Are Graph Embeddings the Panacea?

– an Empirical Survey from the Data Fitness Perspective

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Contents

Problem Statement

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Graph Structure and Network Datasets

Co-existence Networks:

Actors, Amazon Computer, Photos and Ratings
Coauthor CS and Physics, Tolokers, Flickr, Questions

Citation Networks:

CiteSeer, Cora, DBLP, PubMed
WebKG (extended version, nodes hyperlinked)

Social Networks:

BlogCatalog, Github, Twitch (friends or followers)

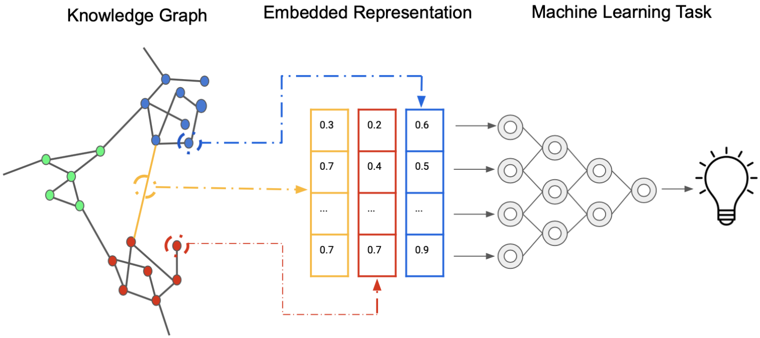
Grid Network:

Minesweeper (adjacent nodes)

Knowledge Graphs:

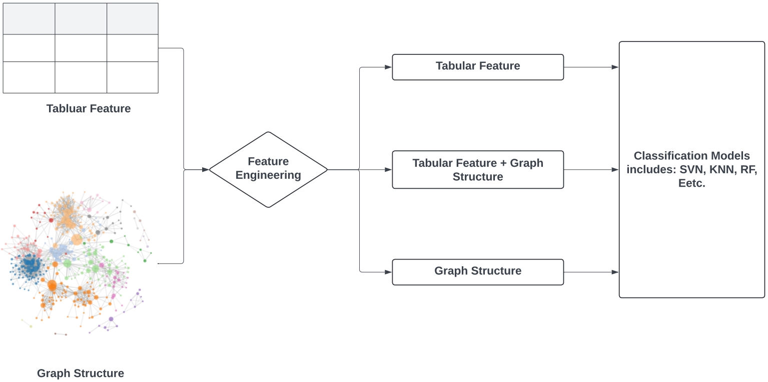
Roman Empire (mini knowledge graph)
Wiki (abstracted into a graph)

Graph Representation Learning for Machine Learning Tasks



Workflow for graph data

Feature Engineering



Feature engineering workflow

Research Questions

For node classification problems

Q1. Is there a potential benefit of applying graph representation learning?

Q2. Is structural information alone sufficient?

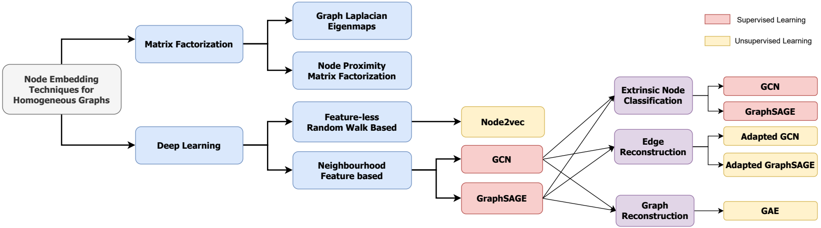
Q3. Which embedding technique would best suit my dataset?

Literature Review

Previous Surveys: Graph embeddings and KG embeddings

- 2017-Now, 6 surveys[1] about graph embeddings and knowledge graph ebemddings
- Objective of the surveys are focusing on graph embedding algorithms and applications.
- There is a lack of research effort on quantifying **the intricate relationship between specific network structure features and the performance of different graph embedding techniques.**

[1] Cai et al., Chen et al., Goyal and Ferrara, Makarov et al., Xu



Node Embedding Techniques for Homogeneous Graphs.[2]

[2]Adapted from Cai et al.

Experiment Setup

Representative Network Characteristics

$\|V\|$	Total number of nodes	$\|E\|$	Total number of edges
d	Dimension of node features	K	Number of classes
$\bar{k}$	Average degree of nodes ($= 2\|E\|/\|V\|$)	k_{var}	Second moment of degree distribution
k_{min}	Minimum node degree	k_{max}	Maximum node degree
L	Average shortest path between all node pairs	D	Diameter (The maximum distance between all possible pairs of nodes)
T	Transitivity (measuring likelihood of triangle formation)	C	Average clustering (quantifying the tendency of nodes to cluster together)
γ	Degree exponent of the power-law degree distribution, $P(k) \sim k^{-\gamma}$		

Network characteristics: notations and definitions

Dataset Categories and Network Types

Network Type	Dataset topic	Description
Co-existence Network (7)	Actor (1)	Wikipedia co-occurrence of actors; Classify into categories.
	Amazon (3)	Product co-purchases, bag-of-words from reviews; Product/review categories.
	Coauthor (CS, Physics) (2)	Authorship network, paper keywords; Study fields classification.
	Tolokers (1)	Toloka worker data, shared tasks; Banned worker prediction.
Citation Network (15)	Cora, etc. (12)	Publications, citations, bag-of-words; Publication classes.
	WebKG (3)	University web pages, hyperlinks, bag-of-words; Page categories.
Social Network (8)	Twitch (6)	Streamers, mutual follows, game embeddings; Language use classification.
	BlogCatalog (1)	Blog platform users and friendships, TF-IDF from blogs; User categories.
	Github (1)	Developer relationships, locations, repos; Web/ML developer classification.
Knowledge Graph (2)	Wiki (1)	Wikidata graph, item relations, one-hot vectors; Item categories.
	Roman Empire (1)	Wikipedia articles, word connections, embeddings; Syntactic roles classification.
Social Knowledge Network (2)	Questions (1)	Yandex Q dataset, answered questions, user profile embeddings; Active user prediction.
	Flickr (1)	Users, images, metadata, text annotations; Tag-based classification.
Grid (1)	Minesweeper (1)	Grid cells, adjacent mines; Mine presence prediction.

Dataset Context, where each number inside the parentheses denotes the number of datasets for that given network type or dataset topic.

Network Characterisation of the Datasets

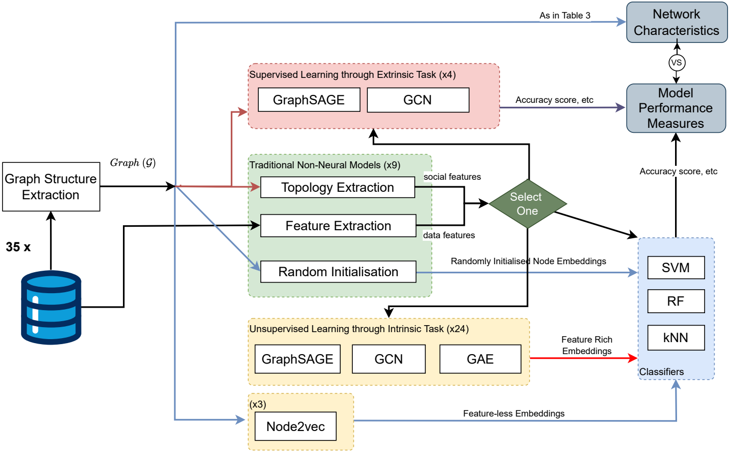
Dataset	$\|V\|$	$\|E\|$	d	K	$\bar{k}$	k_{var}	$k_{\min}$	$k_{\max}$	L	C	T	D	γ
Actor	7,600	30,019	932	5	7.90	400.56	1	1,304	4.11	0.05	0.04	12	2.81
AZ_COMPUTERS	13,752	245,861	767	10	35.76	6,221.40	**0**	2,992	3.38	0.34	0.10	10	2.83
AZ_PHOTO	7,650	119,081	745	8	31.13	3,204.10	**0**	1,434	4.05	**0.40**	0.17	11	2.92
AGD_BlogCatalog	5,196	171,743	8,189	6	66.11	7,376.53	**5**	769	2.51	0.12	0.08	**4**	4.06
AGD_CiteSeer	3,312	4,715	3,703	6	2.85	19.81	1	100	**1.08**	0.07	0.03	28	3.31
AGD_Cora	2,708	5,429	1,433	7	4.00	44.23	1	169	1.17	0.13	0.02	19	3.05
AGD_Flickr	7,575	239,738	**12,047**	9	63.30	21,303.96	1	1,881	2.41	0.33	0.10	4	2.76
AGD_Pubmed	19,717	44,338	500	3	4.50	75.51	1	171	6.34	0.03	0.01	18	4.20
AGD_Wiki	2,405	16,523	4,973	17	13.74	499.01	1	281	3.65	0.32	**0.44**	9	3.82
CF_CiteSeer	4,230	5,337	602	6	**2.52**	20.43	1	85	1.35	0.11	0.08	26	2.83
CF_Cora	19,793	63,421	8,710	**70**	6.41	118.33	1	297	1.16	0.26	0.13	23	3.38
CF_Cora_ML	19,793	63,421	8,710	**70**	6.41	118.33	1	297	1.16	0.26	0.13	23	3.38
CF_DBLP	17,716	52,867	1,639	4	5.96	123.03	1	339	1.16	0.13	0.10	34	3.23
CF_PubMed	19,717	44,324	500	3	4.49	75.43	1	171	6.34	0.06	0.05	18	4.17
CiteSeer	3,327	4,552	3,703	6	2.73	18.92	**0**	99	1.08	0.14	0.13	28	2.63
Coauthor_CS	18,333	81,894	6,805	15	8.93	162.75	1	136	5.42	0.34	0.18	24	5.18
Coauthor_Physics	34,493	247,962	8,415	5	14.38	449.23	1	382	5.16	0.37	0.18	17	4.88
Cora	2,708	5,278	1,433	7	3.89	42.53	1	168	1.17	0.24	0.09	19	2.98
Cora_Full	19,793	63,421	8,710	**70**	6.41	118.33	1	297	1.16	0.26	0.13	23	3.38
GitHub	37,700	289,003	128	**2**	15.33	6,761.61	1	**9,458**	3.25	0.17	0.01	11	2.54
HGD_AZ_Ratings	24,492	93,050	300	5	7.60	93.39	**5**	132	16.24	0.29	0.15	46	3.60
HGD_Minesweeper	10,000	39,402	**7**	**2**	7.88	62.44	3	**8**	46.67	0.22	0.33	99	2.79
HGD_Questions	**48,921**	153,540	301	**2**	6.28	774.50	1	1539	4.29	**0.02**	0.01	16	**1.83**
HGD_Roman_empire	22,662	32,927	300	18	2.91	**9.50**	2	14	**2331.56**	0.19	0.28	**6,824**	**6.34**
HGD_Tolokers	11,758	**519,000**	10	**2**	**88.28**	**33,978.74**	1	2,138	2.78	0.27	0.11	11	3.08
PubMed	19,717	44,324	500	3	4.50	75.43	1	171	6.34	0.06	0.05	18	4.18
TWITCH_DE	9,498	162,636	128	**2**	34.25	8,363.44	3	4,261	2.72	0.20	0.05	7	2.58
TWITCH_EN	7,126	42,450	128	**2**	11.91	634.28	3	722	3.68	0.13	0.04	10	2.79
TWITCH_ES	4,648	64,030	128	**2**	27.55	3,198.91	3	1,024	2.88	0.22	0.08	9	2.58
TWITCH_FR	6,551	119,217	128	**2**	36.40	7,328.28	2	2,042	2.68	0.22	0.05	7	2.61
TWITCH_PT	1,912	33,211	128	**2**	34.74	4,324.69	3	769	2.53	0.32	0.13	7	2.53
TWITCH_RU	4,385	41,689	128	**2**	19.01	2,098.57	3	1,231	3.02	0.17	0.05	9	2.58
WEBKB_Cornell	**183**	**298**	1,703	5	3.26	60.52	1	94	3.20	0.10	0.01	8	3.09
WEBKB_Texas	**183**	325	1,703	5	3.55	75.22	1	104	3.03	0.11	**0.01**	8	2.62
WEBKB_Wisconsin	251	515	1,703	5	4.10	81.85	1	122	3.26	0.11	0.01	8	2.50

Graph Representation Learning

- Node2vec[3]
- GraphSAGE (SAmple and aggreGatE)[4]
- GCN (Graph Convolutional Network)[5]
- GAE (Graph Auto Encoder)[6]

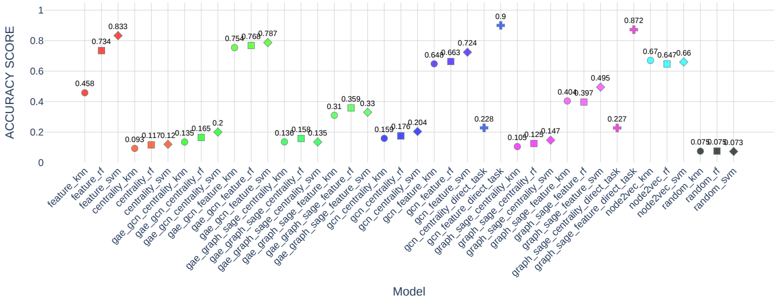
[3] Grover and Leskovec
[4] Hamilton et al.
[5] Pei et al.
[6] Goyal and Ferrara

Survey Experiment Design



Results and Discussion

Results: Dataset Coauthor CS accuracy score



Dataset Coauthor CS accuracy score for models[7]

[7] Code and results available: https://github.com/PascalSun/PAKDD-2024

Q1: Do all datasets benefit from graph structure representation learning?

Evaluation metric: Feature Only models with those integrating node features and graph structure

Results:

- 21 of 35 datasets showed improved performance with graph structures (e.g., Minesweeper, Roman Empire, Twitch).
- Datasets like PubMed, Wiki, and Flickr performed better with Feature Only models.

Highlight: The PubMed dataset has the longest average shortest path among the citation networks, potentially explaining its exceptional performance.

Conclusion: Graph structures enhance performance in many cases but are not always superior.

Q2: Is structural information alone sufficient?

Evaluation Metric: *Structure Only* models with those integrating node features and graph structure.

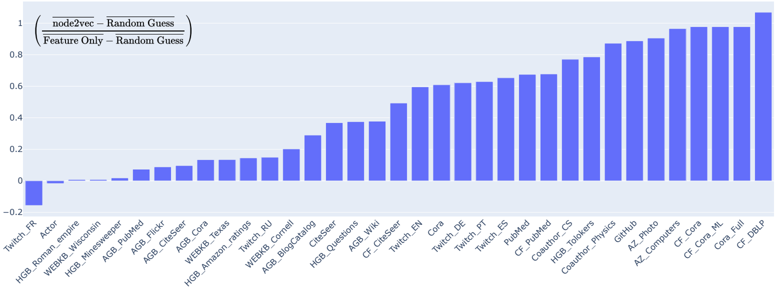
Findings:

- Combined models outperform *Structure Only* models.
- *Node2vec* is on par with *Feature Only* for dense networks.

Highlight: Short-diameter networks favor *Structure Only* models.

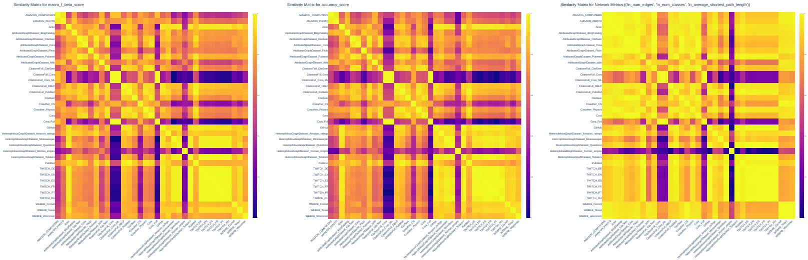
Conclusion: Structural data alone falls short; *Node2vec* excels in specific dense networks.

Q2: Is structural information alone sufficient?



Comparison of classification accuracies of the **node2vec** models versus the **Feature Only** models for all the datasets (the bar symbol represents the average accuracy of the model over the SVM, RF, and KNN classifiers).

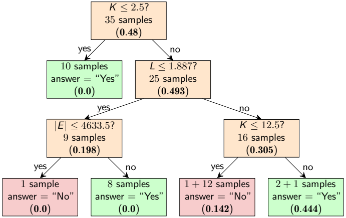
Q3: Which graph embedding representation model(s) suit my dataset?



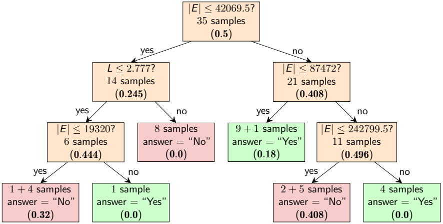
Similarity matrices for: F1 score (left), Accuracy score (middle), Network Parameters ($|E|$, K, L) (right).

Q3: Which graph embedding representation model(s) suit my dataset?

Q1: Do datasets benefit from graph embedding learning?



Q2: Is structural information alone sufficient?



Decision Trees for Q1 and Q2 based on $\mathbf{v}'_{\text{net}} = (|E|, K, L)$. The boldface numbers inside parentheses denote the Gini indices. Each leaf node is coloured in green (or pink) for the "Yes" (or "No") answer to the question.

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Conclusion and Future Work

Graph Network Type and Model Performance

Sparse Networks: These networks have long average shortest path lengths, a large number of classes, and limited edges, making them generally unsuitable for classification tasks via graph representation learning.

Dense Networks: Characterized by their well-connected nature and rich edge information, these networks show excellent performance with random walk-based models such as node2vec, especially compared to attribute-only models.

Best Performers: The most effective models are those that integrate neighbor-attribute-based supervised learning, consistently outperforming others by effectively leveraging both structural and attribute information.

Future work

Enhance Dataset Diversity: Address the dominance of citation networks by expanding to more varied domains, which is crucial for improving dataset diversity.

Advance Feature Representation: Move beyond bag-of-words and one-hot encoding for textual attributes. Implement semantic-enriched content embeddings using Large Language Models (LLM) to leverage recent advancements in this field.

Explore Deeper Networks: While node2vec shows impressive performance, there is a need to develop and study deeper networks inspired by random walks, as our current non-random walk-based models are limited to two layers.

Q & A

THANK YOU

Q & A

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