ICML Topological Deep Learning Challenge 2024: Beyond the Graph Domain

Guillermo Bernárdez [*1,2] **Lev Telyatnikov** [*1,2] **Marco Montagna** [1,2] **Federica Baccini** [1,2] **Mathilde Papillon** [3,2] **Miquel Ferriol-Galmés** [3] **Mustafa Hajij** [3,2] **Theodore Papamarkou** [3,2] **Maria Sofia Bucarelli** [2] **Olga Zaghen** [2] **Johan Mathe** [2] **Audun Myers** [2] **Scott Mahan** [2] **Hansen Lillemark** [2] **Sharvaree Vadgama** [3] **Erik Bekkers** [3] **Tim Doster** [3] **Tegan Emerson** [3] **Henry Kvinge** [3] **Katrina Agate** [4] **Nesreen K Ahmed** [4] **Pengfei Bai** [4] **Michael Banf** [4] **Claudio Battiloro** [4] **Maxim Beketov** [4] **Paul Bogdan** [4] **Martin Carrasco** [4] **Andrea Cavallo** [4] **Yun Young Choi** [4] **George Dasoulas** [4] **Matouš Elphick** [4] **Giordan Escalona** [4] **Dominik Filipiak** [4] **Halley Fritze** [4] **Thomas Gebhart** [4] **Manel Gil-Sorribes** [4] **Salvish Goomanee** [4] **Victor Guallar** [4] **Liliya Imasheva** [4] **Andrei Irimia** [4] **Hongwei Jin** [4] **Graham Johnson** [4] **Nikos Kanakaris** [4] **Boshko Koloski** [4] **Veljko Kovač** [4] **Manuel Lecha** [4] **Minho Lee** [4] **Pierrick Leroy** [4] **Theodore Long** [4] **German Magai** [4] **Alvaro Martinez** [4] **Marissa Masden** [4] **Sebastian Mežnar** [4] **Bertran Miquel-Oliver** [4] **Alexis Molina** [4] **Alexander Nikitin** [4] **Marco Nurisso** [4] **Matt Piekenbrock** [4] **Yu (Demi) Qin** [4] **Patryk Rygiel** [4] **Alessandro Salatiello** [4] **Max Schattauer** [4] **Pavel Snopov** [4] **Julian Suk** [4] **Valentina Sánchez** [4] **Mauricio Tec** [4] **Francesco Vaccarino** [4] **Jonas Verhellen** [4] **Frederic Wantiez** [4] **Alexander Weers** [4] **Patrik Zajec** [4] **Blaž Škrlj** [4] **Nina Miolane** [1]

Editors: *S. Vadgama, E.J. Bekkers, A. Pouplin, S.O. Kaba, H. Lawrence, R. Walters, T. Emerson, H. Kvinge, J.M. Tomczak, S. Jegelka*

Abstract

This paper describes the 2nd edition of the *ICML Topological Deep Learning Challenge* that was hosted within the ICML 2024 ELLIS Workshop on Geometry-grounded Representation Learning and Generative Modeling (GRaM). The challenge focused on the problem of representing data in different discrete topological domains in order to bridge the gap between Topological Deep Learning (TDL) and other types of structured datasets (e.g. point clouds, graphs). Specifically, participants were asked to design and implement topological liftings, i.e. mappings between different data structures and topological domains –like hypergraphs, or simplicial/cell/combinatorial complexes. The challenge received 52 submissions satisfying all the requirements. This paper introduces the main scope of the challenge, and summarizes the main results and findings.

[*]Equal contribution [1]Challenge Organizer [2]Challenge Reviewer [3]Challenge Contributor [4]Challenge Participant. Correspondence to: Guillermo Bernárdez <guillermo_bernardez@ucsb.edu>, Lev Telyatnikov <lev.telyatnikov@uniroma1.it>.

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1. Introduction

The field of Topological Deep Learning (TDL) aims to extend Graph Neural Networks (GNN) (Scarselli et al., 2009) by naturally processing relations between two or more elements (Hajij et al., 2022b; Papillon et al., 2023b; Hajij & Istvan, 2021; Bodnar et al., 2021a;b). In particular, TDL methods allow to go beyond the paradigm of pairwise interactions by encoding higher-order relationships using algebraic topology concepts (Bick et al., 2023; Bodnar, 2023; Battiloro et al., 2023a). Fig. 1 presents a visual comparison of traditional discrete domains (i.e. pointclouds, graphs) versus the standard discrete topological domains used to model n-body relations (simplicial/cellular/combinatorial complexes, hypergraphs).

Despite its recent emergence, TDL is already postulated to become a relevant tool in many research areas and applications, from complex physical systems (Battiston et al., 2021) and signal processing (Barbarossa & Sardellitti, 2020) to molecular analysis (Bodnar et al., 2021c) and social interactions (Schaub et al., 2020), to name a few. However, a current limiting factor in the extensive use of higher-order structures is that most datasets are usually stored as pointclouds or graphs. Although researchers have introduced various mechanisms for extracting higher-order elements (e.g. Xu et al. (2022); Battiloro et al. (2023b); Bernárdez et al. (2023); Elshakhs et al. (2024); Hajij et al. (2022a); Hoppe & Schaub (2024)), it remains unclear how to optimize the process given a specific dataset and task.

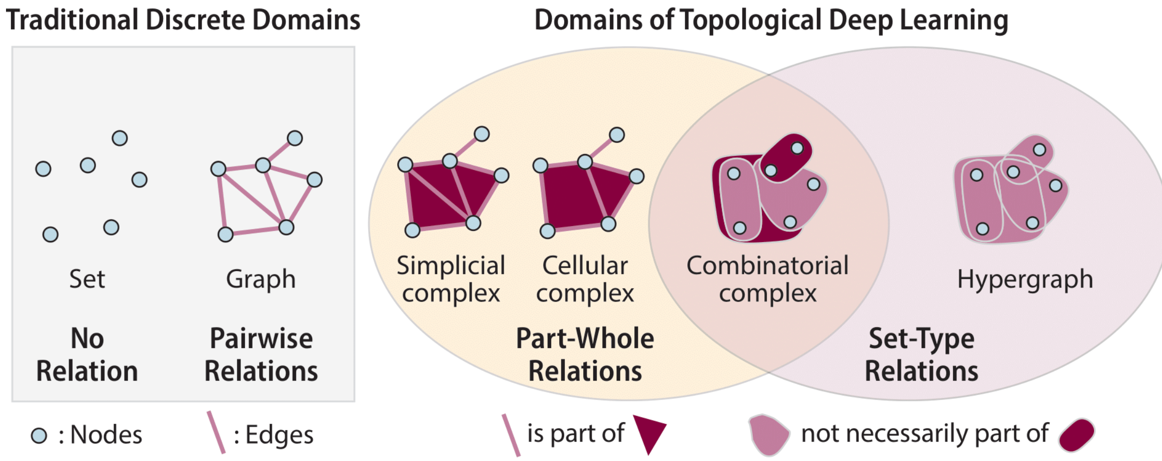

Figure 1. Different discrete domains. Figure adopted from (Papillon et al., 2023b).

In this context, developing tools and methods to move between different discrete (topological) domains represents one of the most pressing open challenges in TDL (Papamarkou et al., 2024). The process of mapping a data structure to a different topological domain is formalized using the concept of *topological lifting* (or, equivalently, *lifting*) (Papillon et al., 2023b). Additionally, a *feature lifting* is a particular lifting that transfers data from an original domain where a signal (node/edge features) exists, to a new domain where new topological structures can emerge, such as simplicial/cell complexes. Fig. 2 depicts some visual examples of different liftings involving several topological domains.

In this framework, the main purpose of the *ICML 2024 Topological Deep Learning Challenge* is to foster new research and knowledge about effective liftings between different topological domains and data structures. The introduction of new topological liftings between different topological domains, as well as an efficient implementation of both new and existing mappings, might help to enforce the impact of TDL to a broader range of use cases and scenarios.

Besides reporting the main organizational aspects of the challenge, this paper aims to give an overview of the main results achieved by participants.

2. Setup of the Challenge

The challenge[1] was hosted by the Geometry-grounded Representation Learning and Generative Modeling (GRaM) Workshop[2] at the International Conference on Machine Learning (ICML) 2024. Participants were asked to implement a topological lifting, apply it to a toy dataset, and test the results with an existing provided model for the considered target domain.

2.1. Guidelines

Participation was free and open to everyone –only principal PyT-Team developers were excluded. To enroll in the challenge it was sufficient to:

- Send a valid Pull Request (PR) –i.e. passing all tests– before the deadline.
- Respect Submission Requirements (see below).

Teams were accepted, and there was no restriction on the number of team members. An acceptable PR automatically subscribed a participant/team to the challenge. A Pull Request could not contain more than one lifting. However, there was no restriction on the number of submissions (i.e. PRs) per participant/team.

Consistent with the aims of an open environment for sharing participation, in this activity was completely voluntary and no support or endorsement of any of the participating parties by any of the other participating parties was provided. All submissions are the views of the individual participants only and should be taken, as is with all faults and without any guarantee, promise or endorsement of any kind.

2.2. Submission Requirements

The submission had to have a valid lifting transformation between any pair of the following data structures: point-cloud/graph, hypergraph, simplicial complex, cell complex, and combinatorial complex. For a lifting to be valid, participants had to implement a mapping between the topological structures of two of the considered domains –*topological lifting*. Participants may optionally implement a procedure

[1]Website: https://pyt-team.github.io/packs/challenge.html
[2]Workshop website: https://gram-workshop.github.io/

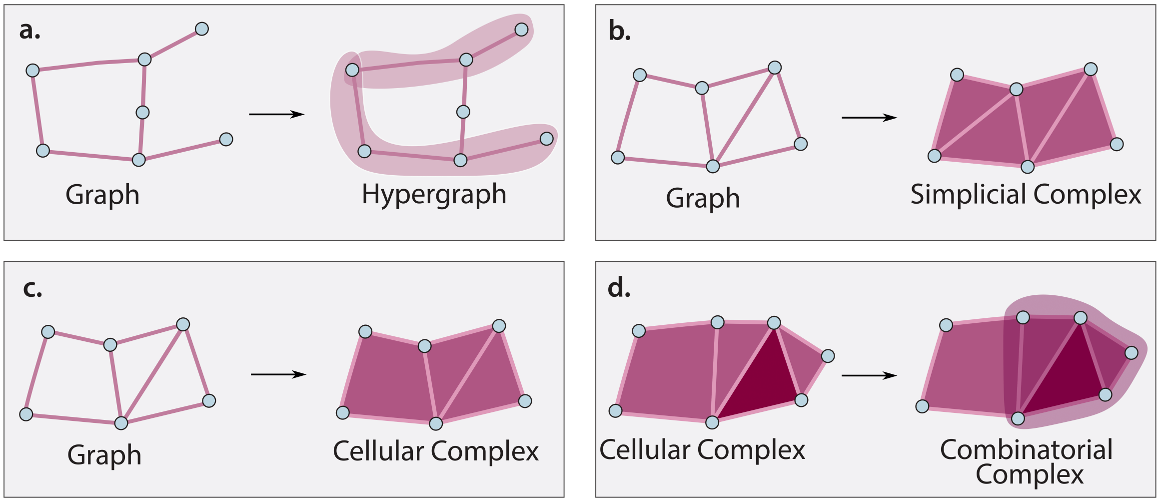

Figure 2. Examples of liftings: (a) A graph is lifted to a hypergraph by adding hyperedges that connect groups of nodes. (b) A graph can be lifted to a cellular complex by adding faces of any shape. (c) Hyperedges can be added to a cellular complex to lift the structure to a combinatorial complex. Figure adopted from (Hajij et al., 2023)

to define the features over the resulting topology –*feature lifting*.

Topology Lifting (Required)

Submissions could implement already proposed liftings from the literature, as well as propose novel approaches. In the case of original liftings, we note that neither the challenge nor its related publications would prevent participants from publishing their work: they keep all the credit for their implementations.

For a lifting from a certain source domain `src` (e.g. graph) to a topological destination `dst` (e.g. simplicial), a submission consisted of a PR to the ICML Challenge repository with the following files:

1. A Python script implementing the topological lifting in a single class using the provided `{src}2{dst}` transform primitives.
2. A configuration file defining the default parameters of the implemented transform.
3. A Jupyter notebook that loads a dataset from the `src` domain, applies the implemented lifting to transform the data into the `dst` domain, and runs a model from `TopoModelX` () over the lifted dataset.
4. A Python script which contains the unit tests for all implemented methods and classes.

Feature Lifting (Optional)

Some TDL models require well-defined features on higher-order structures (e.g. 2-cells, hyperedges); therefore, in their more general formulation, liftings also need to produce initial features for every topological element of the target domain. Participants were more than welcome to implement new feature liftings mappings, although it was optional and only regarded as a bonus.

2.3. Award Categories

Given the lack of an exhaustive analysis of different types of procedures to infer the topological structure within TDL, there was no particular requirement for submitted liftings –apart from a high-quality code implementation. To promote and guide diversity in submissions, we proposed 4 general, non-mutually exclusive Award Categories (ACs) according to the following 2 taxonomies.

By target domain:

- **1st AC:** Best implementation of a lifting to Simplicial of Cell Domain.
- **2nd AC:** Best implementation of a lifting to Combinatorial Complex, Hypergraph, or Graph Domain.

By leveraged information:

- **3rd AC:** Best feature-based lifting, including liftings that leverage both the graph connectivity simultaneously.
- **4th AC:** Best implementation of a lifting using exclusively the graph connectivity.

In addition to the winners' award categories, the challenge also featured honorable mentions. These honorable mentions were determined based on aggregated reviewers' comments.

2.4. Evaluation Method

The Condorcet method was used to rank the submissions and decide on the winners in each category. The evaluation criteria were:

- Does the submission implement the lifting correctly? Is it reasonable and well-defined?
- How readable/clean is the implementation? How well does the submission respect the submission requirements?
- Is the submission well-written? Do the docstrings clearly explain the methods? Are the unit tests robust?

Note that these criteria did not reward the final model performance nor the complexity of the method. Rather, the goal was to implement well-written and accurate liftings that would unlock further experimental evidence and insights in this field.

Selected PyT-Team maintainers and collaborators, as well as each team whose submission(s) respect(s) the guidelines, voted once to express their preference for the best submission in each category. Note that each team was allowed only one vote per category, regardless of the number of team members.

2.5. 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 classes to manage simplicial/cell/combinatorial complexes whenever these topological domains are the target –i.e., destination– of the lifting. Moreover, we highly encouraged the use of TopoX (Hajij et al., 2024) and NetworkX (Hagberg & Conway, 2020) libraries when possible.

3. Submissions and Winners

The challenge received 56 submissions in total, out of which 52 were valid according to the requirements (see Subsection 2.2). Regarding these valid submissions, they come from 31 different teams, with together sum up a total of 57 participants. Each award category accounted for 24, 28, 25, and 27 submissions correspondingly. Table 1 lists all qualifying submissions.

The winners were announced publicly at the ICML Workshop on Geometry-grounded Representation Learning and Generative Modeling, on social media, as well as on the official challenge website. Regardless of the final rankings, we want to emphasize that all the submissions were of exceptionally high quality. We warmly congratulate all participants.

3.1. Award Category Winners

Three prizes were awarded for each category, corresponding to first, second and third places in the Condorcet voting ballot results.

1st AC: Best lifting to Simplicial of Cell Domain.

1. *Random Latent Clique Lifting* (Graph to Simplicial) by Mauricio Tec, Claudio Battiloro, George Dasoulas.
2. *Hypergraph Heat Kernel Lifting* (Hypergraph to Simplicial) by Matt Piekenbrock.
3. *DnD Lifting* (Graph to Simplicial) by Jonas Verhellen

2nd AC: Best lifting to Graph, Hypergraph, or Combinatorial Domain.

1. *Simplicial Paths Lifting* (Graph to Combinatorial) by Manuel Lecha, Andrea Cavallo, Claudio Battiloro.
2. *Matroid Lifting* (Graph to Combinatorial) by Giordan Escalona.
3. *Forman-Ricci Curvature Coarse Geometry Lifting* (Graph to Hypergraph) by Michael Banf, Dominik Filipiak, Max Schattauer, Liliya Imasheva.

3rd AC: Best feature-based lifting.

1. *PointNet++ Lifting* (Pointcloud to Hypergraph) by Julian Suk, Patryk Rygiel.
2. *Kernel Lifting* (Graph to Hypergraph) by Alexander Nikitin.
3. *Mixture of Gaussians + MST Lifting* (Pointcloud to Hypergraph) by Sebastian Mežnar, Boshko Koloski, Blaž Škrlj.

4th AC: Best connectivity-based lifting.

1. *Matroid Lifting* (Graph to Combinatorial) by Giordan Escalona.
2. *Forman-Ricci Curvature Coarse Geometry Lifting* (Graph to Hypergraph) by Michael Banf, Dominik Filipiak, Max Schattauer, Liliya Imasheva.

3. *Hypergraph Heat Kernel Lifting* (Hypergraph to Simplicial) by Matt Piekenbrock.

3.2. Honorable Mentions

Apart from voting for the best implementations in each award category, reviewers were also asked to highlight submissions and/or participants if they found their implementations particularly interesting. Given the high quality of received submissions, reviewers's feedback originated two extra honorable mentions' categories:

Great Contributors: Teams or participants that have submitted several top quality liftings, becoming great contributors of this project.

- Martin Carrasco (PRs 28, 29, 41, 50).
- Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar (PRs 14, 16, 21, 37, 42).
- Theodore Long (PRs 22, 35, 65).
- Jonas Verhellen (PRs 5, 7, 8, 10, 11).
- Pavel Snopov (PRs 6, 9, 18, 20).
- Julian Suk, Patryk Rygiel (PRs 23, 34, 53).

Highlighted Submissions: Original and/or outstanding submissions.

- *Modularity Maximization Lifting* (Graph to Hypergraph) by Valentina Sánchez.
- *Universal Strict Lifting* (Hypergraph to Combinatorial) by Álvaro Martínez.
- *Mapper Lifting* (Graph to Hypergraph) by Halley Fritze, Marissa Masden

4. Conclusion

This white paper presented the motivation and outcomes of the organization of the 2nd edition of the Topological Deep Learning Challenge hosted through the ICML 2024 Geometry-grounded Representation Learning and Generative Modeling (GRaM) Workshop. Challenge submissions implemented a wide variety of topological liftings between different pair of discrete (topological) domains, providing with a rich assortment of tools to infer and exploit higher-order structures. We hope that this community effort will help bridging the gap between TDL and most of the current datasets, stored as pointclouds or graphs. Therefore, the methods implemented in this challenge can potentially foster research and further methodological benchmarks in this growing TDL field.[3]

Last, but not least, we remark that the participation statistics of this 2nd challenge edition almost doubled the numbers of the previous ICML 2023 TDL Challenge (Papillon et al., 2023a) –both in terms of participants and submissions–, indicating a notable increase in interest in the TDL field.

[3] In fact, all challenge submissions are by design compatible with `TopoBenchmarkX` framework (Telyatnikov et al., 2024), which easily allows the use of a diverse set of datasets, models and topological liftings.

Lifting name	ACs	Authors	Source domain	Dest. domain	Feat.-based	Conn.-based
Independent Sets Lifting	1,4	Frederic Wantiez	G	SC		✓
Neighborhood Lifting	1,4	Jonas Verhellen	G	CC		✓
Neighborhood/Dowker Lifting	1,4	Pavel Snopov	G	SC		✓
Vietoris-Rips Lifting	1,3	Jonas Verhellen	G	SC	✓	
Graph Induced Lifting	1,4	Jonas Verhellen	G	SC		✓
Line Lifting	1,4	Pavel Snopov	G	SC		✓
Eccentricity Lifting	1,4	Jonas Verhellen	G	SC		✓
DnD Lifting	1,3	Jonas Verhellen	G	SC	✓	
CellEncoding Lifting	2,4	Alexander Weers	CC	G		✓
KNN Graph Lifting	2,3	Frederic Wantiez	PC	SC	✓	
Molecule Ring-Based Lifting	1,4	Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar	G	CC		✓
Molecule Ring & Close Atoms Lifting	2,3	Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar	G	CCC	✓	✓
Vietoris–Rips Lifting	1,3	Matouš Elphick	PC	SC	✓	
Delaunay Lifting	1,3	Pavel Snopov	PC	SC	✓	
KNN Lifting	2,3	Hongwei Jin	PC	G	✓	
Witness Lifting	1,3	Pavel Snopov, German Magai	PC	SC	✓	
Molecule Ring & Functional Lifting	2,3	Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar	G	CCC	✓	✓
Alpha Complex Lifting	1,3	Theodore Long	PC	SC	✓	
Expander Hypergraph Lifting	2,4	Julian Suk, Patryk Rygiel	G	HG		✓
Cy2C Lifting	1,4	Yun Young Choi, Minho Lee	G	SC		✓
N-Hop Lifting	2,4	Martin Carrasco	G	CCC		✓
Coface Lifting	2,4	Martin Carrasco	SC	CCC		✓
Kernel Lifting	2,3	Alexander Nikitin	G	HG	✓	✓
Matroid Lifting	2,4	Giordan Escalona	G	CCC		✓
Forman-Ricci Curvature Coarse Geometry Lifting	2,4	Michael Banf, Dominik Filipiak, Max Schattauer, Liliya Imasheva	G	HG		✓
Voronoi Lifting	2,3	Julian Suk, Patryk Rygiel	PC	HG	✓	
Feature-Based Rips Complex	1,3	Theodore Long	PC	SC	✓	
Protein Close Residues Lifting	2,3	Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar	G	HG	✓	✓

Random Walks Lifting	2,3	Nikos Kanakaris, Veljko Kovač, Nesreen K Ahmed, Paul Bogdan, Andrei Irimia	PC	G	✓	
Node Attribute Lifting	2,3	Yu Demi Qin, Graham Johnson	G	HG	✓	
Neighbourhood Complex Lifting	1,4	Martin Carrasco	G	SC		✓
PointCloud to Graph Protein Lifting	2,3	Bertran Miquel-Oliver, Manel Gil-Sorribes, Alexis Molina, Victor Guallar	PC	G	✓	
Path-based Lifting	1,4	Salvish Goomanee	G	CCC		✓
Directed Flag Complex Lifting	2,3	Thomas Gebhart	G	SC		✓
Mixture of Gaussians + MST Lifting	2,3	Sebastian Mežnar, Boshko Koloski, Blaž Škrlj	PC	HG	✓	
Node centrality Lifting	2,4	Michael Banf, Dominik Filipiak, Max Schattauer, Liliya Imasheva	G	HG		✓
Universal Strict Lifting	2,4	Alvaro Martinez	HG	CCC		✓
Mapper Lifting	2,4	Halley Fritze, Marissa Masden	G	HG		✓
Modularity Maximization Lifting	2,3	Valentina Sánchez	G	HG	✓	✓
Random Flag Complex Lifting	1,3	Martin Carrasco	PC	SC	✓	
Path lifting	2,4	Pierrick Leroy, Marco Nurisso, Francesco Vaccarino	G	HG		✓
PointNet++ Lifting	2,3	Julian Suk, Patryk Rygiel	PC	HG	✓	
Ball-Pivoting Lifting	1,3	Katrina Agate	PC	SC	✓	
Spin Lifting	1,4	Pengfei Bai	G	PC		✓
Simplicial Paths Lifting	2,4	Manuel Lecha, Andrea Cavallo, Claudio Battiloro	G	CCC		✓
Hypergraph Heat Kernel Lifting	1,4	Matt Piekenbrock	HG	SC		✓
Tangential (Delaunay) Lifting	1,3	Maxim Beketov	PC	SC	✓	
Probabilistic Clique Lifting	2,4	Alvaro Martinez	G	CCC		✓
Random Latent Clique Lifting	1,4	Mauricio Tec, Claudio Battiloro, George Dasoulas	G	SC		✓
Discrete Conf. Complex	1,4	Theodore Long	G	CC		✓
Mapper Lifting	2,3	Patrik Zajec	PC	G	✓	
Spectral Lifting	2,3	Alessandro Salatiello	G	HG	✓	

Table 1: List of valid submissions. Legend for domains: PC $\rightarrow$ pointcloud , G $\rightarrow$ graph, HG $\rightarrow$ hypergraph, SC $\rightarrow$ simplicial, CC $\rightarrow$ cellular, and CCC $\rightarrow$ combinatorial.

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