Network Science meeting Deep Graph Learning
Challenges and Opportunities

HONAI 2025: Higher-Order Networks meets AI Satellite @ NetSci 2025

Christopher Blöcker

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Würzburg, Germany

My random walk through science...

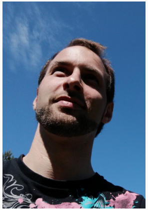
- B.Sc Computer Science, Univ. Appl. Sci. Wedel, Germany, **Discrete Optimisation**
- M.Sc. Computer Science, Univ. Appl. Sci. Wedel, Germany, **Functional Programming**
- “Predoc” Computational Biology, Duke-NUS, Singapore, **Applied Machine Learning**
- PhD Computational Science, Umeå University, Sweden, **Network Science**
  Doctoral Advisor: by Martin Rosvall
- Postdoc **Machine Learning for Complex Networks**
  - University of Zürich, Switzerland
  - University of Würzburg, Germany

ML4Nets Group at University of Würzburg

Ingo Scholtes

Anatol Wegner

Vincenzo Perri



Christopher Blöcker

Chester Tan

Lisi Qarkaxhija

Franziska Heeg

Moritz Lampert

Jan von Pichowski

Insights from Network Science can advance Deep Graph Learning

Christopher Blöcker [1] Martin Rosvall [2] Ingo Scholtes [1] Jevin D. West [3]

Abstract

Deep graph learning and network science both analyze graphs but approach similar problems from different perspectives. Whereas network science focuses on models and measures that reveal the organizational principles of complex systems with explicit assumptions, deep graph learning focuses on flexible and generalizable models that learn patterns in graph data in an automated fashion. Despite these differences, both fields share the same goal: to better model and understand pat-

strated the critical connection between network topology and the collective behaviour of complex systems—one of the enduring themes of network science and now one of the central challenges in deep graph learning.

Surprisingly, the two fields have diverged more than they have converged since Hopfield's influential paper. We see an opportunity for that to change, and argue for better integration of the two research communities. At their core, both fields model and analyze patterns in graphs. However, their needs are different. In deep graph learning, there is a need for methods that augment data to cope with limited train-

Deep Graph Learning (DGL)

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Tasks

- Node Classification ($\neq$ Community Detection)
- (Temporal) Link Prediction
- Graph Classification

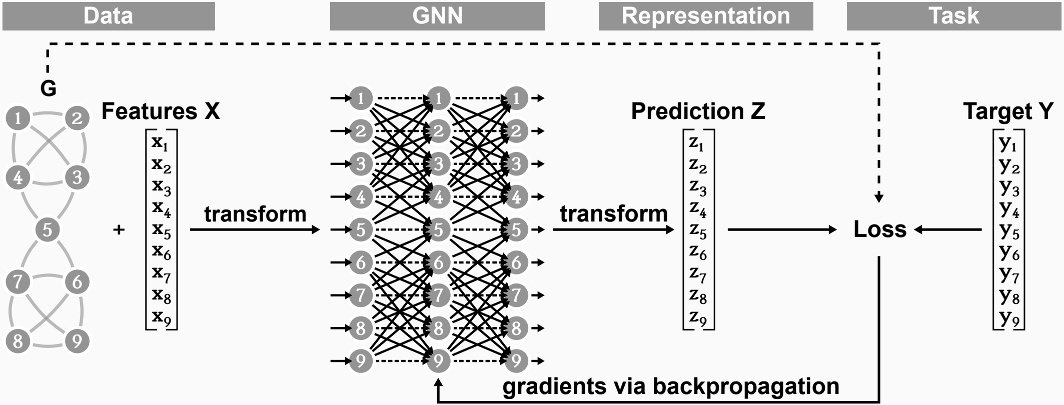
Learning

- Supervised, semi-supervised, or self-supervised
- Unsupervised is uncommon

Datasets

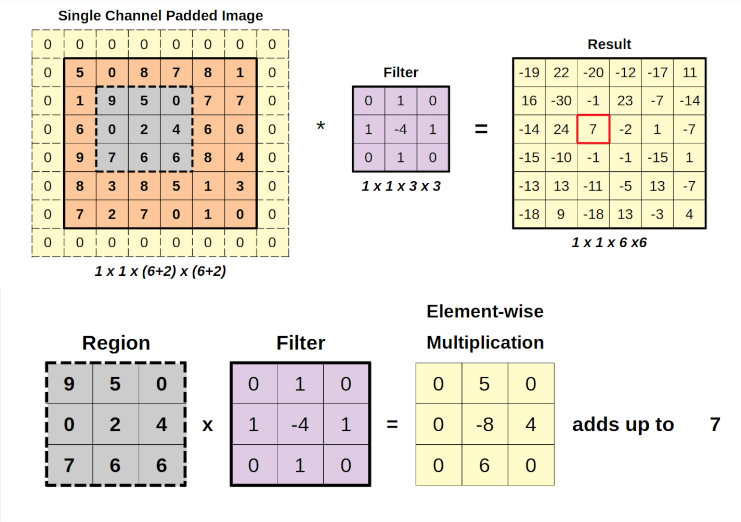
- Focus on empirical datasets with node and/or edge features
- Using synthetic data is also rather uncommon

General Setup (Simplified)



Focus on supervised task-specific training in an end-to-end fashion.

GNNs are inspired by CNNs



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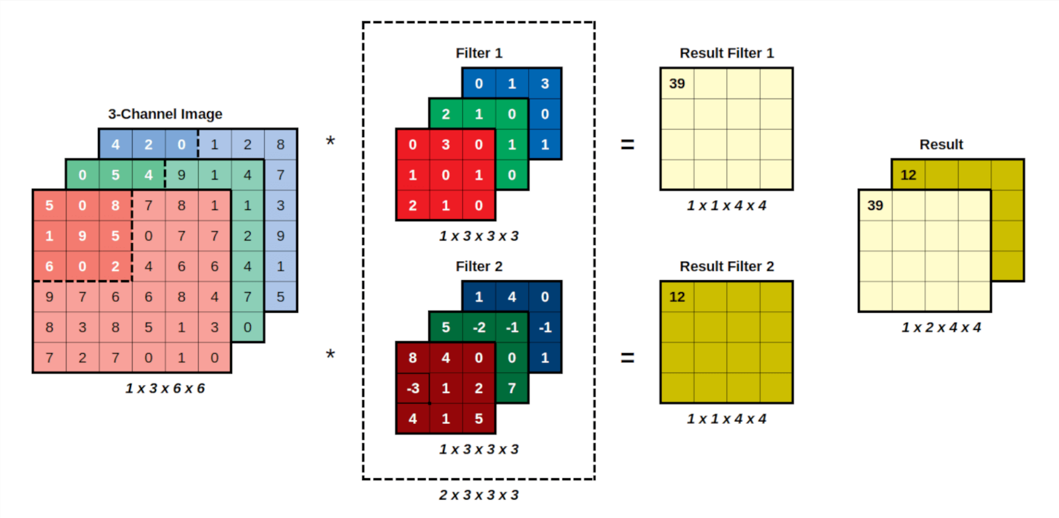

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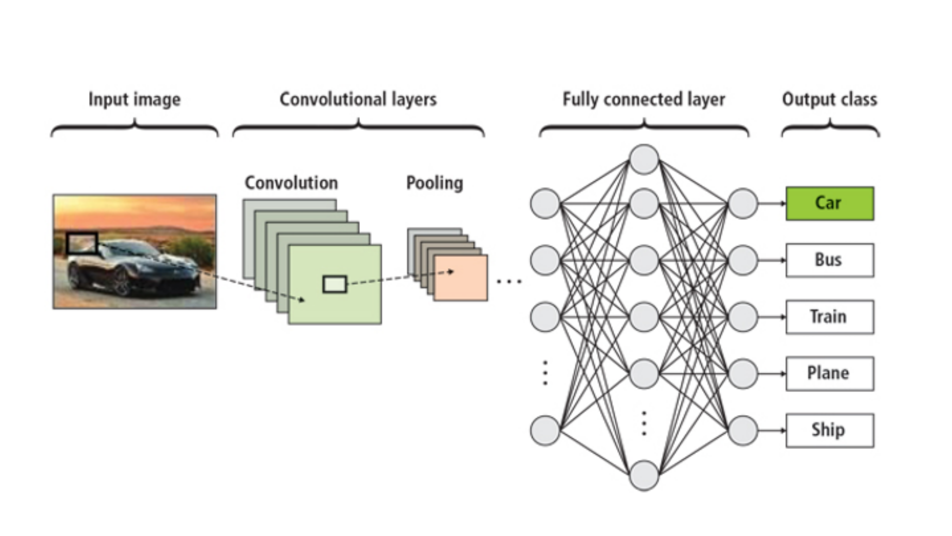
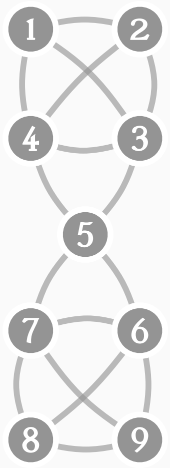


Source: https://www.nvidia.com/en-us/glossary/computer-vision/

How GNNs do it

Problem: Graphs are not “regular” like a grid of pixels.



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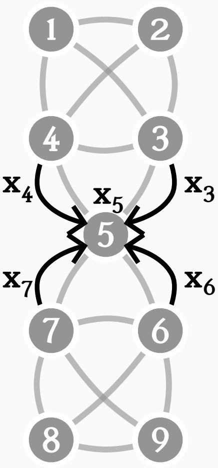

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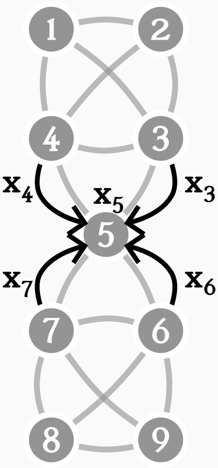
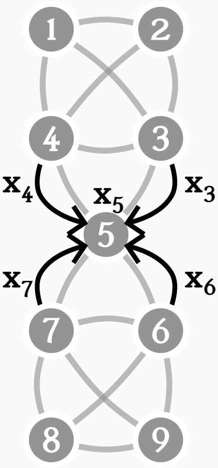


$$\mathbf{x}'_5 = f(\mathbf{x}_5, [\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_6, \mathbf{x}_7])$$

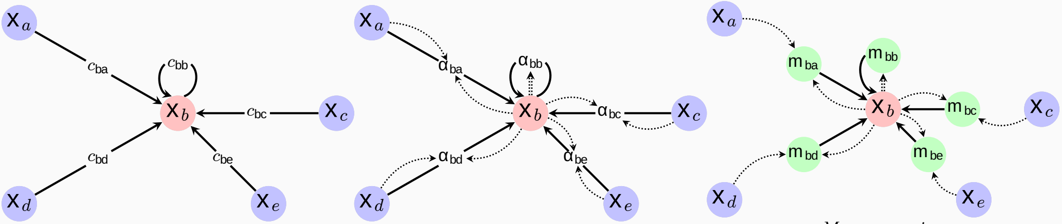
Problem: Graphs are not “regular” like a grid of pixels.



$$\mathbf{x}_5' = f(\mathbf{x}_5, [\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_6, \mathbf{x}_7])$$

$$f = ?$$

Flavours of and Differences between GNNs



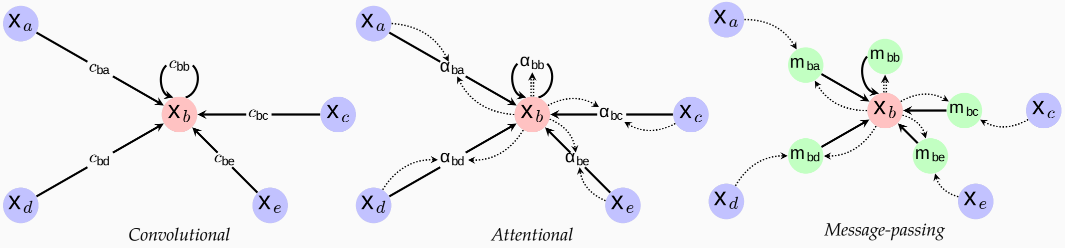
Convolutional *Attentional* *Message-passing*

$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in N_u} c_{uv}\psi\left(\mathbf{x}_v\right)\right) \qquad \mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in N_u} \underbrace{a\left(\mathbf{x}_u, \mathbf{x}_v\right)}_{\alpha_{uv}}\psi\left(\mathbf{x}_v\right)\right) \qquad \mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in N_u} \psi\left(\mathbf{x}_u, \mathbf{x}_v\right)\right)$$

“message”: $\psi\left(\mathbf{x}\right) = \mathbf{W}\mathbf{x} + \mathbf{b}$ “update”: $\phi\left(\mathbf{x}, \mathbf{z}\right) = \sigma\left(\mathbf{W}\mathbf{x} + \mathbf{U}\mathbf{z} + \mathbf{b}\right)$

$\rightarrow$ Bronstein et al., Geometric deep learning: Grids, groups, graphs, geodesics, and gauges; arXiv:2104.13478

Flavours of and Differences between GNNs

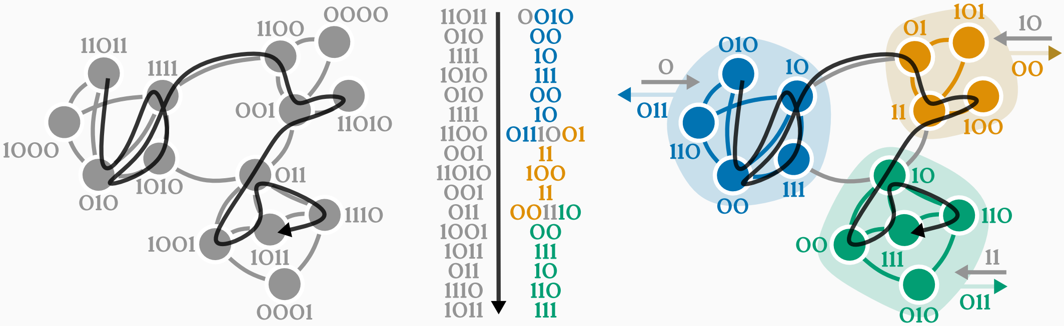


→ Bronstein et al., Geometric deep learning: Grids, groups, graphs, geodesics, and gauges; arXiv:2104.13478

Relevant Papers

- Kipf & Welling, *Semi-Supervised Classification with Graph Neural Networks*, ICLR 2017
- Veličković et al., *Graph Attention Networks*, ICLR 2018
- Gilmer et al., *Neural Message Passing for Quantum Chemistry*, ICML 2017

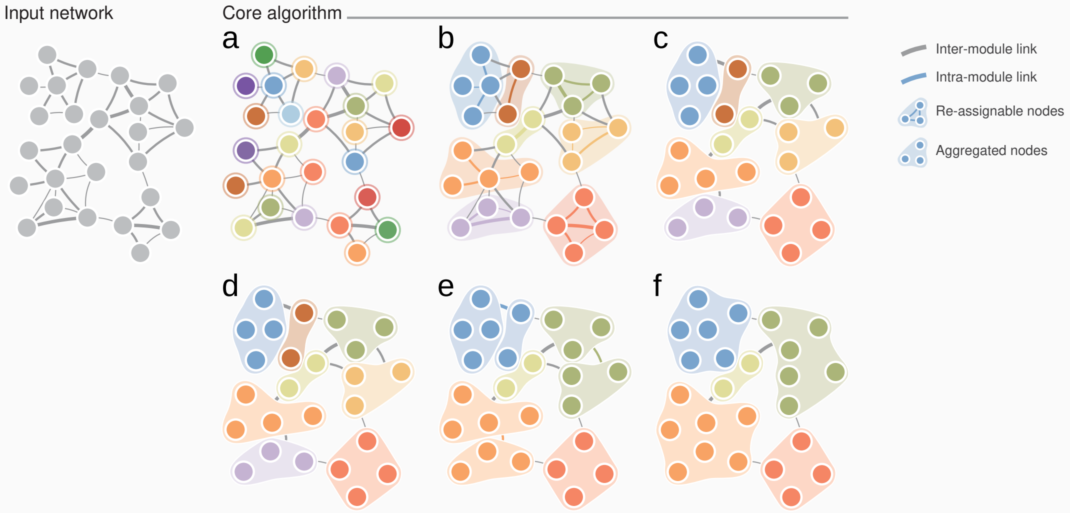
GNNs have Limitations



$$L = H(P)$$

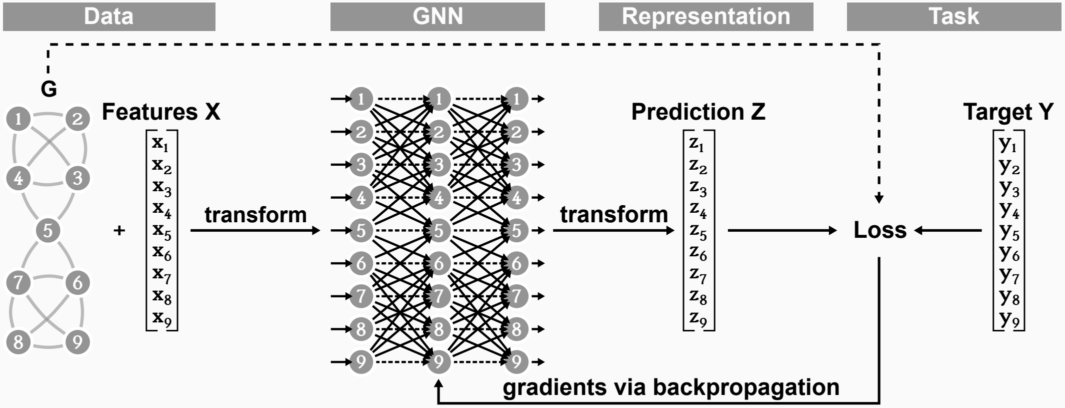
$$L = qH(Q) + \sum_{m} p_m H(P_m)$$

Infomap

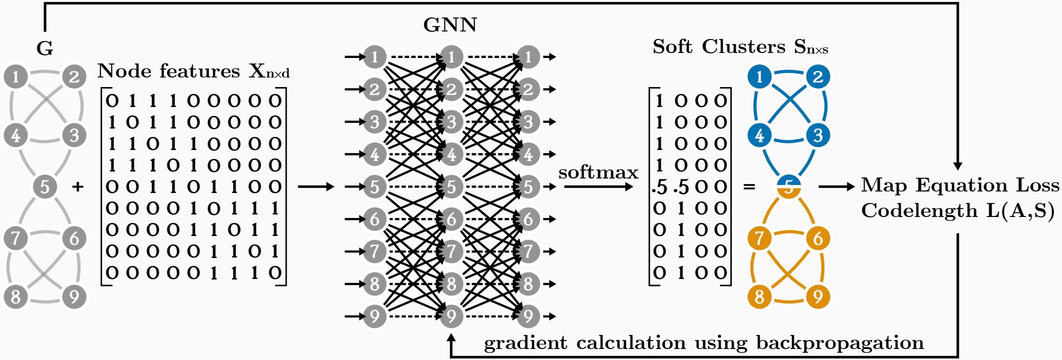


→ Smiljanić et al., Community Detection with the Map Equation and Infomap: Theory and Applications; arXiv:2311.04036

General Setup



Map Equation Setup

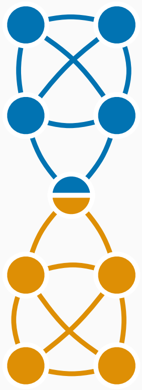


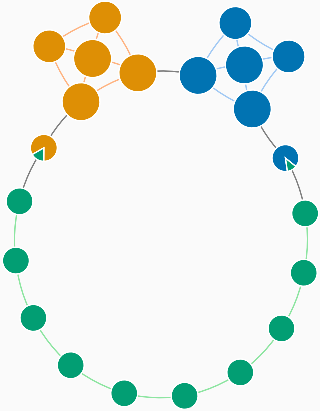
$$C = S^\top F S \quad q = 1 - \operatorname{tr}(C) \quad q_m = C 1_s - \operatorname{diag}(C) \quad m_{exit} = (1_s^\top C)^\top - \operatorname{diag}(C) \quad p_m = q_m + 1_s^\top C$$

$$L(A, S) = q \log_2 q - (q_m \log_2 q_m) 1_s - (m_{exit} \log_2 m_{exit}) 1_s - (p \log_2 p) 1_n + (p_m \log_2 p_m) 1_s$$

→ Blöcker et al., The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks; NeurIPS 2024

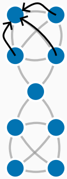
What's the problem?





"This should not work!"

What's the problem? Colour refinement...



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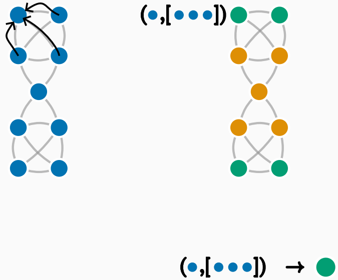

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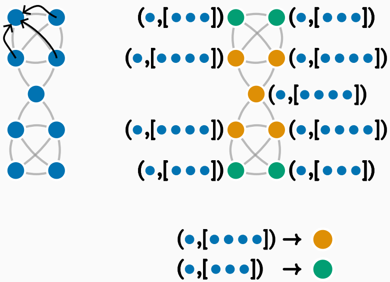

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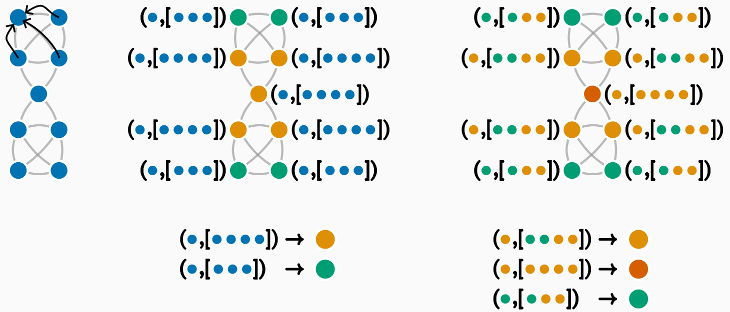

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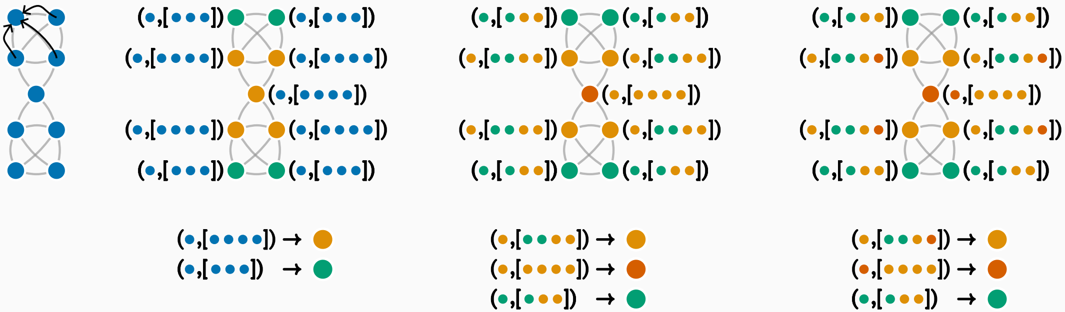

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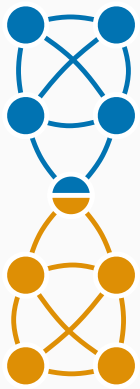

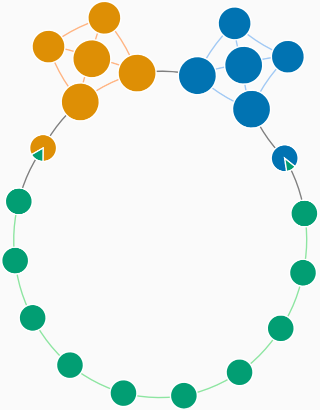

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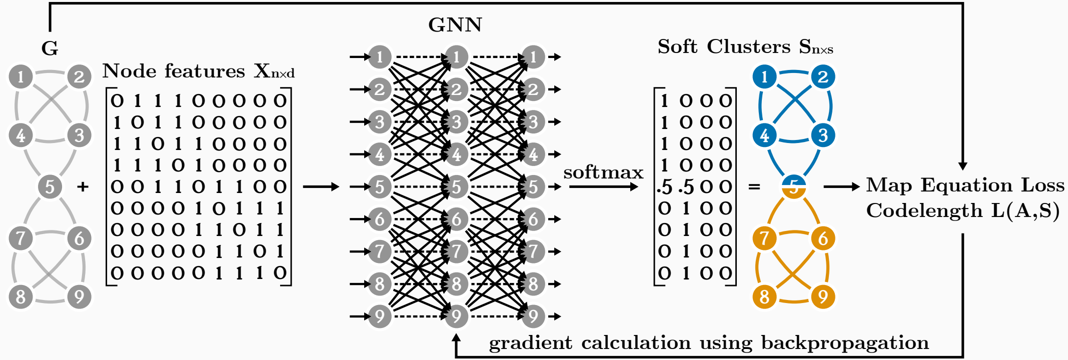
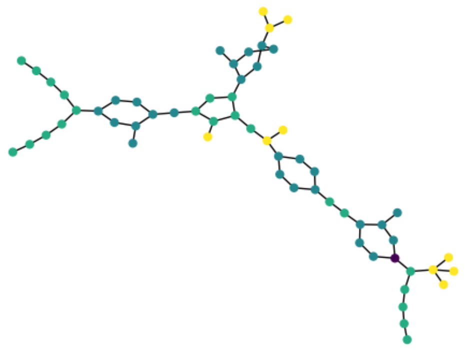


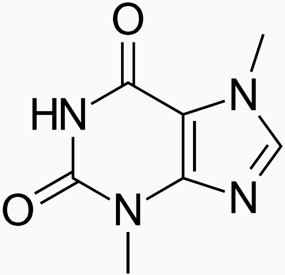
→ Blöcker et al., *The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks*, NeurIPS 2024

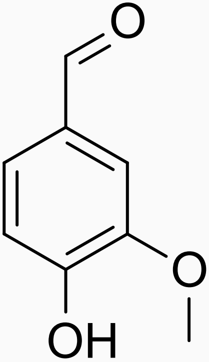
But in inductive settings, we cannot encode node IDs.

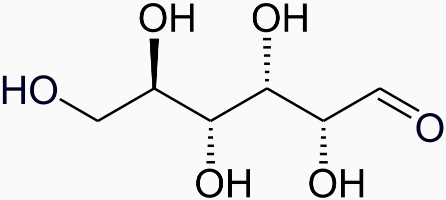
When we cannot enocde node IDs

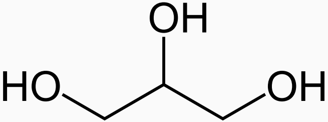


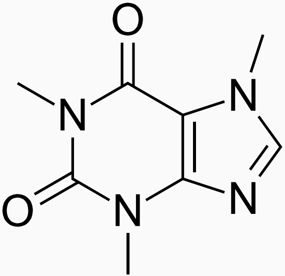
→ von Pichowski et al., MDL-Pool: Adaptive Multilevel Graph Pooling Based on Minimum Description Length; arXiv:2409.10263



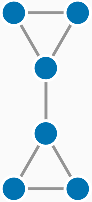


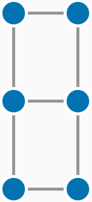






Weisfeiler-Leman Graph Isomorphism Test fails to distinguish some graphs





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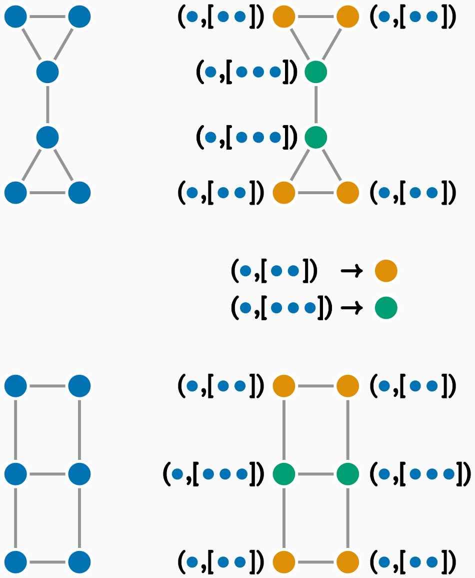

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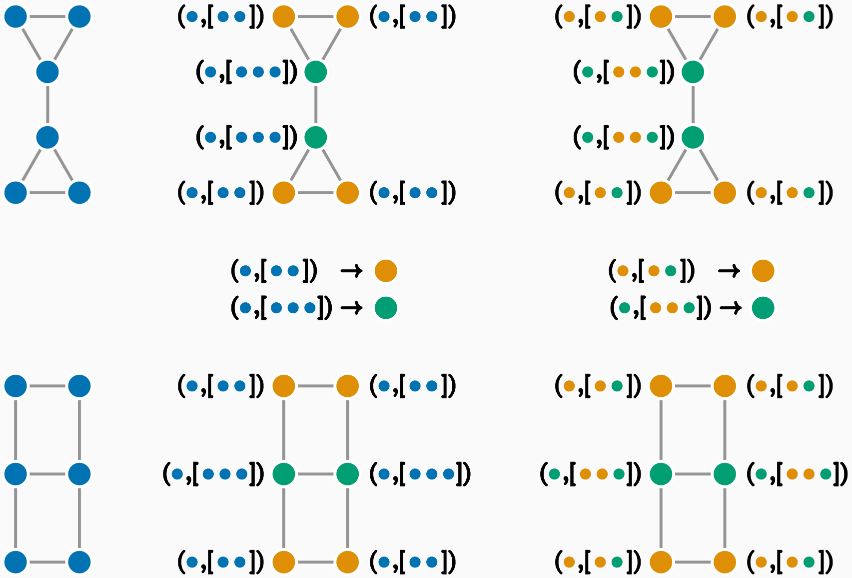


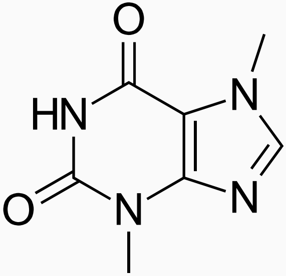
Relevant Papers

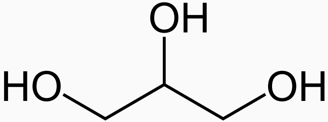
- Xu et al., *How Powerful are Graph Neural Networks?*, ICLR 2019
- Morris et al., *Weisfeiler and Leman Go Neural: Higher-Order Graph Neural Networks*, AAAI 2019
- Sato, *A Survey on the Expressive Power of Graph Neural Networks*, arXiv:2003.04078

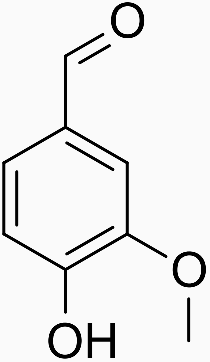
But why does that matter for us?

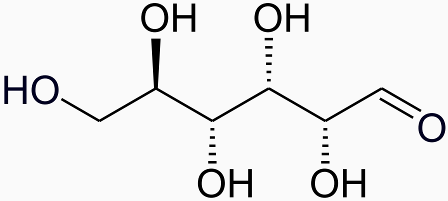
Because we cannot encode the node IDs in inductive settings.

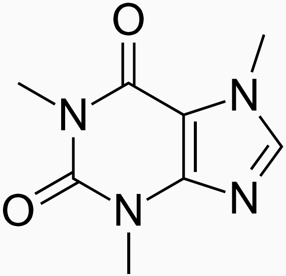
Graph classification











Insights from Network Science can advance Deep Graph Learning

→ Blöcker et al.; arXiv:2502.01177

Insights from Network Science can advance Deep Graph Learning

Christopher Blöcker [1] **Martin Rosvall** [2] **Ingo Scholtes** [1] **Jevin D. West** [3]

3 Feb 2025

Abstract

Deep graph learning and network science both analyze graphs but approach similar problems from different perspectives. Whereas network science focuses on models and measures that reveal the organizational principles of complex systems with explicit assumptions, deep graph learning focuses on flexible and generalizable models that learn patterns in graph data in an automated fashion. Despite these differences, both fields share the same goal: to better model and understand pat-

strated the critical connection between network topology and the collective behaviour of complex systems—one of the enduring themes of network science and now one of the central challenges in deep graph learning.

Surprisingly, the two fields have diverged more than they have converged since Hopfield's influential paper. We see an opportunity for that to change, and argue for better integration of the two research communities. At their core, both fields model and analyze patterns in graphs. However, their needs are different. In deep graph learning, there is a need for methods that augment data to cope with limited train-

“Whereas network science focuses on models and measures that **reveal the organisational principles of complex systems with explicit assumptions**, deep graph learning focuses on **flexible and generalisable models that learn patterns in graph data in an automated fashion**.”

“Despite these differences, both fields share the same goal: to better model and understand petterns in graph-structured data.”

~~Challenges~~ Opportunities and Opportunities (non-exhaustive)

NetSci

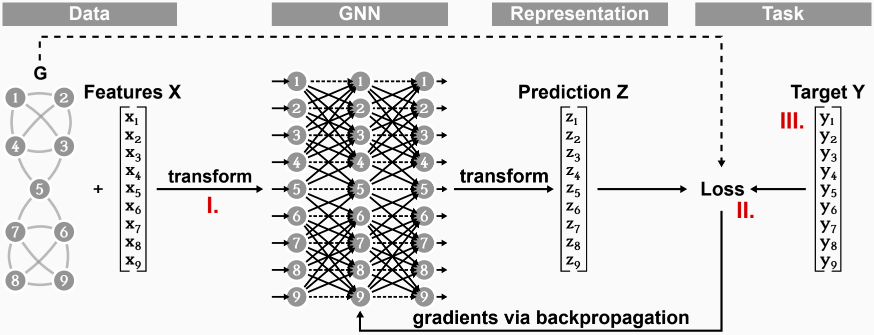
- \+ Transparent models, clear assumptions
- \+ Principled approaches for dealing with unreliable data
- \+ Synthetic datasets with ground truth
- \+ Aiming for mechanistic understanding, unsupervised learning
- +/- Often relying on discrete objectives
- \- No standard set of benchmarks, difficult to compare methods
- \- Scalability to massive datasets

DGL

- \+ Flexible (model-free) approaches
- \+ Strong focus on scalability
- \+ SOTA performance in many scenarios
- \+ Empirical datasets
- \- Synthetic datasets with ground truth
- \- Requires data augmentation
- \- Results often difficult to interpret
- \- Many methods work well, but it is not well understood what they do and what patterns they can learn

Publishing cultures differ

Principled Deep Learning Modelling



Challenges / Opportunities

- I Explicit expectations regarding the data & data augmentation
- II Inductive bias for guiding the learning process
- III Datasets and benchmarks for evaluation

I. Explicit Expectations & Data Augmentation

Probabilistic Generative Models

Probabilistic generative models formulate explicit expectations

The can be used to randomise the graph's topology to study what properties are due to the topology vs. explained by other properties, such as the degree sequence.

- Erdős-Rényi random graphs where edges exist independently with probability p

  → Erdős & Rényi, *On the evolution of random graphs*, 1960
- Graphs with given degree sequence or distribution

  → Molloy & Reed, *A critical point for random graphs with a given degree sequence*, 1995
- Exponential random graphs with a given set of network statistics

  → Robins et al., *An introduction to exponential random graph (p*) models for social networks*, 2007
- SBM for random graphs with given homophilic or heterophilic communities

  → Lee & Wilkinson, *A review of stochastic block models and extensions for graph clustering*, 2019

Data Augmentation

Aim: generate more training data, improve generalisability, mitigate overfitting

Clear approach in computer vision

Original

Blur

Crop

Flip H

Flip V

Data Augmentation for GNNs

Aim: generate more training data, improve generalisability, mitigate overfitting

Currently, a "theory of data augmentation for GNNs" is lacking

→ Morris et al., *Position: Future Directions in the Theory of Graph Machine Learning*, ICML 2024

GNNs work well on homophilic datasets but suffer from over-smoothing.

- Targeted insertion or removal of edges to increase homophilic patterns

  → Zhao et al., *Data augmentation for graph neural networks*, AAAI 2021
- Selectively adding nodes to slow down message passing

  → Azabou et al., *Half-Hop: A graph upsampling approach for slowing down message passing*, ICML 2023
- Spectral gap tuning
  - Insertion and deletion of edges to mitigate oversmoothing and oversquashing

    → Jamadandi et al., *Spectral Graph Pruning Against Over-Squashing and Over-Smoothing*, NeurIPS 2024
  - Community- and/or feature-informed insertion and deletion of edges

    → Rubio-Madrigal et al., *GNNs getting comfy: Community and feature similarity guided rewiring*, ICLR 2025

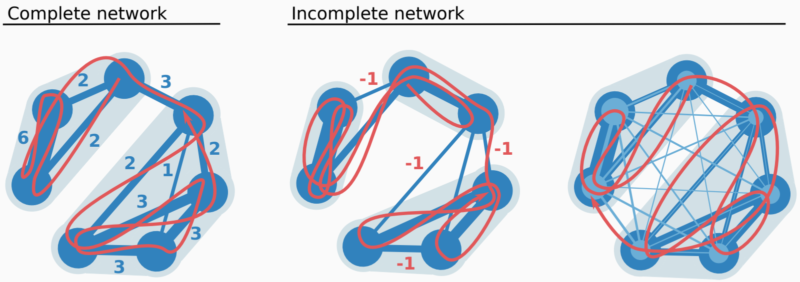
Data Augmentation for GNNs

Empirical data is often unreliable: incomplete or spurious observations

- Bayesian network reconstruction

  → Newman, *Network structure from rich but noisy data*, Nature Physics 2018
- SBM: simultaneous reconstruction and community detection (also Bayesian)

  → Peixoto, *Network reconstruction and community detection from dynamics*, PRL 2019



→ Smiljanić et al., *Mapping Flows on Weighted and Directed Networks with Incomplete Observations*; J. Comp. Net., 2021

Challenge & Opportunity: Integrate probabilistic generative models with GNNs

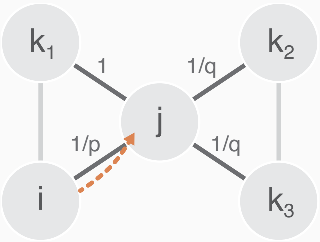
II. Inductive Bias for Guiding the Learning Process

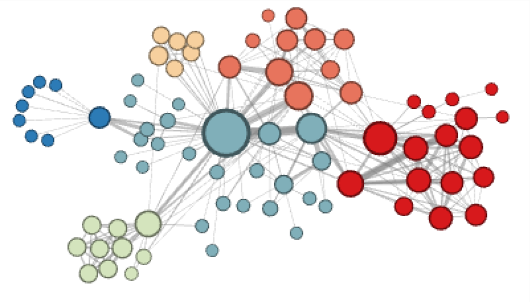
Community Detection

"Standard" approach in DGL

- Learn embeddings (for example, with a GNN)
- Run k-means clustering (with a suitable k → guess or "hyperparameter tuning")

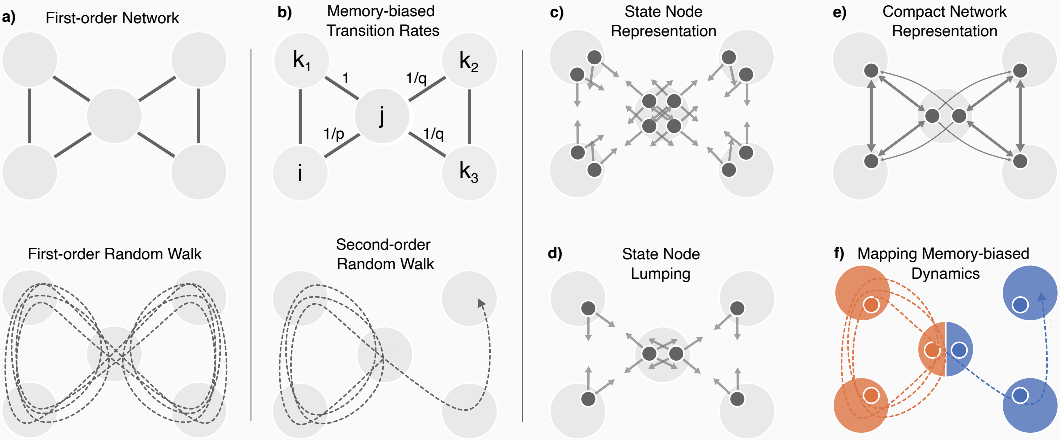
For example, node2vec





→ Grover & Leskovec, *node2vec: Scalable Feature Learning for Networks*, KDD 2016

Using node2vec for Overlapping Communities from 1st-Order Data



→ Lindström et al., *Mapping compact memory-biased dynamics reveals overlapping communities*, arXiv:2304.05775

Maja Lindström, Session Dynamics 2, Thu 12:30 - 12:45

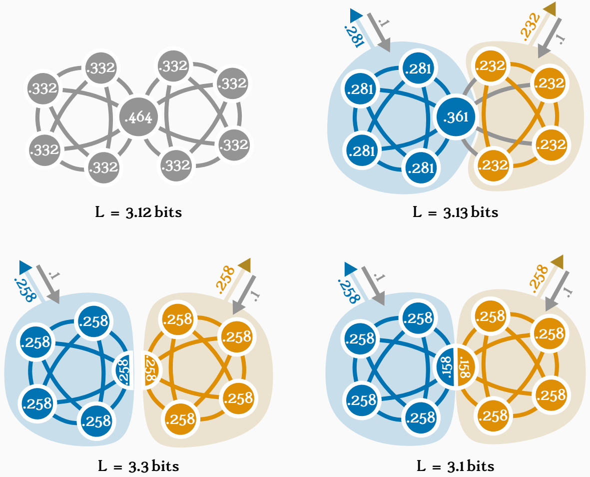
Network Science / Graph Theory inspired Deep Community Detection works

- Min-Cut & Max-Cut
  - $\rightarrow$ Bianchi et al., *Spectral Clustering with Graph Neural Networks for Graph Pooling*, ICML 2020
  - $\rightarrow$ Abate & Bianchi, *MaxCutPool: differentiable feature-aware Maxcut for pooling in graph neural networks* , ICLR 2025
- Modularity
  - $\rightarrow$ Tsitsulin et al., *Graph Clustering with Graph Neural Networks*, JMLR 2023
- The map equation
  - $\rightarrow$ Blöcker et al., *The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks*, NeurIPS 2024

Challenge: Need to define continuous generalisation of discrete objectives
Approach: Usually via soft cluster assignments

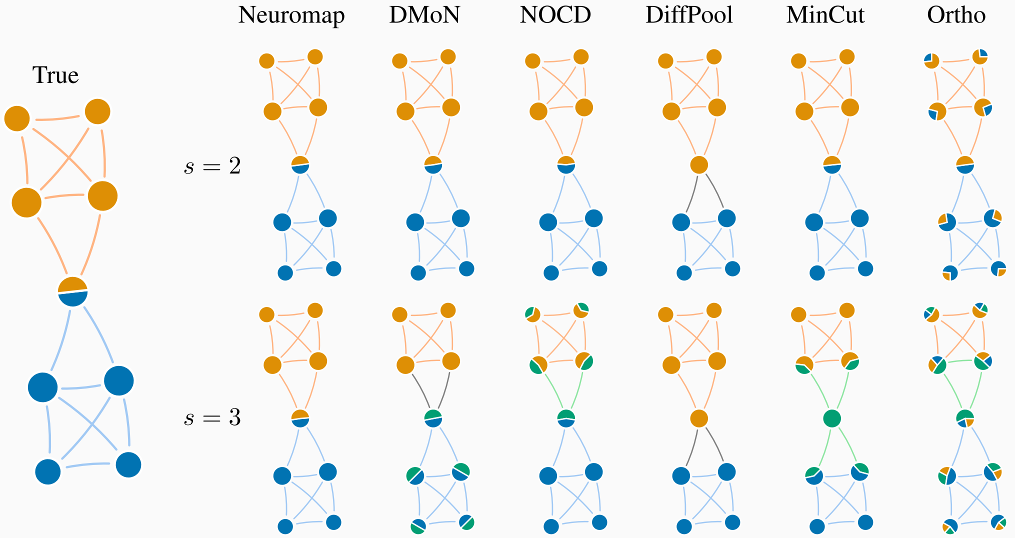
From Discrete to Continuous

Not straightforward, there may be effects on the loss landscape.



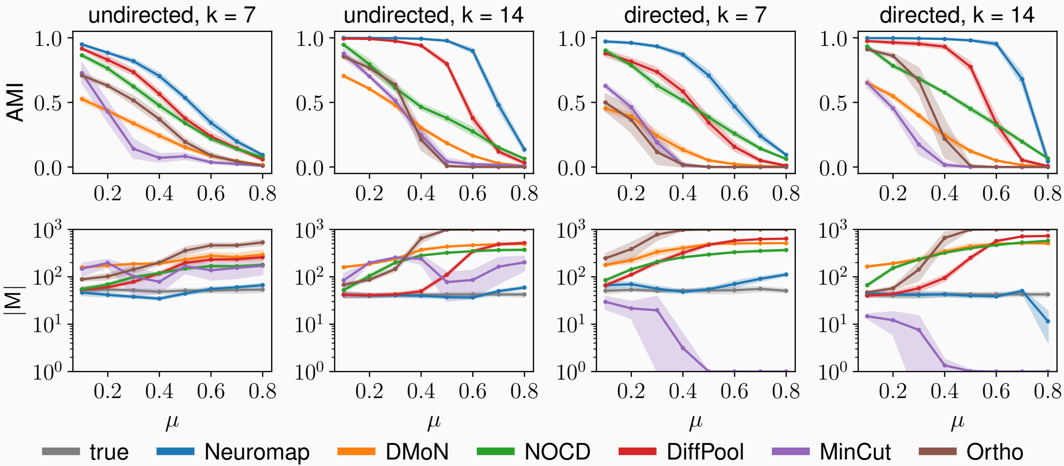
→ Blöcker et al., *The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks*, NeurIPS 2024

Issue: Regularisation is (often) essential (but also often ineffective)



→ Blöcker et al., *The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks*, NeurIPS 2024

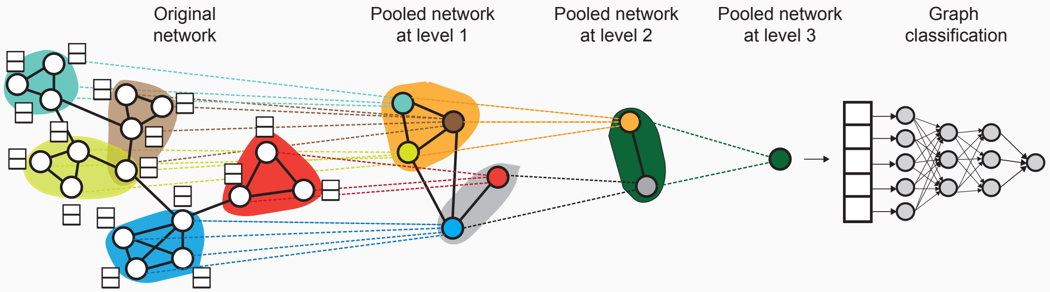
LFR networks with 1000 nodes: Regularisation is ineffective



→ Blöcker et al., *The Map Equation Goes Neural: Mapping Network Flows with Graph Neural Networks*, NeurIPS 2024

DGL currently lacks effective non-parametric methods!

Pooling for Graph Classification (≈ "Hierarchical Community Detection")



→ Ying et al., *Hierarchical Graph Representation Learning with Differentiable Pooling*, NeurIPS 2018

Non-parametric approaches

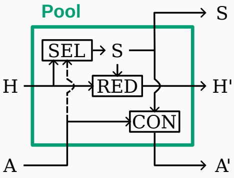
- BN-Pool, based on the so-called stick-breaking process

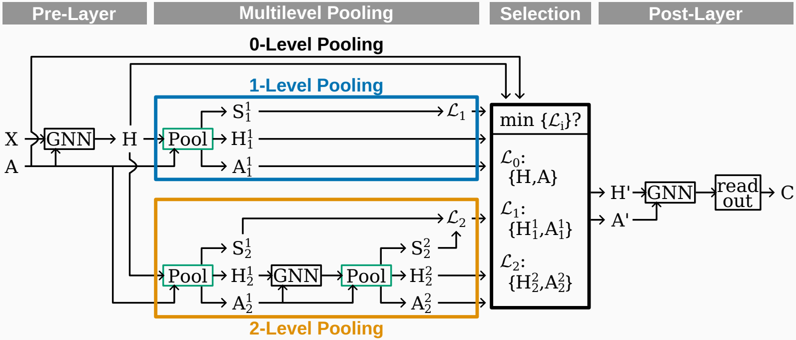
  → Castellana & Bianchi, *BN-Pool: a Bayesian Nonparametric Approach to Graph Pooling*, arXiv:2501.09821

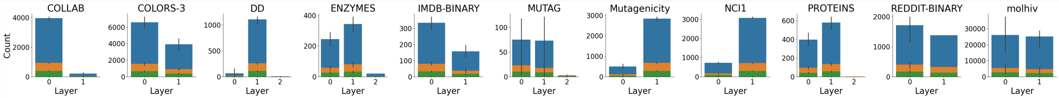
- MDL-Pool, based on the map equation

  → von Pichowski et al., MDL-Pool: Adaptive Multilevel Graph Pooling Based on Minimum Description Length; arXiv:2409.10263

MDL-Pool: Learning a Multilevel Pooling Operator



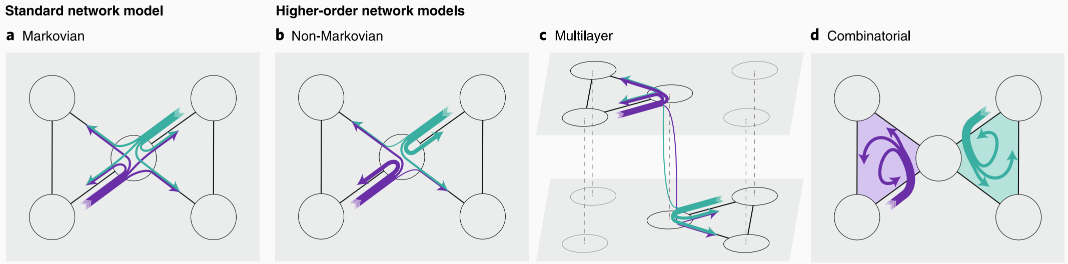




→ von Pichowski et al., *MDL-Pool: Adaptive Multilevel Graph Pooling Based on Minimum Description Length*; arXiv:2409.10263

Higher-Order Models

It is often insufficient to model dyadic interaction in complex networks



→ Lambiotte et al., *From networks to optimal higher-order models of complex systems*, Nature Physics 2019

- Non-Markovian dynamics: sparse memory networks, De Bruijn graphs
  - → Rosvall et al., *Memory in network flows and its effects on spreading dynamics and community detection*, Nat Comm 2014
  - → De Bruijn, *A combinatorial problem*, 1946
- Multi-body interactions: hypergraphs, simplicial complexes
  - → Battiston et al., *Networks beyond pairwise interactions: Structure and dynamics*, Physics Reports 2020

Higher-Order Models

Recent works have started adopting those models

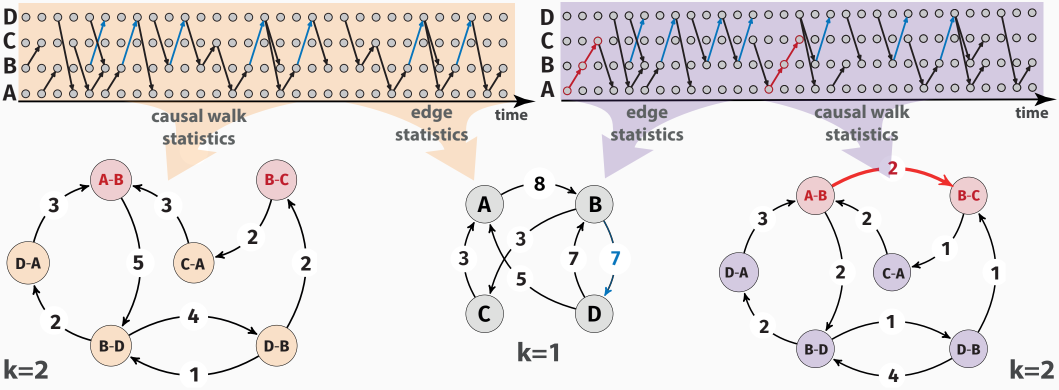
→ Qarkaxhija et al., *De Bruijn goes Neural: Causality-Aware Graph Neural Networks for Time Series Data on Dynamic Graphs*, PMLR 2022

→ Antelmi et al., *A Survey on Hypergraph Representation Learning*, ACM Computing Surveys 2023

→ Frantzen & Schaub, *Learning from Simplicial Data Based on Random Walks and 1D Convolutions*, ICLR 2024

→ Kim et al., *A survey on hypergraph neural networks: An in-depth and step-by-step guide*, KDD 2024

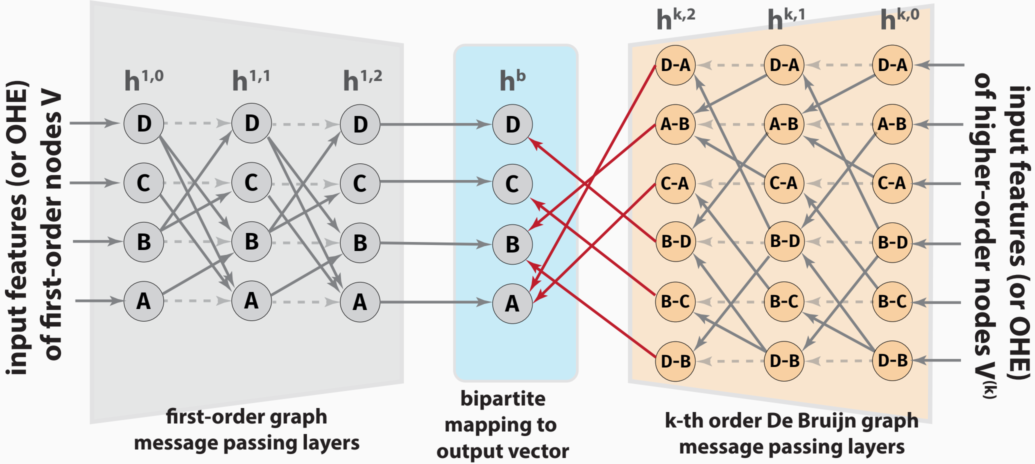
De Bruijn GNN: A Causality-Aware GNN



→ Qarkaxhija et al., *De Bruijn goes Neural: Causality-Aware Graph Neural Networks for Time Series Data on Dynamic Graphs*, PMLR 2022

De Bruijn GNN: A Causality-Aware GNN

The "recipe": message passing on the higher-order network model.



→ Qarkaxhija et al., *De Bruijn goes Neural: Causality-Aware Graph Neural Networks for Time Series Data on Dynamic Graphs*, PMLR 2022

III. Datasets and Benchmarks

Evaluation

Focus on a small set of datasets with the goal to maximise predictive performance.
→ Cora, Pubmed, CiteSeer, OGB, TGB, ...

"Current benchmarking practices often lack focus on transformative, real-world applications [...] many benchmark datasets poorly represent the underlying data [...] an excessive focus on accuracy [...] [incentivizes] overfitting rather than fostering generalizable insights."

→ Bechler-Speicher et al., *Position: Graph Learning Will Lose Relevance Due To Poor Benchmarks*; arXiv:2502.14546

"Recent research has highlighted problems with graph-learning datasets and benchmarking practices—revealing, for example, that methods which ignore the graph structure can outperform graph-based approaches on popular benchmark datasets."

→ Coupette et al., *No Metric to Rule Them All: Toward Principled Evaluations of Graph-Learning Datasets*; arXiv:2502.02379

Opportunity: Network scientists have curated a large body of real-world datasets.

Evaluation of MDL-Pool

Often, “nopool” outperforms methods that consider graph topology, but it is never best.

	Pooler	COLLAB	COLORS-3	D&D	ENZYMES	IMDB-B	MUTAG	Mutag.	NCI1	PROTEINS	REDDIT-B	molhiv (AUROC)
	nopool	75.8 ± 1.4	93.4 ± 2.3	75.1 ± 2.7	41.7 ± 5.1	75.6 ± 6.2	87.1 ± 3.2	81.1 ± 1.5	79.6 ± 2.3	75.9 ± 7.0	92.0 ± 1.8	75.8 ± 2.5
Score,1/K	ECPool	77.0 ± 1.4	82.3 ± 2.6	75.3 ± 1.8	42.3 ± 5.3	76.4 ± 10.9	87.1 ± 3.2	81.4 ± 2.2	**80.6** ± 2.1	74.7 ± 6.3	**93.0** ± 1.0	**77.4** ± 1.0
	Graclus	**77.1** ± 1.6	83.5 ± 2.4	71.4 ± 1.9	42.7 ± 6.8	74.8 ± 8.1	85.7 ± 8.7	**82.3** ± 1.8	79.4 ± 1.5	75.5 ± 5.1	92.5 ± 0.9	77.1 ± 1.2
	k-MIS	74.9 ± 1.4	92.2 ± 1.1	75.6 ± 1.4	40.7 ± 8.5	74.8 ± 7.3	88.6 ± 6.4	80.8 ± 1.6	80.1 ± 1.4	76.5 ± 4.9	92.0 ± 2.4	75.4 ± 2.6
	Top-k	74.3 ± 1.8	77.2 ± 17.0	72.4 ± 4.3	39.7 ± 3.6	74.4 ± 11.6	87.1 ± 9.3	78.0 ± 1.4	77.7 ± 2.1	73.3 ± 4.9	91.0 ± 0.5	75.6 ± 2.9
Clustering	DiffPool	60.8 ± 1.9	76.8 ± 6.2	62.0 ± 5.3	16.3 ± 4.3	72.0 ± 8.7	87.1 ± 9.3	78.6 ± 1.9	70.4 ± 9.3	75.5 ± 4.5	80.5 ± 10.1	73.3 ± 3.2
	DMoN	76.0 ± 0.9	90.9 ± 0.9	77.1 ± 3.8	42.7 ± 5.5	74.8 ± 4.6	**90.0** ± 6.4	80.8 ± 1.7	80.2 ± 2.7	76.5 ± 4.7	91.1 ± 1.1	74.9 ± 0.8
	JBGNN	75.7 ± 1.2	89.0 ± 4.0	77.3 ± 4.3	**45.0** ± 6.8	76.8 ± 7.7	87.1 ± 9.3	81.6 ± 1.2	79.3 ± 1.9	**77.1** ± 3.9	91.8 ± 1.2	75.9 ± 2.1
	MinCut	75.8 ± 1.4	91.8 ± 1.4	78.3 ± 2.8	41.3 ± 5.9	73.6 ± 6.5	87.1 ± 7.8	81.2 ± 0.9	80.0 ± 0.7	76.1 ± 5.4	91.6 ± 1.5	76.5 ± 1.5
Free	BNPool	73.5 ± 0.7	**97.1** ± 0.7	74.7 ± 3.7	38.0 ± 3.6	75.6 ± 6.7	85.7 ± 5.1	80.1 ± 1.9	78.6 ± 1.4	76.3 ± 3.6	90.4 ± 2.0	76.8 ± 2.1
	MDL-Pool (1-LVL)	68.9 ± 6.0	86.5 ± 1.2	77.3 ± 2.0	41.3 ± 5.2	76.0 ± 5.1	**90.0** ± 8.1	80.5 ± 0.8	78.0 ± 1.7	75.9 ± 4.6	91.3 ± 1.8	76.3 ± 1.0
	MDL-Pool	76.3 ± 0.9	87.2 ± 1.8	**79.7** ± 2.5	39.3 ± 3.2	**77.2** ± 5.4	85.7 ± 8.7	80.0 ± 2.0	79.0 ± 1.2	76.1 ± 5.5	91.6 ± 1.1	75.2 ± 2.0

→ von Pichowski et al., *MDL-Pool: Adaptive Multilevel Graph Pooling Based on Minimum Description Length*, arXiv:2409.10263

Evaluation

Deep Graph Learning often uses metadata as “ground truth”, but we know that obtaining the ground truth is infeasible, if not impossible, for empirical dataset

→ Peel et al., *The ground truth about metadata and community detection in networks*, arXiv:2409.10263

Network scientists often use synthetic benchmarks with known ground truth

→ Lancichinetti et al., *Benchmark graphs for testing community detection algorithms*, PRE 2008

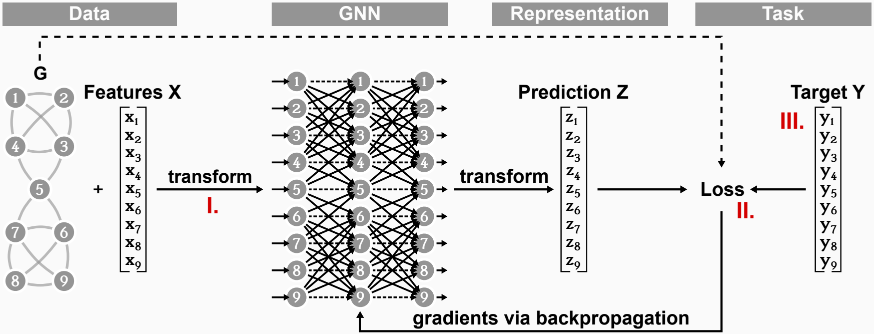
→ Peixoto, *Bayesian stochastic blockmodeling*, Advances in Network Clustering and Blockmodeling 2019

→ Kaminski et al., *Artificial Benchmark for Community Detection (ABCD)—Fast random graph model with community structure*, Network Science 2021

Opportunity: synthetic benchmarks to pinpoint what exact patterns a DGL model learns

Conclusion

Principled Deep Learning Modelling



Challenges / Opportunities

- I Explicit expectations regarding the data & data augmentation
- II Inductive bias for guiding the learning process
- III Datasets and benchmarks for evaluation

Conclusion

Network science and deep graph learning share the same goal: to better model and understand petterns in graph-structured data.

The two fields take different approaches

- Network science focuses on transparent models and aims for mechanistic untերstanding
- DGL emphasises flexibility and scalability, often achieving SOTA performance

Combining their respective strengths holds immense potential for mutual benefits.

Thank you for your attention!