A Comprehensive Study on Text-attributed Graphs: Benchmarking and Rethinking

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NeurIPS 2023 Datasets and Benchmark track

CONTENT

BACKGROUND

- Graphs are ubiquitous in real word

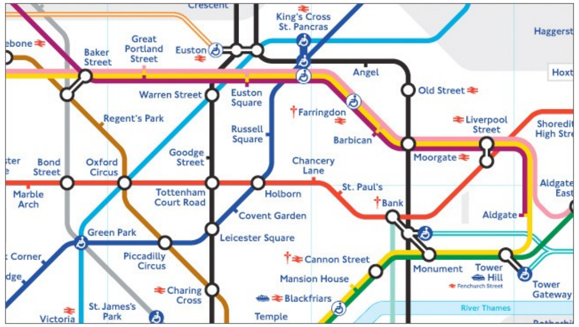


Image credit: visitlondon.com

- Underground Networks

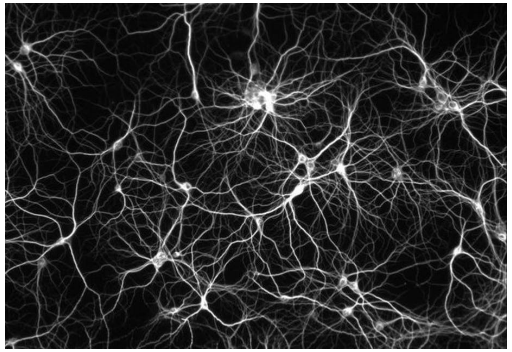


Image credit: The Conversation

- Networks of Neurons

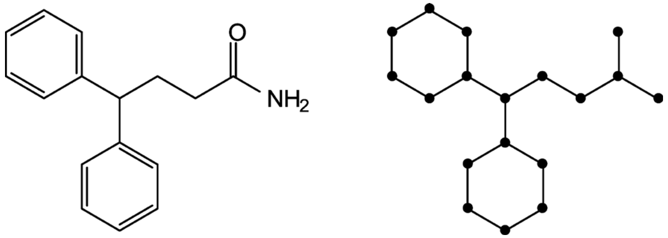


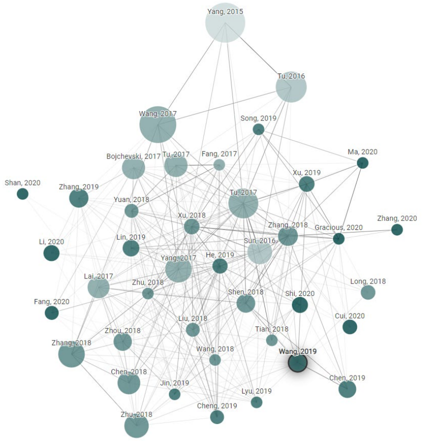
Image credit: MDPI

- Molecules

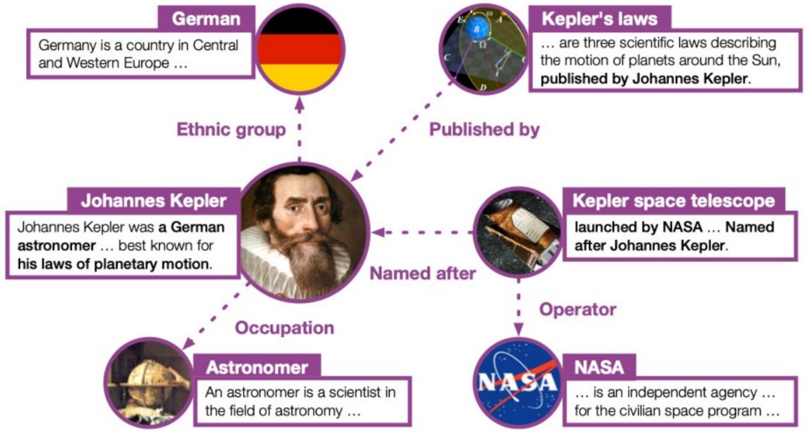
- Text-attributed graphs (TAGs): Nodes are often associated with text attributes

Image credit: Medium

- Social Networks



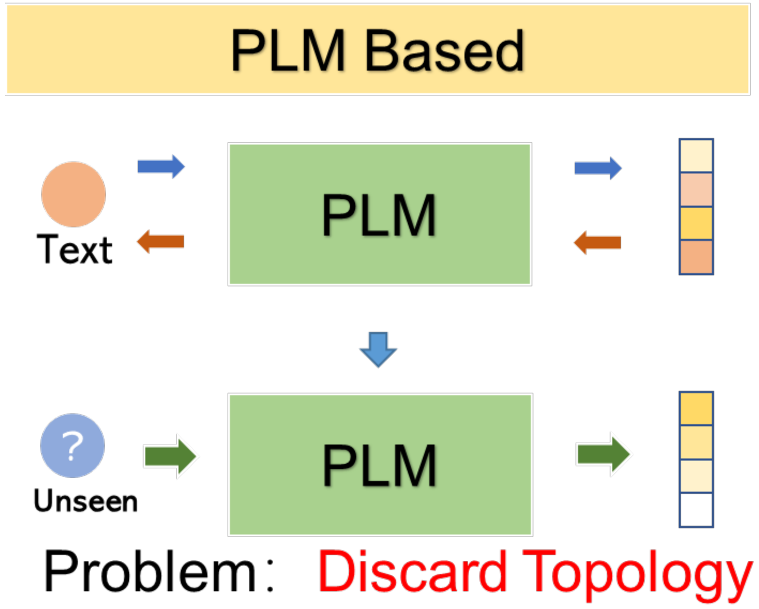
- Citation Networks



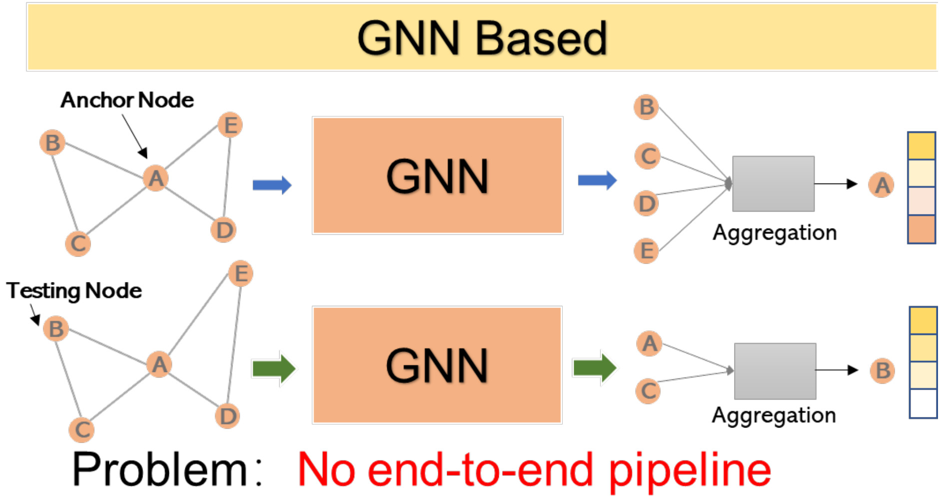
- Knowledge Graph

BACKGROUND

- Representation Learning on TAGs
  - Pre-trained Language Model (PLM) based
    - PLMs (Encoder-only) : BERT, ELECTRA, DeBERTa, RoBERTa.
    - Problem: The knowledge of topology is largely discarded



  - Graph Neural Network (GNN) based
    - GNNs (Message-Passing): GCN, GraphSAGE, GAT.
    - Problem: Modeling of node attributes and graph topology is disconnected

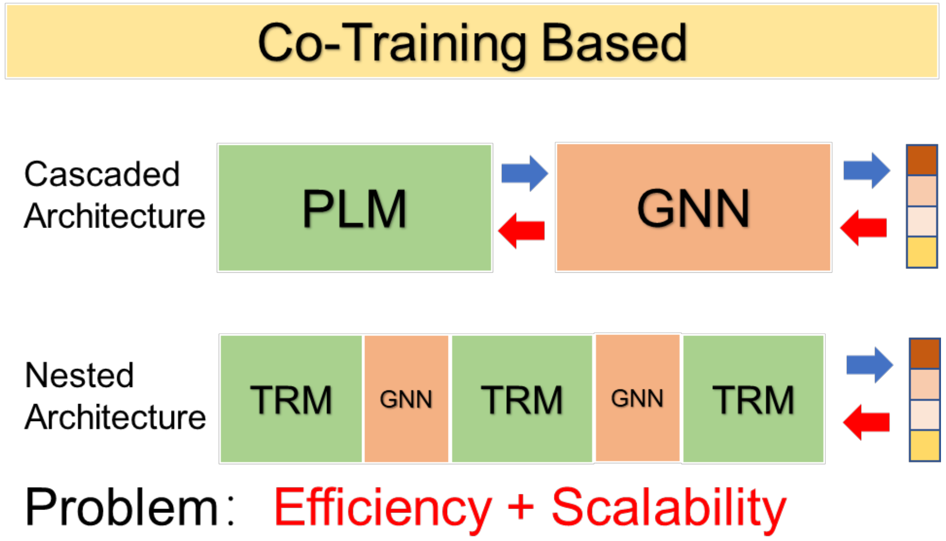


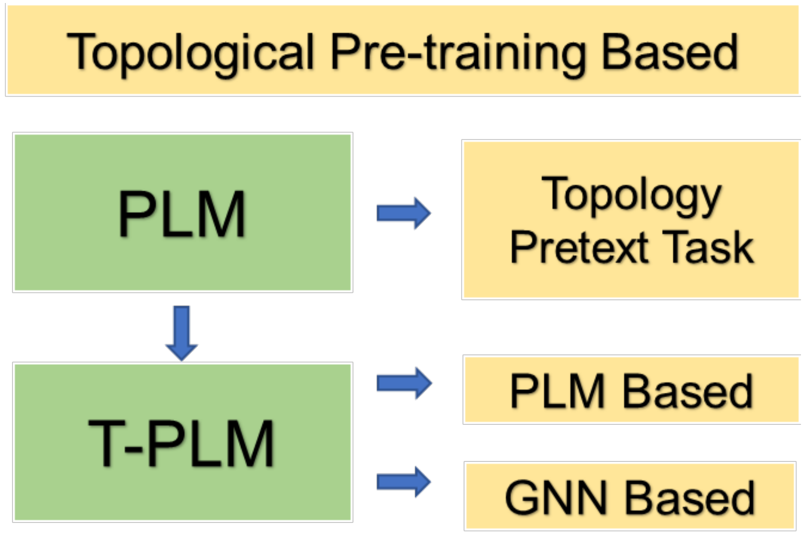
BACKGROUND

- Representation Learning on TAGs
  - Co-Training based
    - An end-to-end training paradigm to jointly model the node attributes and graph topology

$$f_{\Theta}(A,T) = GNN_{\omega}\left(A, LM_{\psi}(T)\right), \Theta = \{\omega, \psi\}$$

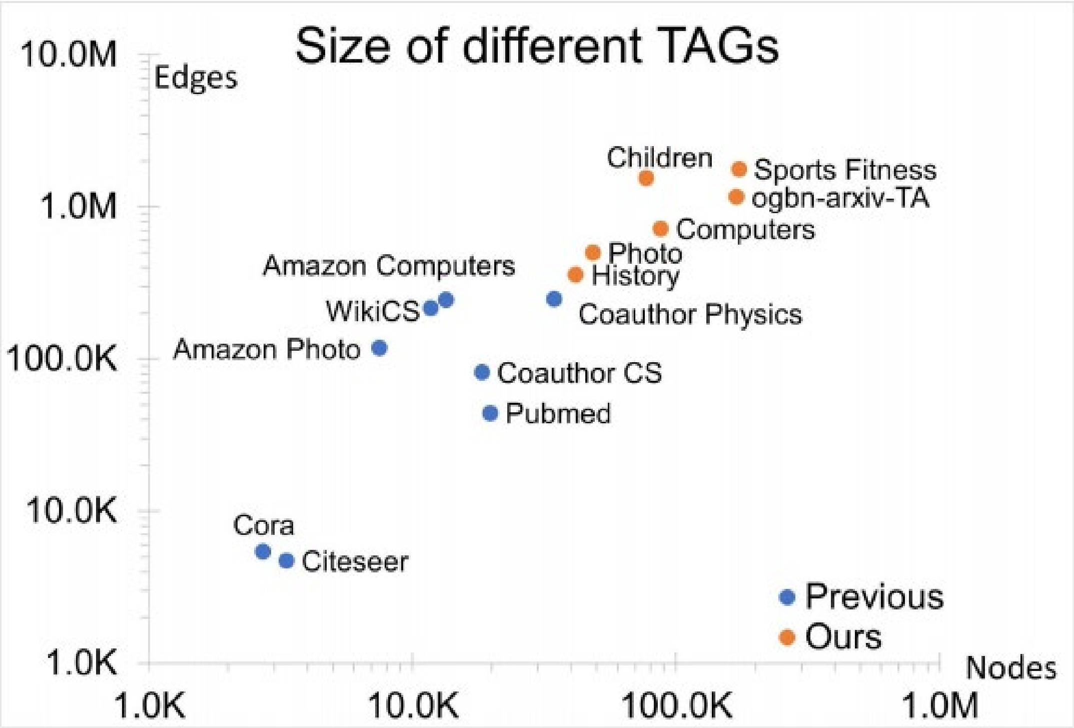
    - Problem: Scalability issues
  - Topological Pre-training based
    - Can we pre-train the LMs to understand the graph topology ?
    - How to design the pre-training tasks ?





DATASET

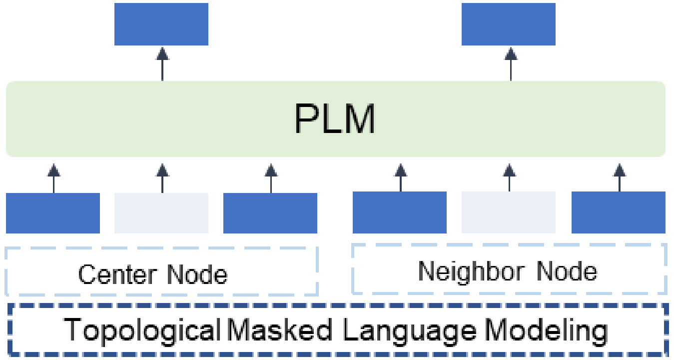
- Previous Datasets
  - Lack the availability of raw textual information
  - Overlook the exploration of text attribute modeling's impact on GNNs
  - These datasets are predominantly small in scale



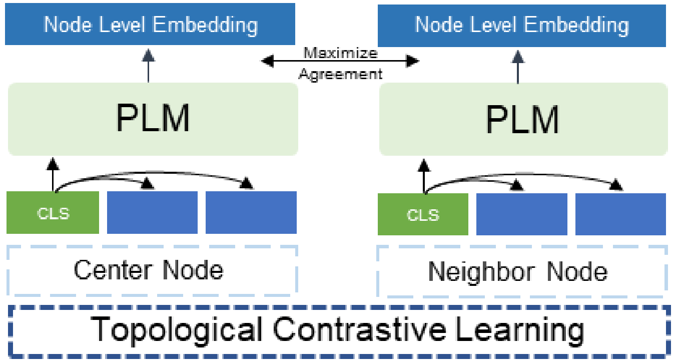
- CS-TAG
  - Keeping raw textual information
  - Modeling text-attributes: different PLMs
  - Scale larger

METHODS

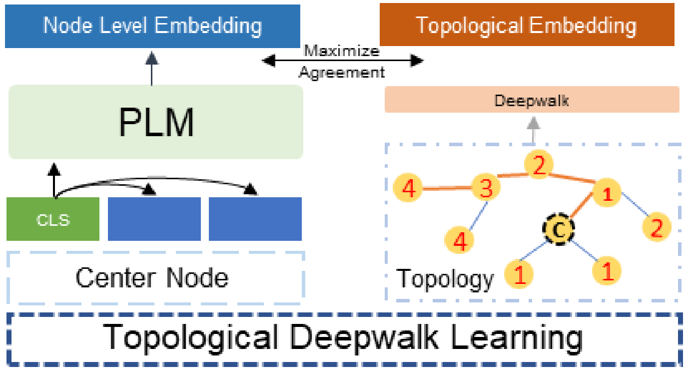
- Topological Masked Language Model (TMLM)
  - The first-order topological information in the token-level



- Topological Contrastive Learning (TCL)
  - The first-order topological information in the node-level



- Topological Deepwalk Learning (TDK)
  - The higher-order topological information in the node-level



EXPERIMENT

- GNNs with different PLM's features

Scale	PLMs	Arxiv GCN	GAT	SAGE	RevGAT	NFormer	GIN	JKNet	APPNP	MoNet	MLP
Small	BERT-Tiny	72.03	72.25	72.35	**72.52**	71.91	68.42	69.50	71.63	45.13	57.22
	ELECTRA	68.45	70.97	69.63	**71.12**	69.45	58.09	62.87	59.55	36.65	36.58
	DistilBERT	73.39	73.48	74.48	**74.68**	**73.56**	72.30	**71.44**	74.01	**50.51**	68.11
Base	ELECTRA	70.81	71.67	70.82	**71.96**	70.43	64.88	63.41	65.62	38.91	48.56
	BERT	73.30	73.40	74.14	**74.59**	72.80	71.94	70.08	73.90	46.90	67.35
	RoBERTa	73.56	73.38	74.52	**74.82**	73.12	72.63	69.40	74.01	44.53	69.31
	DeBERTa	68.15	66.56	67.58	**68.26**	67.11	62.05	44.16	52.37	29.67	47.07
Large	ELECTRA	70.44	71.01	70.72	**72.56**	70.04	64.47	58.34	64.52	37.26	47.72
	BERT	73.25	73.37	74.15	**74.68**	73.12	71.88	68.70	73.53	43.31	66.85
	RoBERTa	**73.95**	**73.72**	**74.64**	**74.99**	73.12	**73.10**	68.10	**74.17**	44.01	**69.51**
	DeBERTa	72.57	71.50	73.22	**73.59**	71.88	71.25	54.41	69.28	33.53	66.28
	Diff	5.80	7.16	7.06	7.54	6.45	15.01	27.28	21.80	20.84	32.93

EXPERIMENT

- Analyzing the performance of the Co-Training paradigm

Way	PLM-Based		GNN-Based				Co-Training Based	
	Tiny	Base	T-GCN	B-GCN	T-SAGE	B-SAGE	GCN(T)	SAGE(T)
Arxiv	70.83	72.96	72.03	73.30	72.35	**74.14**	69.22↓	73.57↑
Children	49.85	**59.91**	57.07	58.11	57.57	58.74	54.75↓	59.70↑
History	83.06	**86.09**	84.52	85.04	84.79	85.12	83.52↓	85.09↑
Photo	73.75	77.53	82.42	82.70	83.25	83.27	83.32↑	**86.64**↑
Computers	58.32	60.40	87.43	87.86	87.90	**88.30**	83.93↓	86.04↓
Sports	81.47	86.02	84.93	86.16	87.06	**87.34**	85.06↑	85.87↓

Datasets	BERT-Tiny						BERT-Base					
	Co-Training			TCL			Co-Training			TCL		
	Acc	Memory	Time	Acc	Memory	Time	Acc	Memory	Time	Acc	Memory	Time
Arxiv	73.57	76.27%	44.0	71.55	27.59%	7.0	-	OOM	-	**74.87**	70.73%	130
Children	59.70	97.28%	15.5	54.11	19.76%	2.0	-	OOM	-	**60.73**	80.99%	30
History	85.09	85.74%	5.7	86.06	14.69%	1.3	-	OOM	-	**86.80**	98.73%	18
Photo	**86.64**	97.83%	14.6	73.86	22.75%	3.1	-	OOM	-	82.85	70.65%	120
# Average	76.25	89.38%	19.95	71.40	21.20%	3.4	-	OOM	-	**76.31**	80.28%	74.50

EXPERIMENT

- Node classification results

Scale	Model	Arxiv						History					
		PLM	GNNs	TMLM	TDK	TCL	TMDC	PLM	GNNs	TMLM	TDK	TCL	TMDC
Small	BERT-Tiny	70.83	**72.52**	70.83	71.50	71.55	71.17	83.06	85.03	85.76	85.79	86.06	**86.88**
	ELECTRA	71.26	71.12	72.65	72.83	73.06	**73.71**	84.18	83.11	84.54	84.42	84.57	**85.18**
	DistilBERT	72.50	74.68	73.53	74.38	74.89	**75.50**	85.81	85.67	85.76	86.29	86.28	**86.88**
Base	ELECTRA	72.67	71.96	73.51	74.33	74.26	**75.56**	85.64	83.79	85.77	85.88	**86.62**	86.41
	BERT	72.96	74.59	73.97	74.23	74.87	**76.11**	86.09	85.28	86.24	86.46	86.80	**86.82**
	RoBERTa	73.10	74.82	74.25	74.57	75.37	**75.97**	85.85	85.69	86.19	86.32	86.95	**86.96**
	DeBERTa	73.82	68.26	74.26	75.01	75.15	**75.99**	86.16	82.31	86.00	86.46	**87.01**	86.94
Large	ELECTRA	72.42	72.56	74.76	73.82	74.17	**75.58**	86.13	83.56	86.39	86.49	**86.82**	86.28
	BERT	73.24	74.68	75.01	74.31	75.15	**75.75**	86.24	85.15	86.47	86.73	86.93	**86.94**
	RoBERTa	73.83	74.99	75.18	74.58	75.48	**75.73**	86.41	85.23	86.72	86.75	87.11	**87.22**
	DeBERTa	74.57	73.59	75.92	75.20	75.58	**76.20**	87.00	84.89	87.11	87.26	87.30	**87.32**
Scale	**Model**	**Children**						**Photo**					
		PLM	GNNs	TMLM	TDK	TCL	TMDC	PLM	GNNs	TMLM	TDK	TCL	TMDC
Small	BERT-Tiny	49.85	**57.86**	54.27	53.43	54.11	54.66	73.75	**84.12**	74.30	73.99	73.86	74.92
	ELECTRA	57.03	56.42	57.35	56.92	56.88	**58.55**	76.58	**83.12**	76.09	76.89	77.74	77.83
	DistilBERT	59.90	59.33	60.03	60.23	60.60	**61.38**	77.51	**84.34**	77.81	79.69	81.85	82.52
Base	ELECTRA	59.09	56.42	59.93	60.27	60.21	**60.83**	77.84	**82.98**	78.27	80.18	81.47	82.82
	BERT	59.91	58.74	60.34	60.43	60.73	**61.43**	77.53	**84.46**	78.54	81.04	82.85	84.09
	RoBERTa	59.80	59.01	60.19	60.71	61.47	**61.83**	78.11	**84.59**	78.33	81.26	82.47	83.04
	DeBERTa	60.26	50.72	60.73	61.39	61.92	**62.20**	78.37	81.44	79.27	81.34	83.07	**83.80**
Large	ELECTRA	58.28	56.59	60.51	59.31	59.29	**61.31**	77.25	**83.00**	79.21	78.44	79.56	81.32
	BERT	60.65	58.90	60.84	61.15	61.50	**62.06**	77.72	**84.21**	78.95	79.26	80.74	81.14
	RoBERTa	60.93	59.26	62.11	61.95	62.06	**63.24**	79.60	**85.12**	80.32	80.82	81.47	82.55
	DeBERTa	61.61	56.34	61.91	**62.51**	62.37	62.46	79.63	82.55	80.45	81.33	82.33	**82.70**

CONCLUSION

- First comprehensive benchmark on TAGs: CS-TAG.
  - Collect and provide text-attributed graph datasets.
  - Comprehensive evaluation of different learning paradigms.
- Topological Pre-training of Language Models
  - TMLM, TDK, TCL, TMDC

NEURAL INFORMATION PROCESSING SYSTEMS

THANKS