Network Science Meets AI

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The intersection of Network Science and Artificial Intelligence presents great opportunities for advancing our understanding of complex systems and developing better predictive models for graph-structured data.

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- Network Science = Physics + graph theory + algorithms + data science on graph

Some recent trends in NetSci

- Go beyond pairwise static interactions
- Analyze the evolution of networks
- Network Generation & Synthesis
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Some recent trends in NetSci

- Go beyond pairwise static interactions <-> Develop GNNs for temporal, heterogeneous, high-order interactions
- Analyze the evolution of networks <-> Forecasting temporal networks
- Network Generation & Synthesis <-> Generative models for graphs
- Study the local/meso-scale structure of the networks <-> Representation learning for subgraphs

Network Science meets AI

The contamination is already happening and it's beneficial for both fields!

- High-order models for network science helps temporal graph learning to leverage the causal topology of networks [1]
- Representation learning for subgraphs is leveraged to approximate exact algorithms for mining motifs in networks [2]

[1] De Bruijn goes Neural: Causality-Aware Graph Neural Networks for Time Series Data on Dynamic Graphs – LOG 2022

[2] Representation Learning for Frequent Subgraph Mining – ICML Workshop 2024

Network Science meets AI

Neural networks are instance of complex systems!

- Existing insights into the topology of complex networks can greatly assist the design of deep neural networks. (Already happening through graph rewiring and augmentation, e.g. [3])
- Network science methods can be used to understand or optimize the structure of deep neural networks. (e.g. [4])
- Methods for the analysis of dynamics processes can advance the comprehension of the learning processes

[3] Cayley Graph Propagation – LOG 2024

[4] Epitopological learning and Cannistraci-Hebb network shape intelligence brain-inspired theory for ultra-sparse advantage in deep learning – ICLR 2024

Network Science meets AI

SOME OF OUR CONTRIBUTIONS

- AI helps Network Science
  - Can Graph Neural Networks learn node-level structural features? – ICLR 2024
- Network Science helps AI
  - Link prediction heuristics for temporal graph benchmark – ESANN 2024

Can Graph Neural Networks learn node-level structural features?

Manuel Dileo and Matteo Zignani
Dept. of Computer Science, University of Milan

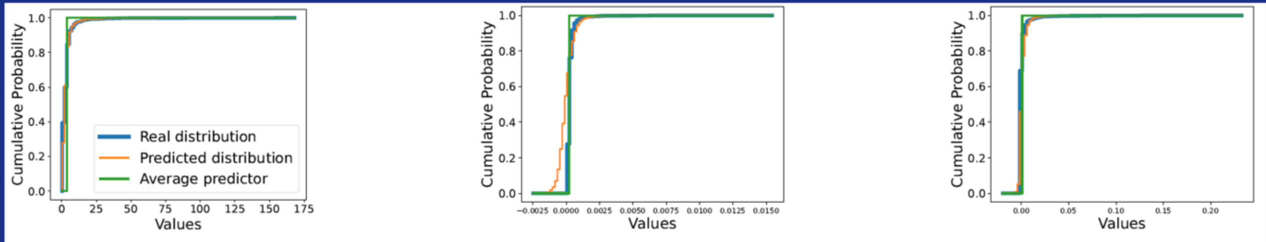
Intro

- GNNs perform feature learning on graphs.
- Network science metrics are features on graphs
- Which network science metrics GNNs can automatically learn?

Method

1. Given a graph dataset, we compute some well-known node-level metrics in network science that serve as target values to predict.
2. We model the problem as a node-regression task.
3. We limit our analysis to standard 1-hop MPNNs with random initialized node embeddings.

GNNs + Random features reconstruct PageRank, learn shortest path distances but struggle to compute clustering coefficient and neighboring features.



(a) Out-degree (b) Pagerank (c) Betweenness centrality
(d) Closeness centrality (e) Clustering coefficient (f) Avg. neighbor degree

Scan to read the full paper

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Tabular Results

Feature	Cora	CiteSeer	Pubmed
In-degree	0.89 ±0.20	0.69 ±0.16	1.52 ±0.13
Out-degree	1.01 ±0.33	0.68 ±0.45	1.46 ±0.37
PageRank	0.06 ±0.02	0.08 ±0.01	0.07 ±0.01
Betweenness	0.06 ±0.01	0.05 ±0.02	0.06 ±0.02
Closeness	0.04 ±0.01	0.04 ±0.01	0.05 ±0.01
Clustering coeff.	0.24 ±0.02	0.22 ±0.01	0.17 ±0.01
Avg. Neigh.degree	6.72 ±1.30	05.45 ±0.43	10.74 ±2.30

Low homophily ⇏ Low performance

Feature	Homophily (Cora)
PageRank	-0.08
Betweenness	-0.04
Closeness	0.89
Clustering	0.33
Avg. Neigh. Degree	0.05

Our results open up the possibility of using pre-trained GNNs to efficiently approximate structural features that are computationally expensive.

Computation of betweenness centrality:

Dataset	Compute	Training	Inference
Cora	3.36s	2.13s	27.2ms
CiteSeer	3.38s	807ms	12.7ms
PubMed	6.21min	6.17s	39ms

GNNs training + inference much faster than standard computation!

Can GNNs learn network science metrics?

RELATED AND FUTURE WORKS

- Linking theoretical results on GNN expressiveness with network science features

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RELATED AND FUTURE WORKS

- Linking theoretical results on GNN expressiveness with network science features
- Leverage GNNs to compute network science metrics in a fast way
- Pre-train GNNs for learning representations based on network science principles

Link prediction heuristics for TGB

TGB

- TGB represents a widely adopted collection of benchmarks for link prediction on temporal networks.
- The TGB leaderboard shows that Deep Learning models exhibit high variability in the performance over the different datasets
- Lack of proper baselines, which makes difficult to argue that we are making progress.

Temporal Graph Benchmark

TGB FOCUSES ITS LEADERBOARD ON DEEP LEARNING MODELS ONLY

Link prediction heuristics

Given two nodes u and v, Preferential Attachment and Common Neighbors' score are defined as:

$$PA(u,v) = |N(u)| \cdot |N(v)|$$

$$CN(u,v) = |N(u) \cap N(v)|$$

Where $|N(u)|$ is the number of u's neighbors.

- Very easy to interpret and to compute
- Effective solutions on static graphs
- They could be extended considering temporal neighborhood

WE COMPARE NETSCI HEURISTICS AGAINST SOTA METHODS FOR LINK PREDICTION ON TGB

Link prediction heuristics for TGB

- Comparable performance with TGNN
- Insights on TGL
  - PA is a crucial mechanism
  - Distinguish link structural roles over time

Model	TGBL-WIKI	TGBL-COIN	TGBL-COMMENT
TGN	0.396 ± 0.06	**0.586 ± 0.04**	**0.379 ± 0.02**
CAW	**0.711 ± 0.001**	OOM	OOM
DyRep	0.050 ± 0.02	0.452 ± 0.05	**0.289 ± 0.03**
PA	**0.488 ± 0.00**	**0.584 ± 0.00**	0.124 ± 0.00
CN	N/A	0.408 ± 0.00	0.242 ± 0.00

CONSIDER NETWORK SCIENCE RESEARCH WHEN DEALING WITH LINK PREDICTION

Link prediction heuristics for TGB

FUTURE WORKS

- Extend the set of heuristics to give more insights into TGL models
  - Link triadic closure
  - Spectral centralities

Link prediction heuristics for TGB

FUTURE WORKS

- Extend the set of heuristics to give more insights into TGL models
  - Link triadic closure
  - Spectral centralities
- Develop a neural model that leverages key findings
  - Bias the link representation using network science principles

Network Science meets AI

EVENTS AND INIATIATIVES

- Special Session at ESANN 2025 [Deadline expired]
- Special Issue "Bridging Network Science and AI" on Springer Applied Network Science
  - Deadline: 30/06/2025

Network Science meets AI

GITHUB REPOSITORY

github.com/manuel-dileo/awesome-netsai

Thanks for your attention