1 and 9 in Category A.2.
- **Mission B (Advancing the Data Infrastructure):** 10 submissions total, evenly split with 5 in Category B.1 and 5 in Category B.2.

These submissions originated from a diverse group of teams and participants from 12 institutions worldwide. The high engagement level underscores the growing interest in formalizing and expanding the data landscape for Topological Deep Learning.

The winners were announced publicly at the first Topology, Algebra, and Geometry in Data Science (TAG-DS) Conference, on social media, and on the official challenge website. These announcements emphasized that regardless of final rankings, the challenge organizers and reviewers were exceptionally impressed by the high quality of the submissions and their significant contributions to the `TopoBench` ecosystem. We warmly congratulate all participants.

3.1 Award Category Winners and Honorable Mentions

Awards were presented to the top submission in each category. Additionally, honorable mentions were awarded to the runners-up (second place) based on the Condorcet method's rankings.

Category A.1: Broadening Benchmarks

- **Winner:** *Amiiza team*. Their implementation of *ATLAS Top Tagging* brings a novel benchmark from the particle physics community into the TDL ecosystem.
- **Honorable Mentions:** *MappingComplexityLab* for the HypBench Dataset and *Loris* for the Graphland Benchmark.

Category A.2: Natively Higher-Order Datasets

- **Winner:** *Hugo Walter* for the implementation of Cornell Labeled Nodes Hypergraphs, consisting of 8 single-labeled hypergraph datasets, representing a significant step forward for hypergraph benchmarking.
- **Honorable Mentions:** *IgPa* for the Conjugated Molecule dataset and *TJPaik* for Analog Circuits implementations.

Category B.1: Large-Scale Inductive Infrastructure

- **Winner:** *DLLB team.* This team successfully tackled the challenge of migrating to `OnDiskDataset` support in the transductive setting.
- **Honorable Mention:** *DLLB team.* The team received a special acknowledgement for their impressive strides in scalable data loading for the inductive setting as well.

Category B.2: Pioneering New Benchmark Tasks

- **Winner:** *DLLB team.* They introduced Link Prediction to the benchmark suite, establishing a new standard for the field.
- **Honorable Mention:** *NeuroTriangles team.* Recognized for proposing higher-order cell tasks on a neuroscience dataset.

3.2 Internship Opportunities

Based on the quality and impact of their contributions, the following teams have been offered internship opportunities at the Geometric Intelligence Lab (UC Santa Barbara) and the IMOS Lab (EPFL): DLLB team, NeuroTriangles, HugoWalter.

4 Discussion

The outcomes of Mission A have expanded `TopoBench`'s dataset scope to be more comprehensive and reflective of the community's interests. As noted by Papamarkou et al. [2024], the field has historically lacked a unified benchmark suite for objective comparison across datasets. `TopoBench` now bridges this gap by harmonizing three critical components: the diverse models and topological liftings developed in previous years' challenges [Papillon et al., 2023a, Bernárdez et al., 2024], the platform's native unified evaluation pipeline, and the new heterogeneous datasets contributed in this edition. This integration guarantees the fair assessment and rigorous reproducibility required to advance the field. Consequently, a straightforward yet critical avenue for future research is to perform systematic benchmarking across these diverse datasets. To date, it remains unclear which topological domains and which topological liftings are most suitable for specific applications. In this context, `TopoBench` [Telyatnikov et al., 2025a] provides the necessary ecosystem for understanding where and why different topological settings excel, enabling the rigorous analysis of intrinsic data properties (like higher-order homophily [Telyatnikov et al., 2025b]) and grounding theoretical advances in experimental evidence (e.g. TopoTune [Papillon et al.], HOPSE [Carrasco et al., 2025]).

Simultaneously, the contributions from Mission B have resolved the significant infrastructural constraints highlighted as "Open Problem 6" (Scalability) and "Open Problem 4" (Software Availability) in Papamarkou et al. [2024]. Prior to this challenge, there had been no systematic attempts to build an infrastructure capable of handling large-scale topological workloads. The outcomes of this challenge propose several novel solutions in this regard. Specifically, the successful implementation of robust `OnDiskDataset` loaders directly unlocks scalable workflows for both transductive and inductive settings. When coupled with the platform's established batching mechanisms, these advancements provide the necessary architecture to perform Topological Deep Learning at scale. This infrastructure opens new frontiers for the field, specifically enabling the exploration of cross-domain pretraining and the development of topological foundation models, research directions that were previously intractable due to memory limitations.

5 Conclusion

This white paper details the outcomes of the 2025 *Topological Deep Learning Challenge: Expanding the Data Landscape*. This initiative was specifically designed to tackle the critical bottlenecks identified in the recent position paper by Papamarkou et al. [2024], namely the scarcity of higher-order datasets and the lack of standardized benchmarking infrastructure. The challenge successfully yielded 44 valid submissions that have substantially enriched the `TopoBench` ecosystem, effectively addressing these foundational issues.

We hope that this community effort bridges the gap between TDL and the broader machine learning landscape. By resolving the infrastructure and data challenges that previously constrained the field, the methods and datasets implemented in this challenge constitute a foundational step toward the next generation of topology-aware artificial intelligence.

#PR	Dataset Name	Team Name	Team Members
182	Wiki-CS [Mernyei and Cangea, 2020]	aweers	Alexander Weers
183	HypBench [Aliakbarisani et al., 2024]	MappingComplexityLab	Robert Jankowski
192	GraphLand [Bazhenov et al., 2025]	Loris	Loris Cino
197	WebKB [Pei et al., 2020]	DLLB	David Leko, Luka Benić
212	QM9 [Ramakrishnan et al., 2014]	Perelyn GDL	Michael Banf, Dominik Filipiak
214	Facebook Page Page[Rozemberczki et al., 2021]	GAAIMC	Ixchel Meza-Chávez, Gabriela Aguilar-Argüello
215	Twitch [Rozemberczki et al., 2021]	LangDiff	Jonas Müller
216	LastFM Asia [Rozemberczki and Sarkar, 2020]	GAAIMC	Ixchel Meza-Chávez, Gabriela Aguilar-Argüello
217	Github [Rozemberczki et al., 2021]	GAAIMC	Ixchel Meza-Chávez, Gabriela Aguilar-Argüello
218	CDC-climate, US-county-fb [Jia and Benson, 2022]	TG	Thomas Grapentin
219	Open Circuit Benchmark [Dong et al., 2023]	TJPaik	Taejin Paik
222	Coauthor_CS [Shchur et al., 2018]	thomasvf	Thomas Vaitses Fontanari
223	BA2Motif [Luo et al., 2020]	ghasemi	Ali Ghasemi
224	MoleculeNet [Wu et al., 2018]	neervana	Dario Loi
225	CityNetwork [Liang et al., 2025]	ox_longrange	Haitz Sáez de Ocáriz Borde, Huidong Liang
229	Deezer Europe [Rozemberczki and Sarkar, 2020]	GAAIMC	Ixchel Meza-Chávez, Gabriela Aguilar-Argüello
232	ogbn-arxiv and ogbn-products [Hu et al., 2020]	Guris	Giovanni B. da Rosa, Alexsandro Santos da Rosa Jr
233	OC20/OC22 [Chanussot et al., 2021, Tran et al., 2023]	MatTheo	Théo Saulus
236	WS1000_gamma [Katsman et al., 2024]	Tlaloc	Eric Rubiel Dolores Cuenca
237	Large-Scale Multipurpose Benchmark Datasets for Water Distribution Networks [Tello et al., 2024]	SPAICOM_CattDiN	Leonardo Di Nino, Tiziana Cattai
242	Semantic CIFAR-10	SPAICOM_semantic	Mario Edoardo Pandolfo, Enrico Grimaldi
243	Dynamical Activity Complex [Lecha et al., 2025]	MaAnCla	Andrea Cavallo, Manuel Lecha, Claudio Battiloro
246	Atlas Top Tagging [Collaboration]	Amiiiza	Amirreza Akbari
248	GraphUniverse [Van Langendonck et al., 2025]	louisvl	Louis Van Langendonck
249	Metamath	ProofTruth	Jared Able

Table 1: Submissions for Category A.1

#PR	Dataset Name	Team Name	Team Members
198	RHG-3 [Feng et al., 2024, Gao et al., 2022]	DLLB	David Leko, Luka Benić
220	DAWN [Benson et al., 2021]	AP	Abhijeet Dutta, Patrick Liu
221	Cornell Labeled Nodes Hypergraphs	HugoWalter	Hugo WALTER
227	Simplicial PPI (HIGH-PPI SHS27k + CORUM) [Gao et al., 2023]	TG	Thomas Grapentin
240	Analog Circuits [Mehradfar et al., 2024]	TJPaik	Taejin Paik
244	OMol25 Metals subset [Levine et al., 2025]	NREL-Insightcenter	Yu (Demi) Qin, Graham Johnson
245	ConjugatedMoleculeDataset [Chen and Schwaller, 2024]	IgPa	Pavel Snopov, Igor Morgunov
247	3D2M [Dasgupta, 2024]	GAAIMC	Ixchel Meza-Chávez, Gabriela Aguilar-Argüello
253	MIPLIB [Gleixner et al., 2021]	Snopoff	Pavel Snopov

Table 2: Submissions for Category A.2

#PR	Dataset Name	Team Name	Team Members
213	FakeDataset	DLLB	David Leko, Luka Benić
231	Reddit [Hamilton et al., 2017]	DLLB	David Leko, Luka Benić
250	ogbn-products [Hu et al., 2020]	TG	Thomas Grapentin
251	ogbg-molpcba [Hu et al., 2020]	TG	Thomas Grapentin
254	MUTAG [Morris et al., 2020]	HT	Henry Tsay

Table 3: Submissions for Category B.1

#PR	Dataset Name	Team Name	Team Members
226	Fit-Predict Wrapper	Loris	Loris Cino
230	Simplicial PPI (HIGH-PPI SHS27k + CORUM) [Gao et al., 2023]	TG	Thomas Grapentin
234	PPI [Gao et al., 2023]	DLLB	David Leko, Luka Benić
238	Chordonomicon [Kantarelis et al., 2024]	NPL	Pierrick Leroy, Henrique M. Borges, Xuan-Chen Liu, Raj Deshpande
252	Mouse Auditory Cortex [Bowen et al., 2024]	NeuroTriangles	Maria Yuffa Meshcheryakova

Table 4: Submissions for Category B.2

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