TopER: Topological Graph Embeddings

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Why TopER?

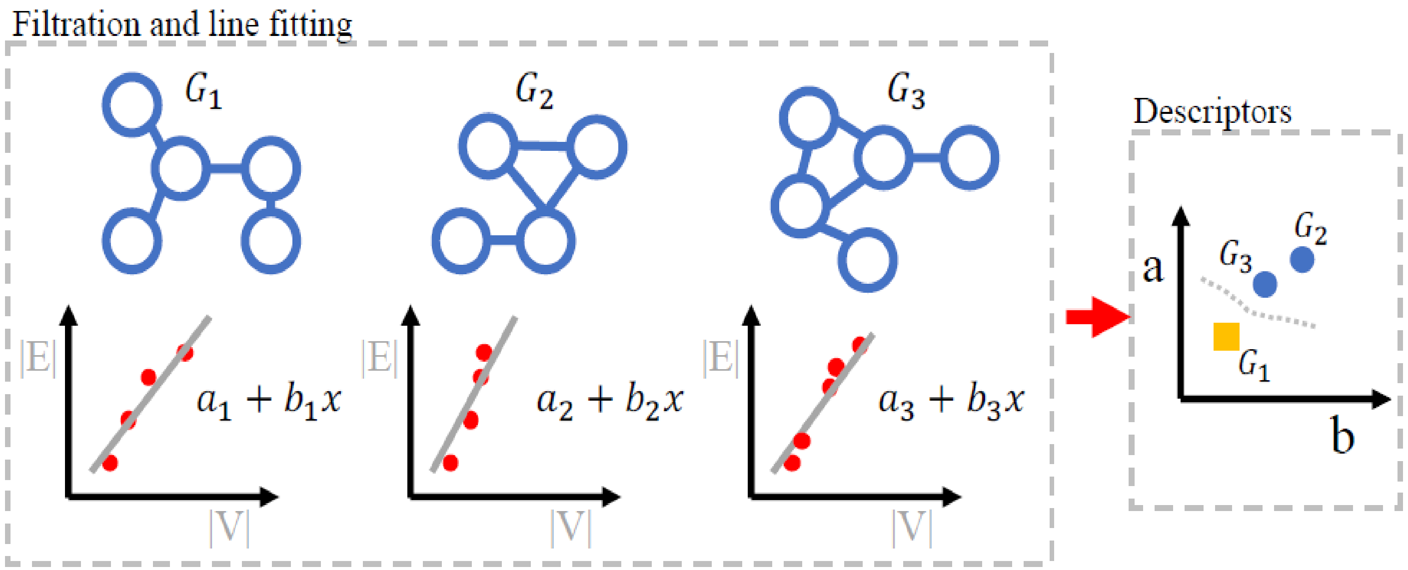
- Standard graph embeddings are high-dimensional and mainly useful for visualizing datasets, **not individual graphs**.
- Existing node-level embedding methods enable visualization of a single graph, but **low-dimensional graph-level embeddings** are largely missing.
- **Persistent Homology** encodes rich topological information but produces complex, hard-to-interpret outputs.
- By leveraging the **filtration process**, we can derive simple and informative low-dimensional summaries that effectively capture topological changes.

TopER: Interpretable Graph Embeddings

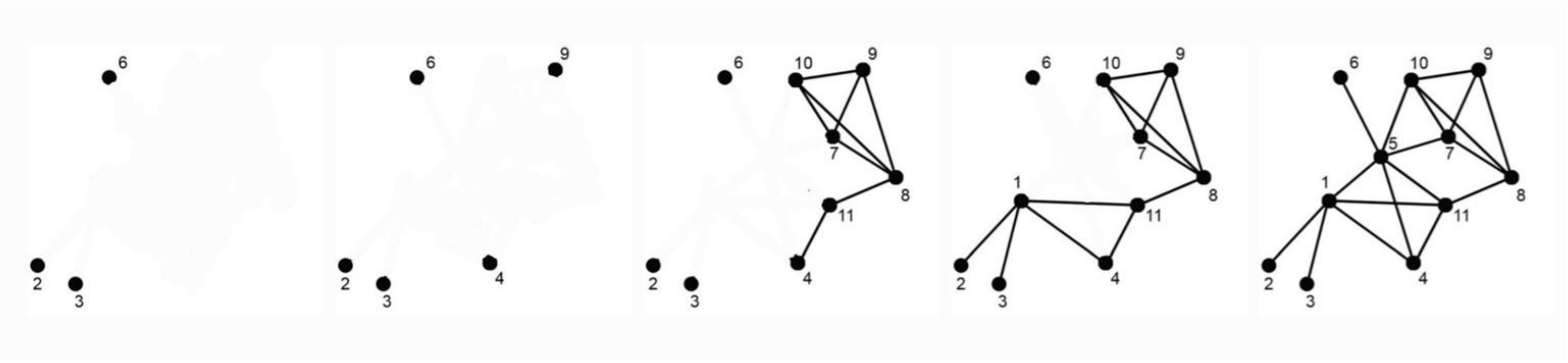
- **TopER** is inspired by the idea of Persistent Homology, which assumes data has a shape and we can quantify it.
- **TopER** tracks how graph shapes change over time.
- It is a low-dimensional Graph Embedding, which can serve as a vectorization of PD.
- It consists of three steps:
  - **Filtration Sequence**
  - **Relative Diagram $\mathcal{A}$**
  - **Evolution**

TopER: Low Dimensional Graph Invariant

- **Filtration Sequence**
  - For a given graph G, we built a nested sequence of subgraphs
$$G_1 \subseteq G_2 \subseteq \cdots \subseteq G_n = G$$
- **Relative Diagram $\mathcal{A}$**
  - $\mathcal{A} = \{(x_i, y_i)\}_{i=1}^{M}$, where x_i = number of 0-cells (nodes), y_i = number of 1-cells (edges) at each threshold α_i.
- **Evolution**
  - We use the Least-Squares method to compute the **linear fit** coefficients a and b of L(x) = a + bx (from evolution of the subgraphs), and then set [a,b] as the graph's feature vector.



Visualization of TopER

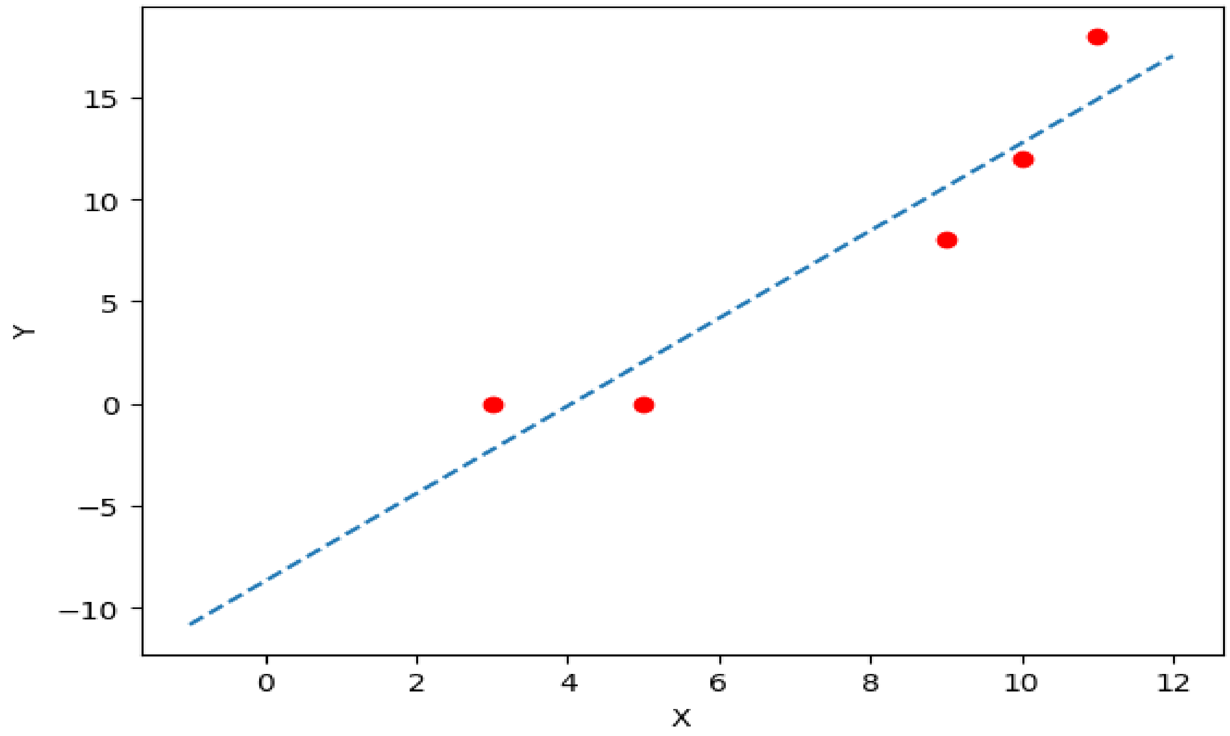


$\mathcal{G}_1$ $\mathcal{G}_3$ $\mathcal{G}_4$ $\mathcal{G}_5$ $\mathcal{G}_6$

$$\mathcal{A} = \{(3,0),(5,0),(9,8),(10,12),(11,18)\}$$

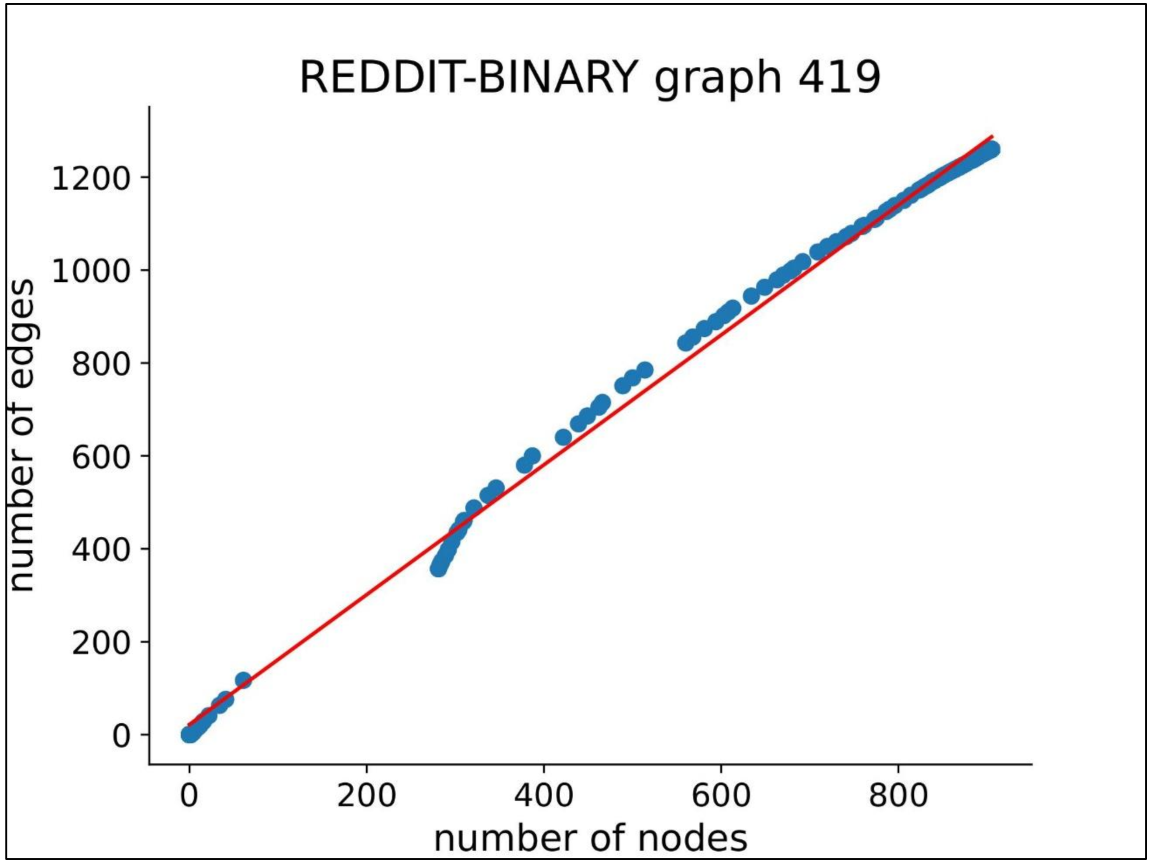
#nodes #edges

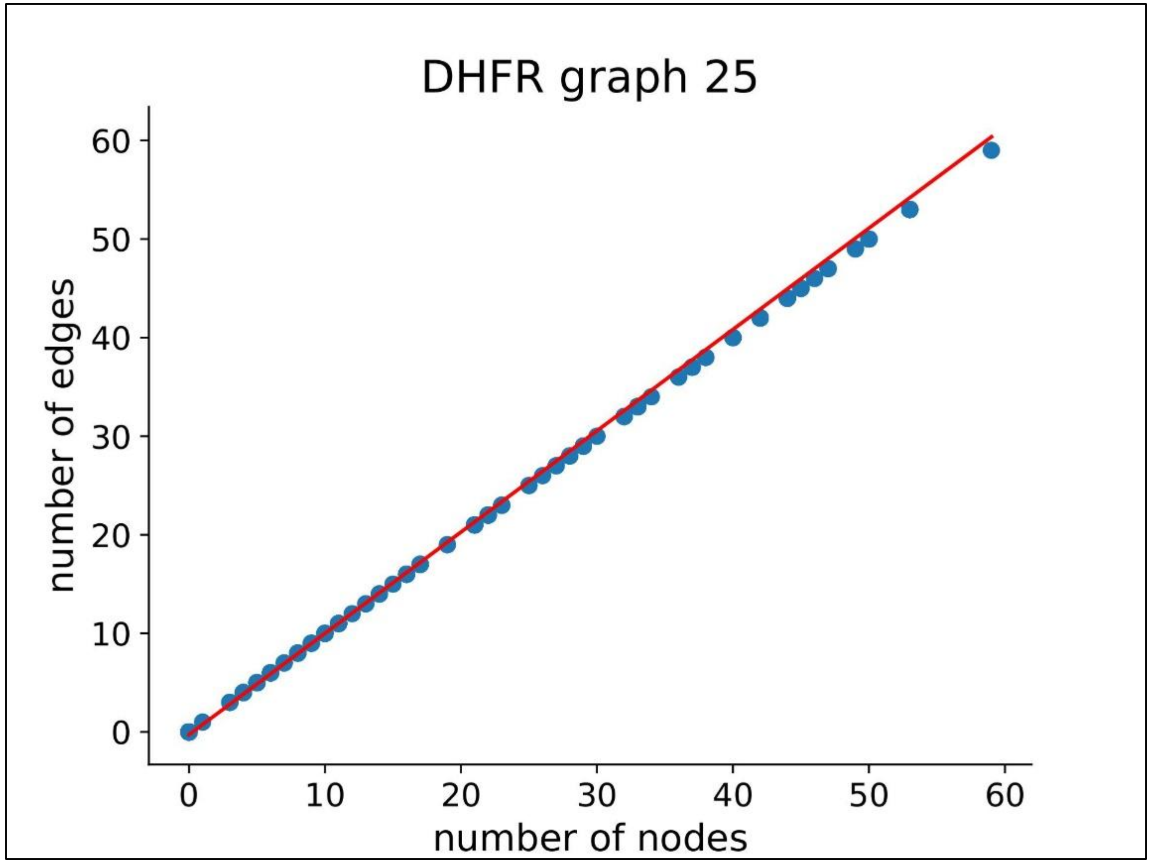
Visualization of TopER (contd.)



For a given graph G, we decompose it into subgraphs $\mathrm{G}_1 \subseteq \mathrm{G}_2 \subseteq \cdots \subseteq \mathrm{G}_\mathrm{n} = \mathrm{G}$, and extract pairs (x_i, y_i) where x_i is the number of nodes and y_i is the number of edges in $\mathrm{G_i}$.
Using the least squares fit, we obtain (a, b) a 2D embedding representing graph G.

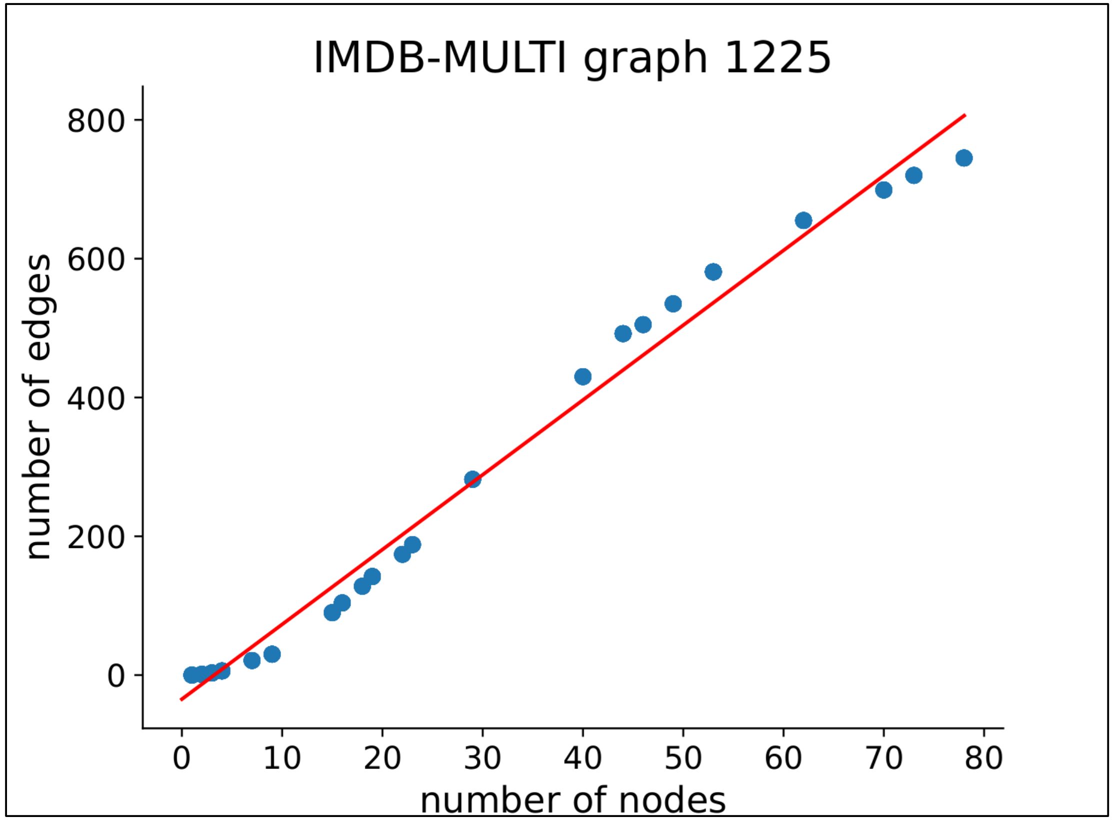
Real Datasets Representations



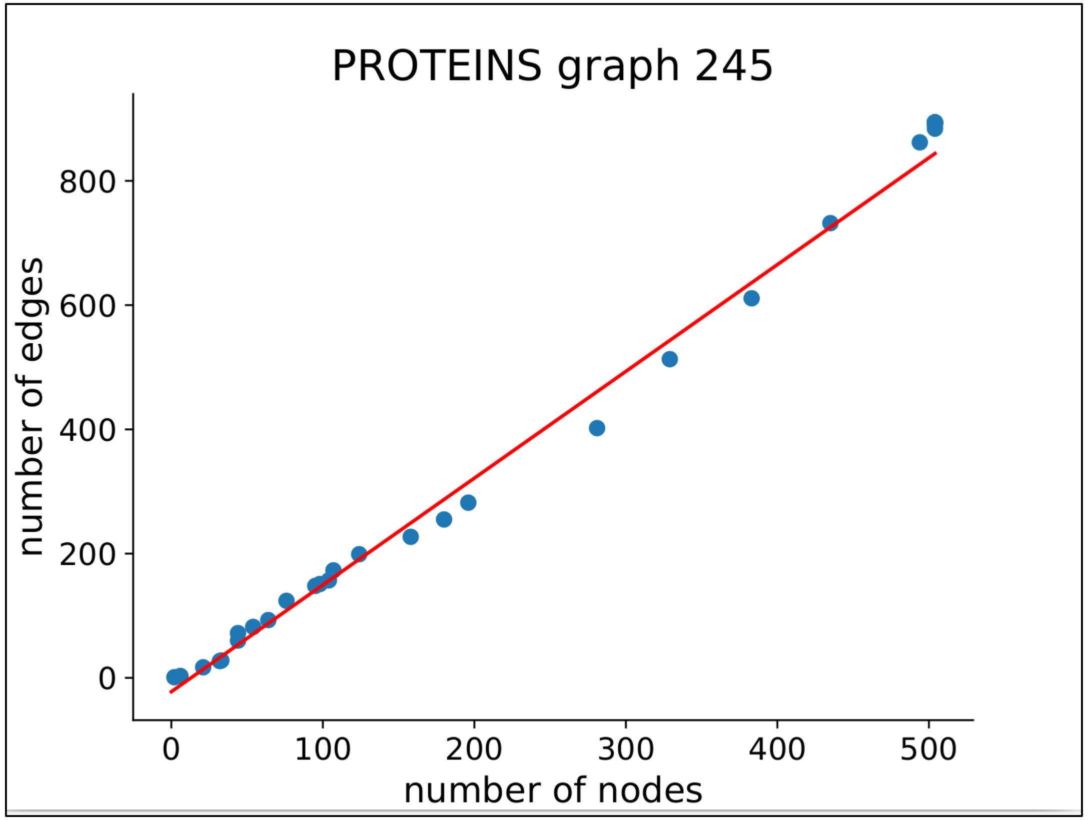


Closeness filtration

Real Datasets Representations



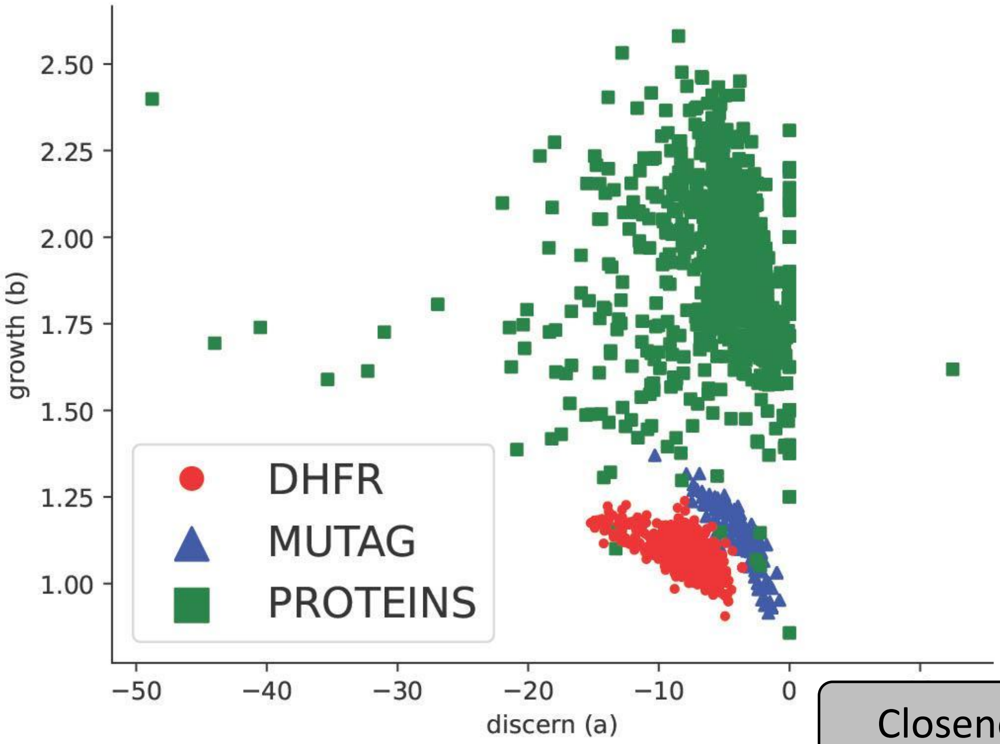
Degree Centrality filtration

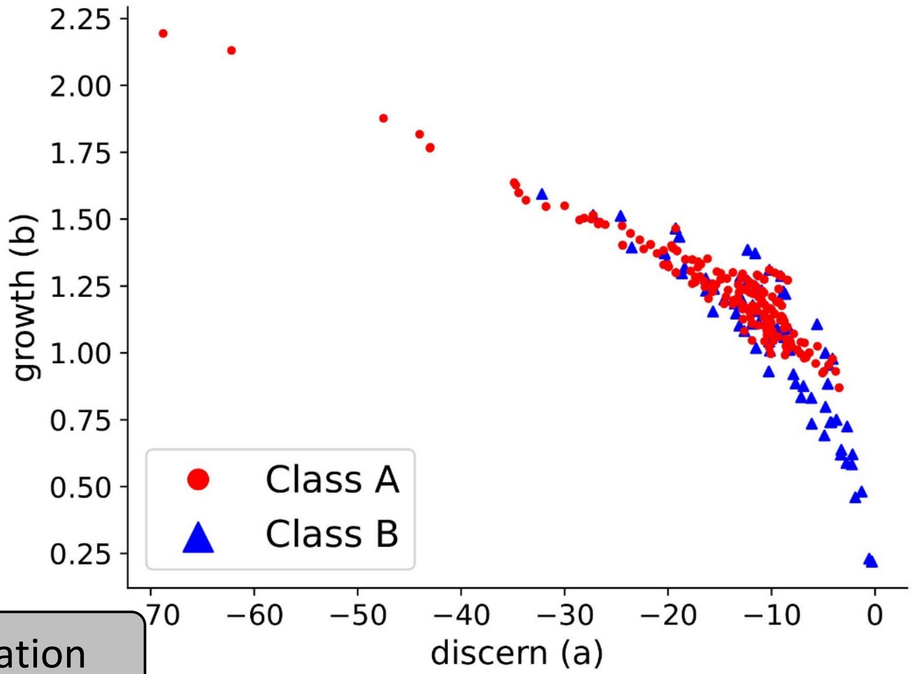


Forman Ricci filtration

Advantages of TopER

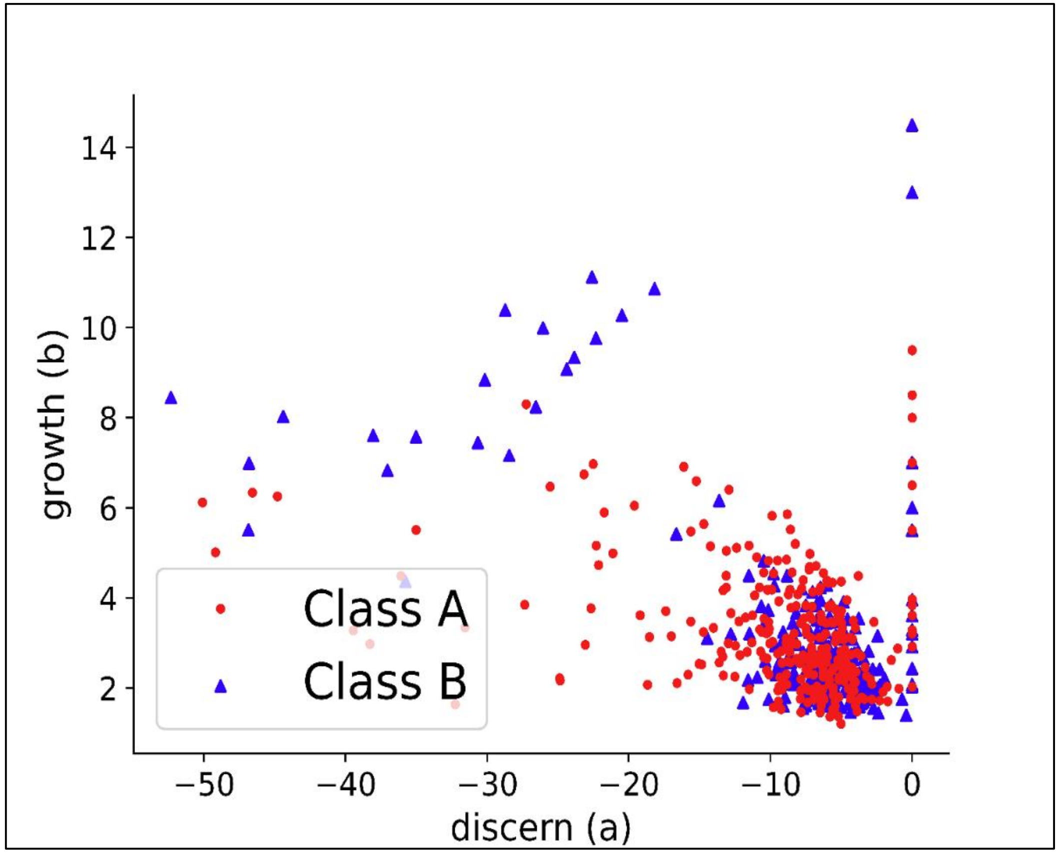
- Enables clear visualization of graph clusters and outliers.
- Simple, fast, and interpretable method.
- Achieves accuracy competitive with SOTA models.
- Fixed-size embeddings can support structural transfer in graph learning.



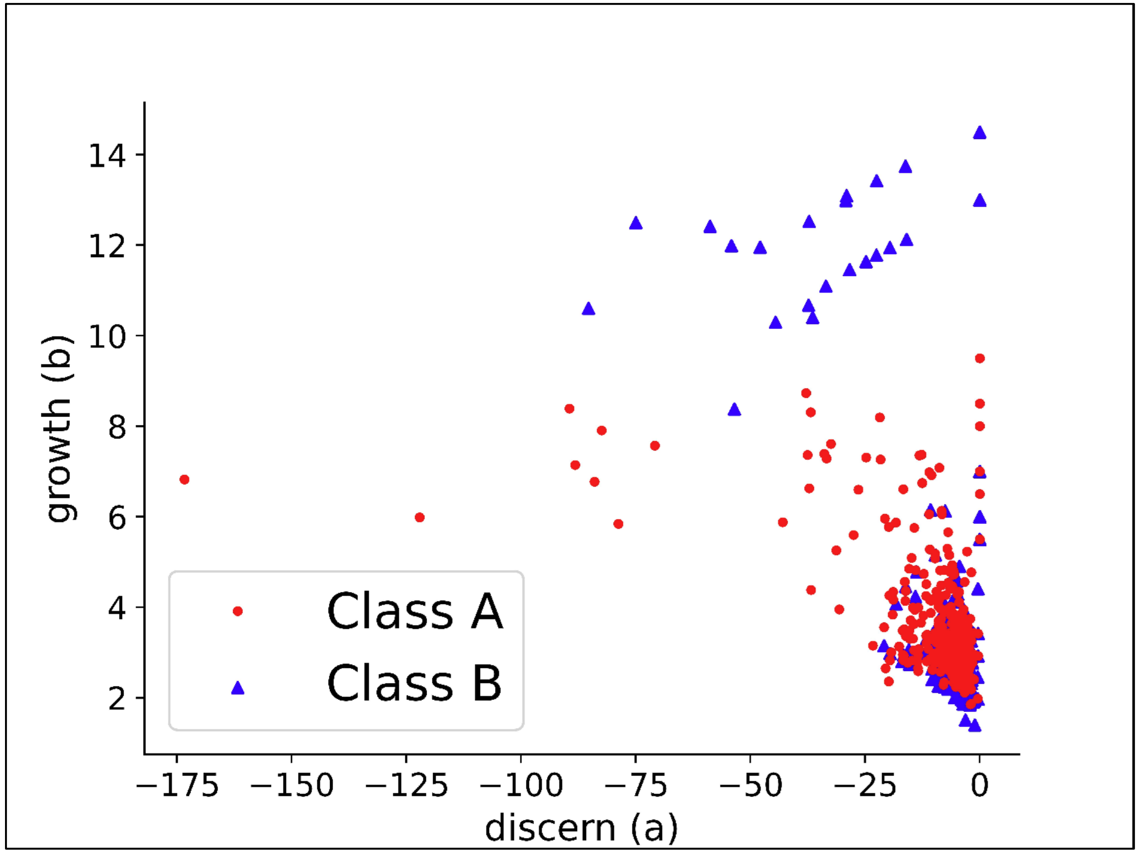


Closeness filtration

IMDB-B visualization

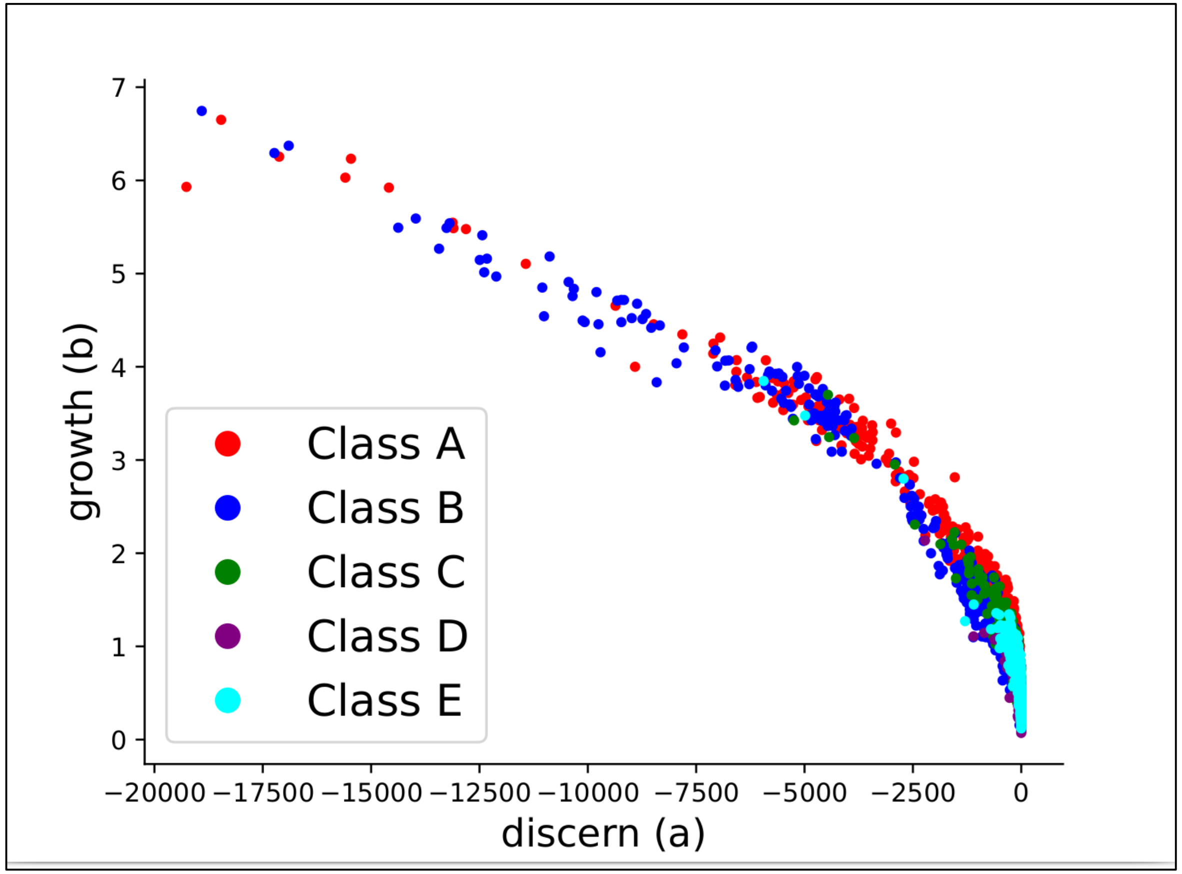


Degree-Centrality filtration

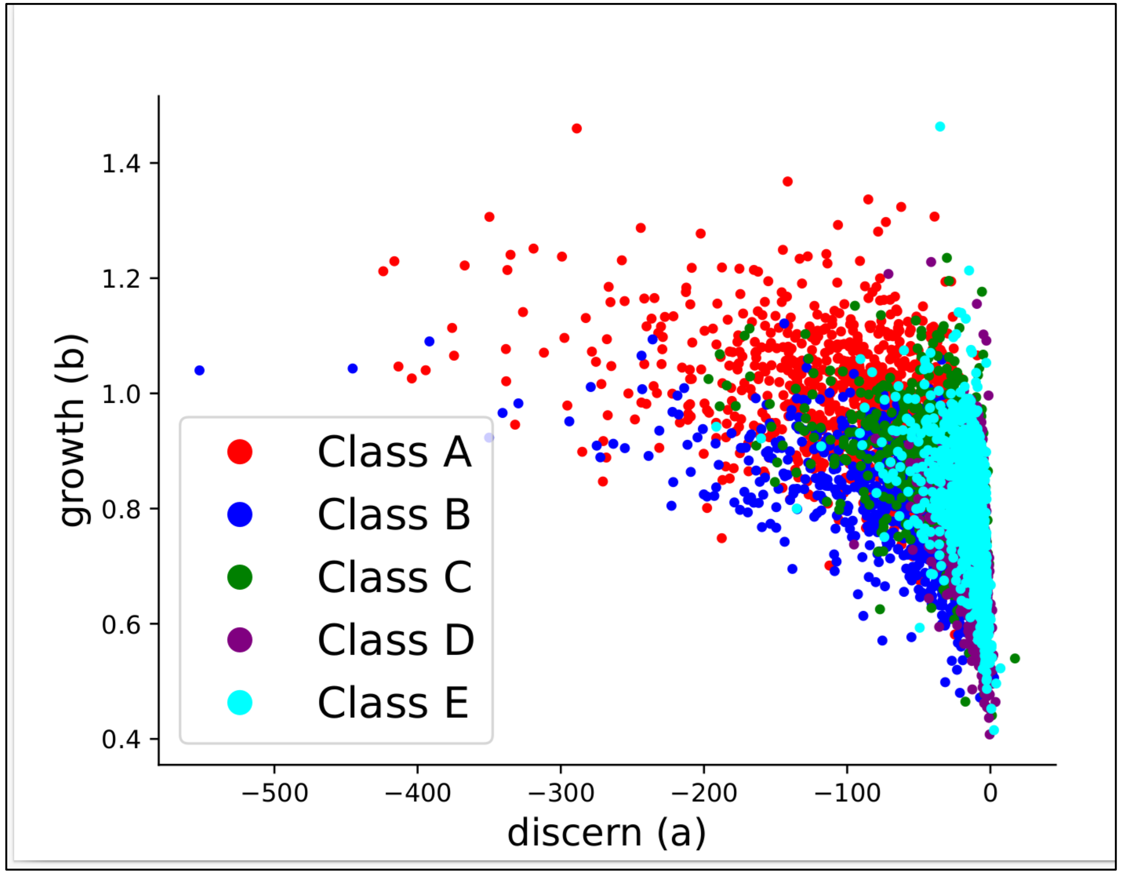


Forman Ricci filtration

Reddit-5K visualization



Degree-Centrality filtration



Closeness filtration

Graph Classification Performance

Model	BZR	COX2	MUTAG	PROTEINS	IMDB-B	IMDB-M	REDDIT-B	REDDIT-5K	Avg.↓
DiffPool	83.93 ± 4.41	79.66 ± 2.64	79.22 ± 1.02	73.63 ± 3.60	68.60 ± 3.10	45.70 ± 3.40	79.00 ± 1.10	--	8.06
P-WL-C	--	--	90.51 ± 1.34	75.27 ± 0.38	--	--	--	--	2.08
SAGPool	82.95 ± 4.95	79.45 ± 2.98	76.78 ± 2.12	71.86 ± 0.97	74.87 ± 4.09	49.33 ± 4.90	84.70 ± 4.40	--	6.61
Top-k	79.40 ± 1.20	80.30 ± 4.21	67.61 ± 3.36	69.60 ± 3.50	73.17 ± 4.84	48.80 ± 3.19	79.40 ± 7.40	--	9.70
1-GIN (GFL)	--	--	--	74.10 ± 3.40	74.50 ± 4.60	49.70 ± 2.90	90.20 ± 2.80	55.70 ± 2.90	2.09
6 GNNs	--	--	80.42 ± 2.07	75.80 ± 3.70	71.20 ± 3.90	49.10 ± 3.50	89.90 ± 1.90	56.10 ± 1.60	4.13
MinCutPool	82.64 ± 5.05	80.07 ± 3.85	79.17 ± 1.64	76.62 ± 2.58	70.77 ± 4.89	49.00 ± 2.83	87.20 ± 5.00	--	5.82
DMP	--	--	84.00 ± 8.60	75.30 ± 3.30	73.80 ± 4.50	50.90 ± 2.50	86.20 ± 6.80	51.90 ± 2.10	4.20
FC-V	85.61 ± 0.59	81.01 ± 0.88	87.31 ± 0.66	74.54 ± 0.48	73.84 ± 0.36	46.80 ± 0.37	89.41 ± 0.24	52.36 ± 0.37	4.01
SubMix	86.34 ± 2.00	84.68 ± 3.70	80.99 ± 0.60	67.80 ± 2.00	70.30 ± 1.40	46.47 ± 2.50	--	--	6.15
G-Mix	84.15 ± 2.30	83.83 ± 2.10	81.96 ± 0.60	66.28 ± 1.10	69.40 ± 1.10	46.40 ± 2.70	--	--	6.91
RGCL	84.54 ± 1.67	79.31 ± 0.68	87.66 ± 1.01	75.03 ± 0.43	71.85 ± 0.84	49.31 ± 0.42	90.34 ± 0.58	56.38 ± 0.40	3.56
AutoGCL	86.27 ± 0.71	79.31 ± 0.70	88.64 ± 1.08	75.80 ± 0.36	72.32 ± 0.93	50.60 ± 0.80	88.58 ± 1.49	**56.75 ± 0.18**	3.08
FF-GCN	89.00 ± 5.00	78.00 ± 8.00	71.00 ± 4.00	62.00 ± 1.00	63.00 ± 8.00	--	--	--	11.53
WWLS	88.02 ± 0.61	81.58 ± 0.91	88.30 ± 1.23	75.35 ± 0.74	**75.08 ± 0.31**	51.61 ± 0.62	--	--	2.26
EPIC	88.78 ± 2.30	**85.53 ± 1.60**	82.44 ± 0.70	69.06 ± 1.00	71.70 ± 1.00	47.93 ± 1.30	--	--	4.67
EMP	--	--	88.79 ± 0.63	72.78 ± 0.54	74.44 ± 0.45	48.01 ± 0.42	91.03 ± 0.22	54.41 ± 0.32	2.97
MP-HSM	--	77.10 ± 3.00	85.60 ± 5.30	74.60 ± 2.10	74.80 ± 2.50	47.90 ± 3.20	--	--	4.67
TopoGCL	87.17 ± 0.83	81.45 ± 0.55	90.09 ± 0.93	**77.30 ± 0.89**	74.67 ± 0.32	**52.81 ± 0.31**	90.40 ± 0.53	--	1.76
PGOT	87.32 ± 3.90	82.98 ± 5.21	**92.63 ± 2.58**	73.21 ± 2.59	62.90 ± 3.05	51.33 ± 1.76	--	--	3.85
RePHINE	--	--	--	71.25 ± 1.60	69.40 ± 3.78	--	--	--	5.86
GPSE	80.49 ± 4.18	78.37 ± 2.62	87.19 ± 8.66	72.15 ± 3.66	69.30 ± 3.61	47.40 ± 5.40	80.40 ± 3.40	--	7.27
TopER	**90.13 ± 4.14**	82.01 ± 4.59	90.99 ± 6.64	74.58 ± 3.92	73.20 ± 3.43	50.00 ± 4.02	**92.70 ± 2.38**	56.51 ± 2.22	**1.60**

Clustering Performances

Clustering Performances. Comparison of Spectral Zoo vs. TopER.

Metric	Method	BZR	COX2	MUTAG	PROT.	IMDB-B	IMDB-M	REDD-B	REDD-5K
Silh ↑	Spec. Zoo	0.05	0.049	**0.344**	0.050	**0.097**	**-0.024**	0.108	-0.121
	TopER	**0.249**	**0.414**	0.258	**0.086**	0.064	-0.032	**0.196**	**-0.067**
CH ↑	Spec. Zoo	3.51	6.13	**120.73**	38.77	**85.24**	**30.98**	269.94	119.81
	TopER	**42.58**	**26.00**	72.52	**151.64**	60.52	11.77	**446.12**	**1209.95**
DB ↓	Spec. Zoo	7.25	6.07	0.95	4.55	2.78	10.73	2.20	25.74
	TopER	**1.93**	**2.29**	**0.88**	**1.54**	**2.19**	**6.87**	**1.32**	**2.78**

TopER vs. Persistent Homology in graph classification tasks

Method	BZR	COX2	PROTEINS	IMDB-B	IMDB-M	RED-5K
PH	88.4 ± 0.6	**82.0 ± 0.6**	74.0 ± 0.4	69.5 ± 0.5	46.5 ± 0.3	54.1 ± 0.1
TopER	**90.1 ± 4.1**	**82.0 ± 4.6**	**74.6 ± 3.9**	**73.2 ± 3.4**	**50.0 ± 4.0**	**56.5 ± 2.2**

Future Work

- **Temporal Graph Learning**
  - Extend TopER to dynamic/temporal graphs
  - Capture evolving graph trajectories and user behavior over time

- **Integration with Graph Foundation Models**
  - As fixed sized embedddings, incorporate TopER embeddings into large-scale graph pre-training for structural transfer

- **Multi-Modal Graph Analysis**
  - Combine TDA features with text, images, or node attributes
  - Improve performance in heterogeneous information networks

Thank You

Contact Us

- **Email:** astrittola@gmail.com
- **GitHub:** https://github.com/AstritTola/TopER