How Powerful are Graph Neural Networks?

(EE531 Final Project - Graph)

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Table of Contents

Outline

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- But why GNNs work? Why are they so powerful?
- Most interestingly, *how powerful are they?*

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Previous / Related Works

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- Above works focus on a specific architecture and **do not easily generalize to other architectures**.
- This paper presents a general framework for analyzing/characterizing the expressive power of a broad class of GNNs!

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Each $v \in V$ has an associated label y_v.
Goal: Learn a representation vector h_v of v such that $y_v = f(h_v)$ i.e. such that v's label can be predicted.

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Graph Classification Problem

A set of graphs $\{G_1, \ldots, G_N\} \subset \mathcal{G}$ is given, along with their labels $\{y_1, \ldots, y_N\} \subset \mathcal{Y}$.
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- k-th layer of a GNN is

$$a_v^{(k)} = \text{AGGREGATE}^{(k)}\left(\left\{h_u^{(k-1)} : u \in \mathcal{N}_G(v)\right\}\right)$$

$$h_v^{(k)} = \text{COMBINE}^{(k)}\left(h_v^{(k-1)}, a_v^{(k)}\right)$$

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- Different choices of AGGREGATE$^{(k)}$ and COMBINE$^{(k)}$ have led to different GNN variants/architectures.

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$$a_v^{(k)} = \text{MAX}\left(\left\{\text{ReLU}\left(Wh_u^{(k-1)}\right) : u \in \mathcal{N}_G(v)\right\}\right)$$

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- Graph Convolutional Networks, or GCN[5]:

$$h_v^{(k)} = \text{ReLU}\left(W\,\text{MEAN}\left\{h_u^{(k-1)} : u \in \mathcal{N}_G(v) \cup \{v\}\right\}\right)$$

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- READOUT can be a simple permutation invariant function, or something more sophisticated[6][7]

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- This seemingly harmless problem has harassed researchers for decades!

Graph Isomorphism Problem

Here are some facts related to GI:

- Not known to be of class NP-complete nor tractable!
  (Researchers have actually defined a new complexity class **GI**)

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- But it is not practical!
- Some practical algorithms: McKay (1981), Schmidt & Druffel (1976), Ullman (1976)...etc.

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Weisfeiler-Lehman test

- Weisfeiler-Lehman test of graph isomorphism[9], or simply WL test, is a combinatorial algorithm for GI.

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- WL test is proved to be successful (and computationally efficient) in isomorphism testing for a broad class of graphs[10]
- There are some cases (ex. regular graphs) when the WL test fails[11]

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- 1-dimensional form of the WL test ("naïve vertex refinement") is *based on neighbor aggregations*, analogous to the GNNs!
- Overview of the algorithm:
  - Aggregate the labels of nodes and their neighborhoods
  - Hashes the aggregated label into *unique* new labels
  - If at some iteration the labels of the nodes between the two graphs differ, then the two graphs are non-isomorphic.

1-dim WL test

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$$c_l^{(0)} = l, \; c_l^{(t)}(v) = \text{HASH}\left(\left(c_l^{(t-1)}(v), \{\{c_l^{(t-1)}(u) | u \in \mathcal{N}(v)\}\}\right)\right)$$

(HASH bijectively maps the above pair to a unique value in Σ that hasn't been used in previous iterations)

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- Run above algorithm in parallel for the two input graphs.
- If at some iteration, the two graphs have a different number of nodes colored $\sigma \in \Sigma$, conclude that the graphs are not isomorphic.
  (This why this 1-dim version is commonly called the *color refinement algorithm*)

WL subtree kernel

- Graph kernel: kernel function that defines *inner product on graphs*[12][13][14]
  (Function measuring the similarity of a pair of two given graphs)

[12] Thomas Gärtner, Peter A. Flach, and Stefan Wrobel. "On Graph Kernels: Hardness Results and Efficient Alternatives". In: *Computational Learning Theory and Kernel Machines, 16th Annual Conference on Computational Learning Theory and 7th Kernel Workshop, COLT/Kernel 2003, Washington, DC, USA, August 24-27, 2003, Proceedings*. 2003, pp. 129–143.

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[14] S. V. N. Vishwanathan et al. "Graph Kernels". In: *J. Mach. Learn. Res.* 11 (2010), pp. 1201–1242.

[15] Nino Shervashidze and Karsten M. Borgwardt. "Fast subtree kernels on graphs". In: *Advances in Neural Information Processing Systems 22: 23rd Annual Conference on Neural Information Processing Systems 2009. Proceedings of a meeting held 7-10 December 2009, Vancouver, British Columbia, Canada*. 2009, pp. 1660–1668.

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- ex. *random walk graph kernel*, *marginalized graph kernel*
- Weisfeiler-Lehman subtree kernel[15][16]: counts common *original and compressed labels* (resulting from 1-dim WL test) in two graphs.

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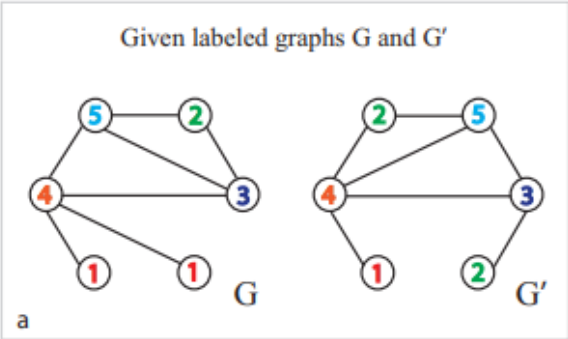
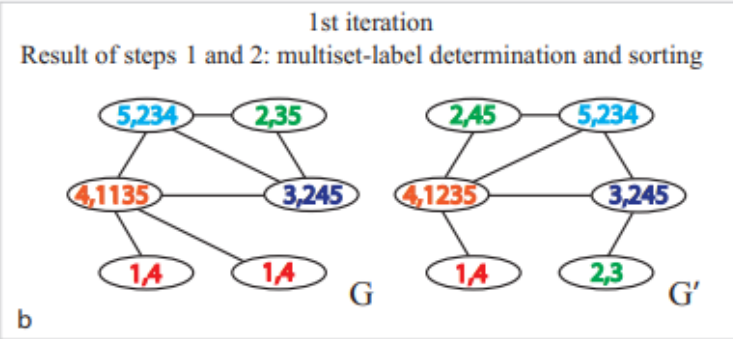
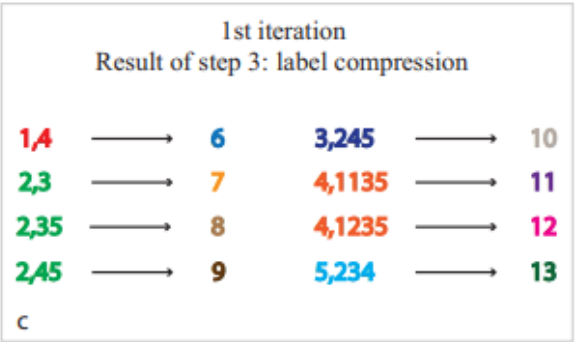
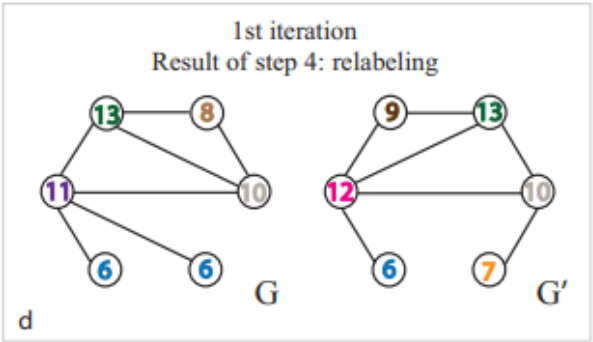
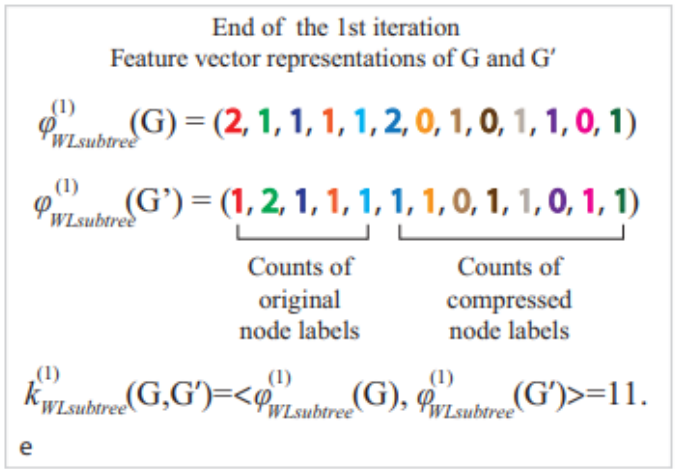
WL subtree kernel











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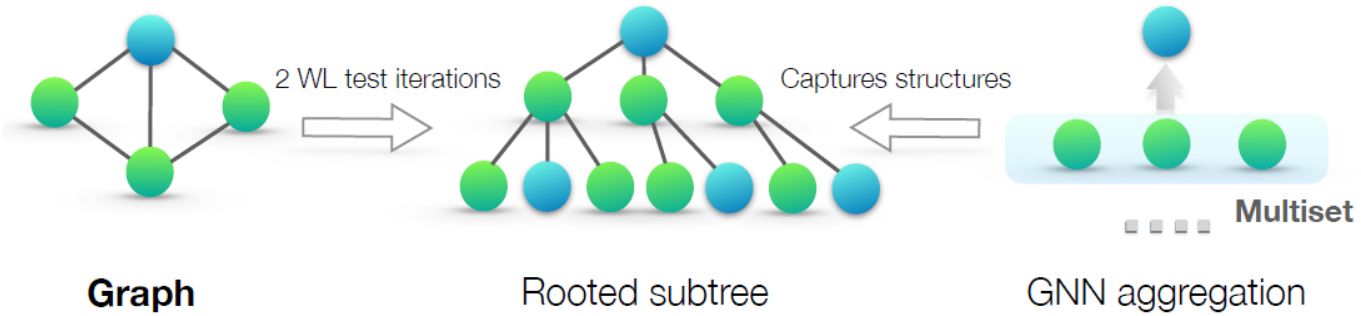
- Is it related to GNN? Yes!
- The kernel uses the *counts of node labels* at different iterations of the WL test as the *feature vector* of a graph.
- Intuitively, a node's label at the k-th iteration of the 1-dim WL test represents a subtree structure of height k rooted at the node.



- Thus, the graph features considered by the WL subtree kernel are essentially counts of different rooted subtrees in the graph!

k-dim WL test

- k-dim WL test is a generalization of the 1-dim WL test; it colors tuples from $V(G)^k$ instead of nodes.

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- In this work, we only focus on 1-dim WL test.

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Outline

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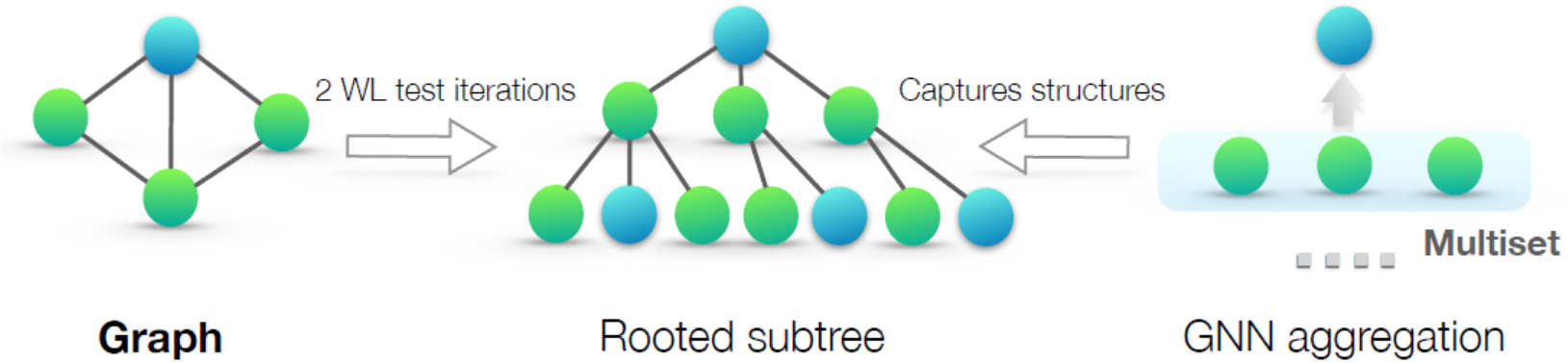

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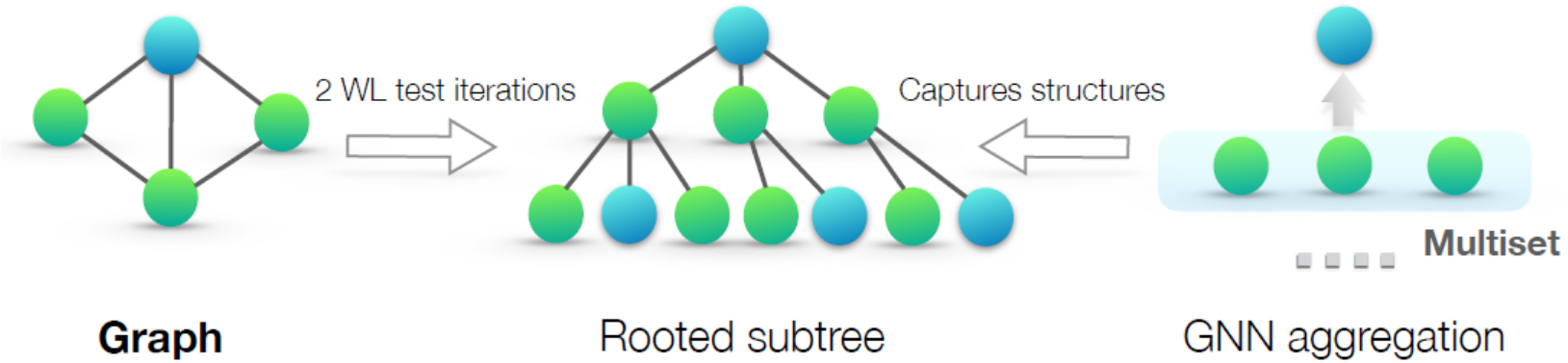

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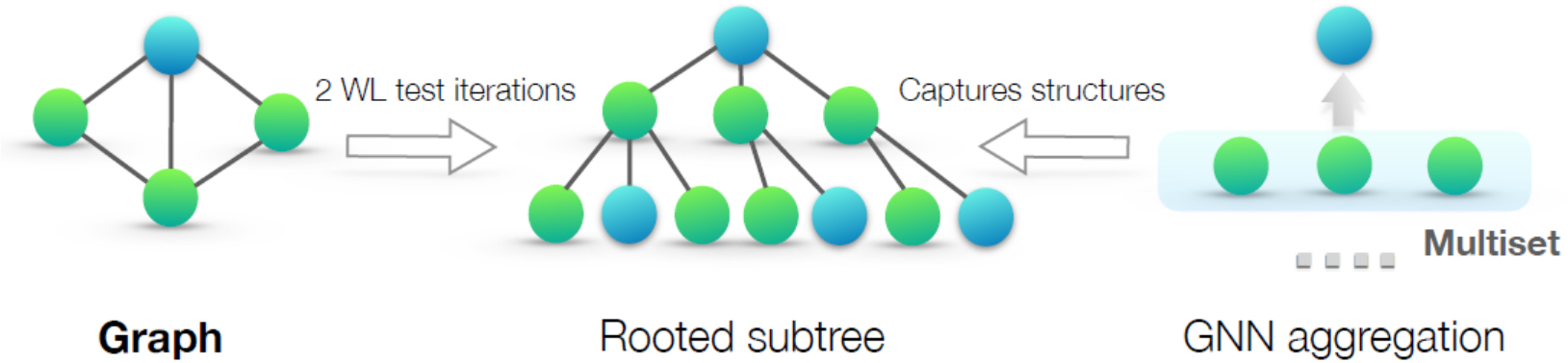

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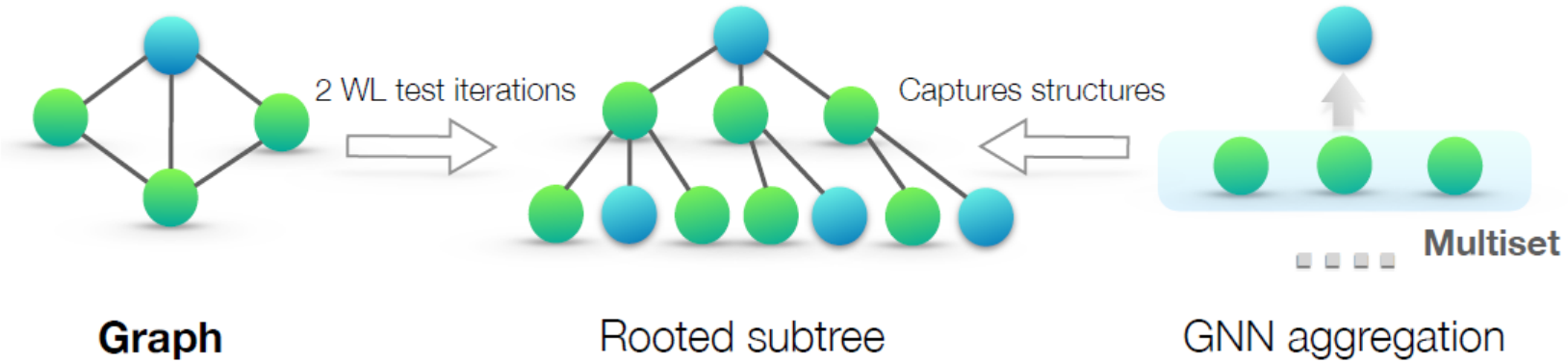

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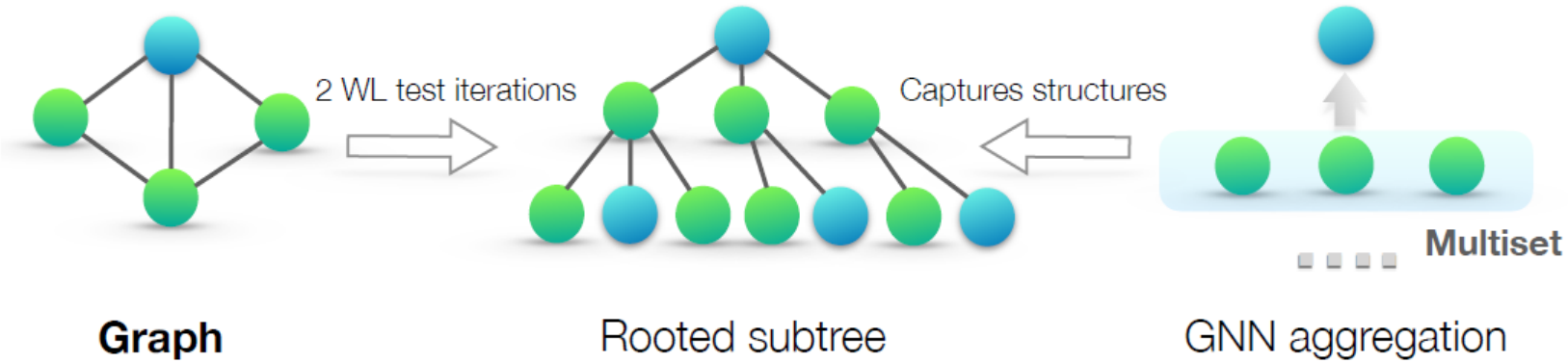

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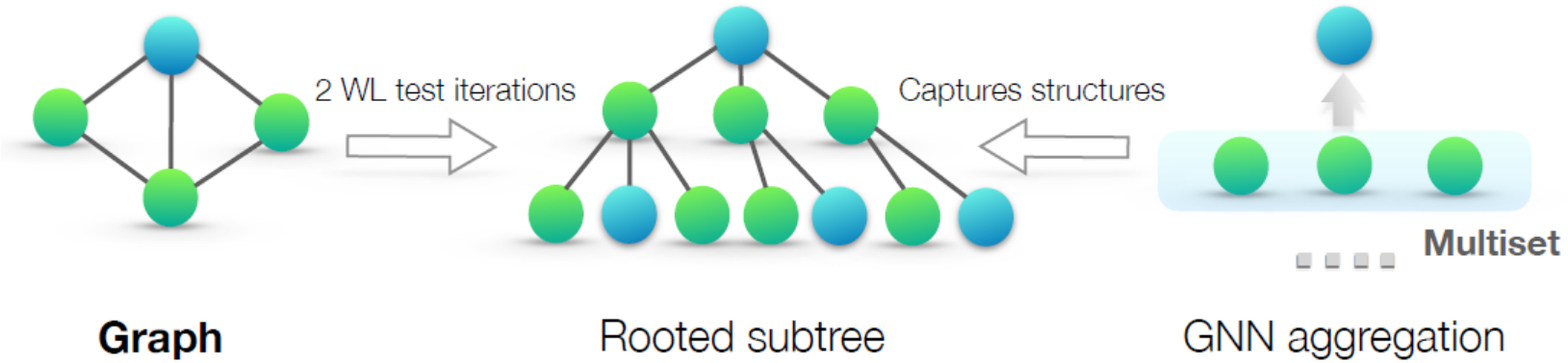

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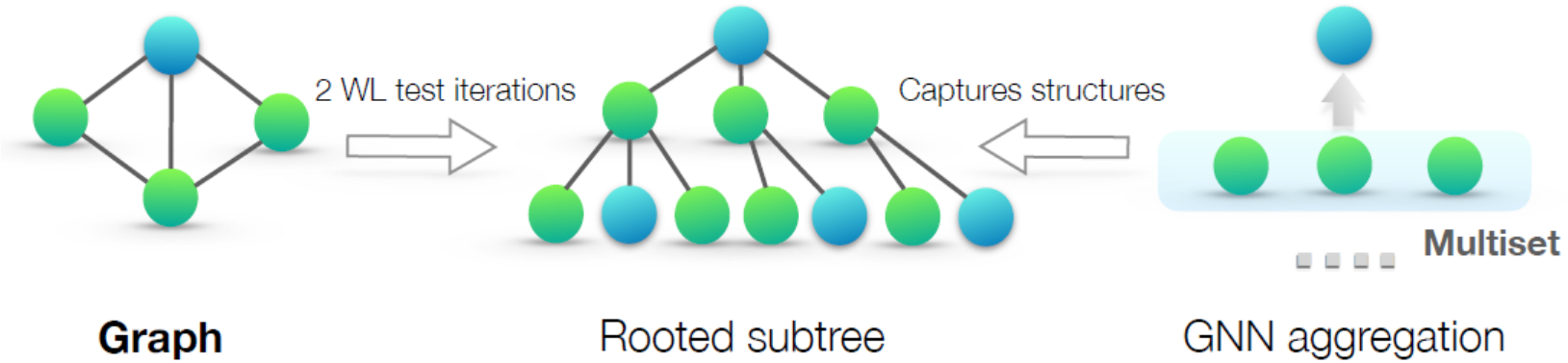

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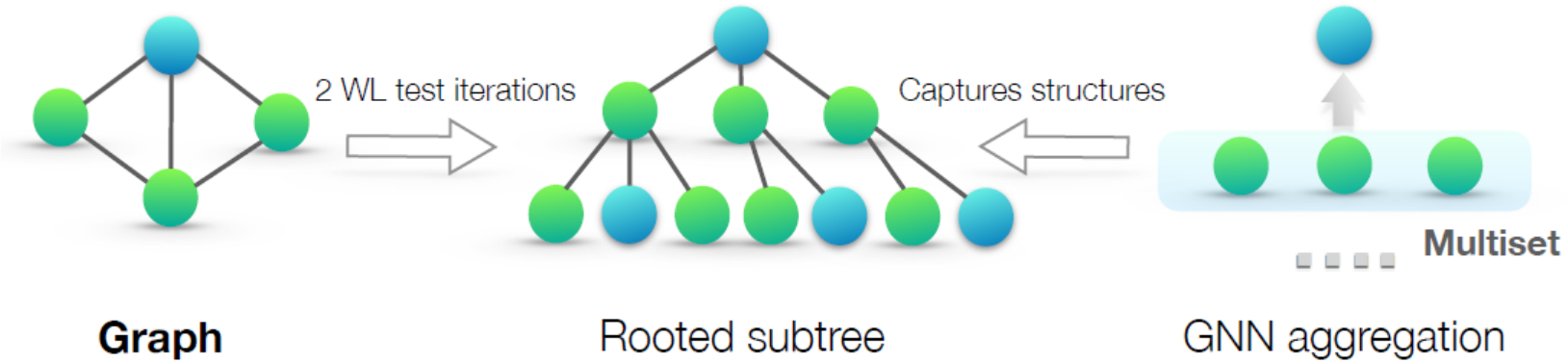

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- GNN's aggregation scheme: *class of functions over multisets that their neural networks can represent*

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Representational capacity of GNNs

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- It says that any aggregation-based GNN is *at most* as powerful as the WL test in distinguishing different graphs.

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Theorem 3

Let $\mathcal{A} : \mathcal{G} \to \mathbb{R}^d$ be a GNN.
With a sufficient number of GNN layers, $\mathcal{A}$ maps any G_1 and G_2 that the Weisfeiler-Lehman test of isomorphism decides as non-isomorphic, to different embeddings if the following conditions hold:

- $\mathcal{A}$ aggregates and updates node features iteratively with

$$h_v^{(k)} = \phi\left(h_v^{(k-1)}, f\left(\left\{h_u^{(k-1)} : u \in \mathcal{N}_G(v)\right\}\right)\right)$$

  where the functions f, which operates on multisets, and ϕ are *injective*.

- $\mathcal{A}$'s graph-level readout, which operates on the multiset of node features $\left\{h_v^{(k)}\right\}$, is *injective*.

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- Node feature vectors in the WL test are essentially one-hot encodings, and thus cannot capture similarity between subtrees!

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- Especially useful when co-occurence of subtrees is sparse across different graphs, or there are noisy edges and node features.[18]

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- Idea: deep multisets[19] *i.e.* parametrizing universal multiset functions with neural networks.

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Lemma 5

Assume $\mathcal{X}$ is countable. There exists a function $f : \mathcal{X} \to \mathbb{R}^n$ so that $h(X) = \sum_{x \in X} f(x)$ is unique for each multiset $X \subset \mathcal{X}$ of bounded size. Moreover, any multiset function g can be decomposed as $g(X) = \phi\left(\sum_{x \in X} f(x)\right)$ for some function ϕ.

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- This lemma tells us that sum aggregators can represent injective, in fact, *universal* functions over multisets.
- Thus, we can conceive aggregation schemes that can represent universal functions over a node and the multiset of its neighbors, satisfying the *injectiveness condition* (a) in Theorem 3!

Graph Isomorphism Network (GIN)

- Here is a simple and concrete formulation of the previous discussion:

Corollary 6

Assume $\mathcal{X}$ is countable. There exists a function $f : \mathcal{X} \to \mathbb{R}^n$ so that for infinitely many choices of ϵ, including all irrational numbers, $h(c, X) = (1+\epsilon)f(c) + \sum_{x \in X} f(x)$ is unique for each pair (c, X), where $c \in \mathcal{X}$ and $X \subset \mathcal{X}$ is a multiset of bounded size.
Moreover, any function g over such pairs can be decomposed as $g(c, X) = \varphi\left((1+\epsilon)f(c) + \sum_{x \in X} f(x)\right)$ for some function φ.

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- We can use MLPs to model and learn f and φ, thanks to the Universal Approximation Theorem[2021].

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How powerful is MLP?

Universal Approximation Theorem (Hornik, 1991)

Define

$$\mathcal{N}_k^{(n)}(\psi) = \left\{ h : \mathbb{R}^k \to \mathbb{R} \middle| h(x) = \sum_{j=1}^{n} \beta_j \psi(a_j' x - \theta_j) \right\}$$

as the set of all functions implemented by such a network with n hidden units, where ψ is the common activation function of the hidden units.
If ψ is continuous, bounded and nonconstant, then $\mathcal{N}_k^{(n)}(\psi)$ is dense in $\mathcal{C}(X)$ for all compact subsets X of $\mathbb{R}^k$.

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- The choice of the activation function doesn't matter; it's the multilayer feedforward architecture that gives neural networks the potential of being universal approximators.

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- Then, GIN updates node representations as:

$$h_v^{(k)} = \text{MLP}^{(k)}\left(\left(1+\epsilon^{(k)}\right) h_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)}\right)$$

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- Node embeddings, learned by the GIN, can be directly used for node classification and link prediction.

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- Use information from *all* depths/iterations of the model[22]!

$$h_G = \text{CONCAT}\left(\text{READOUT}\left(\left\{h_v^k | v \in V(G)\right\}\right) \middle| k = 0, 1, \ldots, K\right)$$

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- Use information from *all* depths/iterations of the model[22]!

$$h_G = \text{CONCAT}\left(\text{READOUT}\left(\left\{h_v^k | v \in V(G)\right\}\right) \middle| k = 0, 1, \ldots, K\right)$$

- Note that if GIN replaces READOUT with summing all node features from the same iteration, it provably generalizes the WL test and the WL subtree kernel.

[22] Keyulu Xu et al. "Representation Learning on Graphs with Jumping Knowledge Networks". In: *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*. 2018, pp. 5449–5458.

Outline

Overview

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Outline

MLP?

- The function f in Lemma 5 helps map distinct multisets to unique embeddings.

[23] Kurt Hornik. "Approximation capabilities of multilayer feedforward networks". In: *Neural Networks* 4.2 (1991), pp. 251–257.

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- f can be parametrized by MLPs, as shown by the Universal Approximation Theorem[23]

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- Unlike models using MLPs, 1-layer perceptron (even with the bias term) is not a universal approximator of multiset functions.

Outline

GCN

- As described previously, Graph Convolutional Network[24] takes the form:

$$h_v^{(k)} = \text{ReLU}\left(W \,\text{MEAN}\left\{h_u^{(k-1)} : u \in \mathcal{N}_G(v) \cup \{v\}\right\}\right)$$

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Corollary 8

Assume $\mathcal{X}$ is countable. There exists a function $f : \mathcal{X} \to \mathbb{R}^n$ so that $h(X) = \frac{1}{|X|} \sum_{x \in X} f(x)$, $h(X_1) = h(X_2)$ *if only if* multisets X_1 and X_2 hav e the same distribution. That is, assuming $|X_2| \geq |X_1|$, we have $X_1 = (S, m)$ and $X_2 = (S, km)$ for some $k \in \mathbb{N}$.

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- This is as powerful as the sum aggregator if the node features are diverse and rarely repeat, and thus *effective for node classification*.

Outline

GraphSAGE

- As described previously, GraphSAGE[25] takes the form:

$$a_v^{(k)} = \text{MAX}\left(\left\{\text{ReLU}\left(Wh_u^{(k-1)}\right) : u \in \mathcal{N}_G(v)\right\}\right)$$

$$h_v^{(k)} = W\left[h_v^{(k-1)}, a_v^{(k)}\right]$$

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Summary

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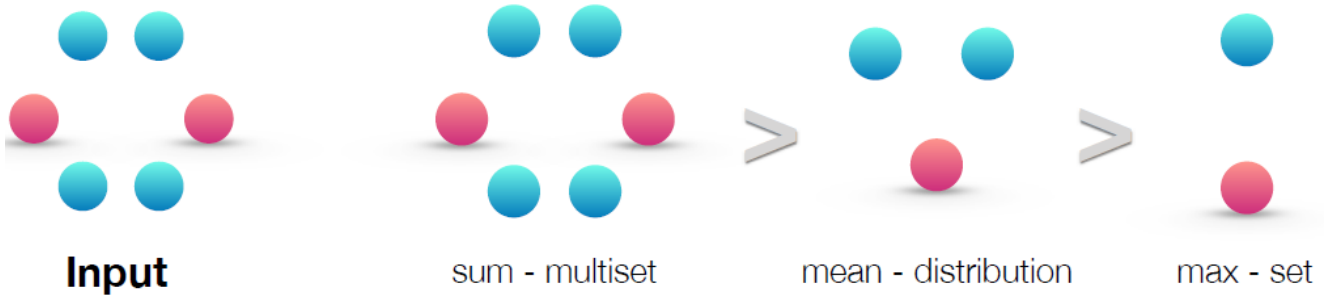

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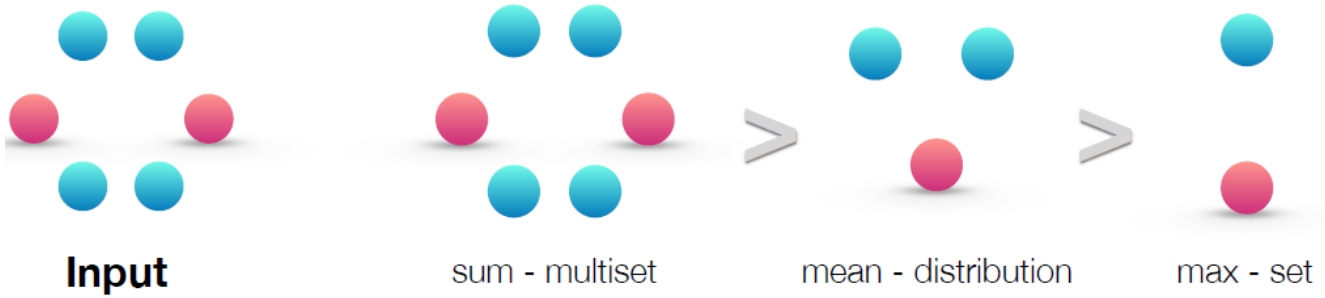

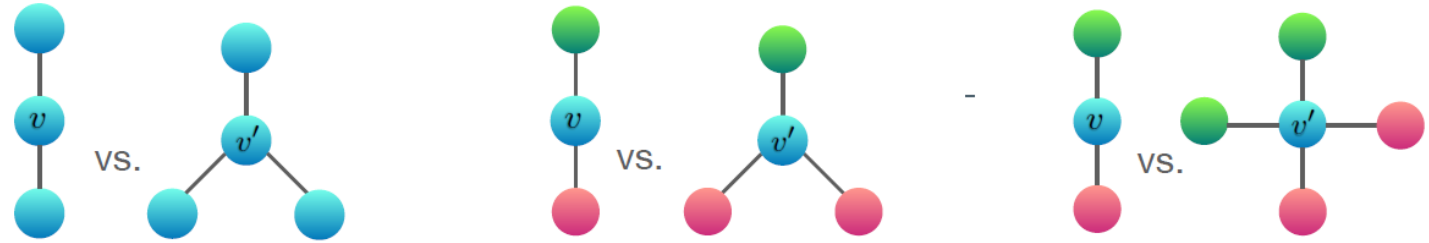

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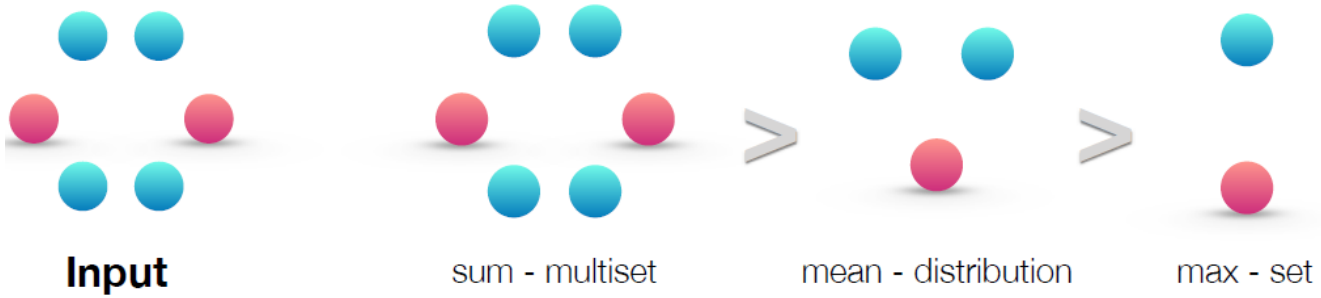

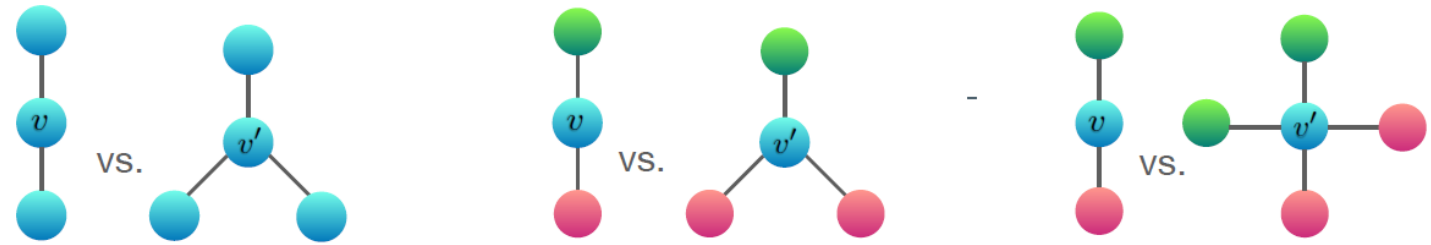

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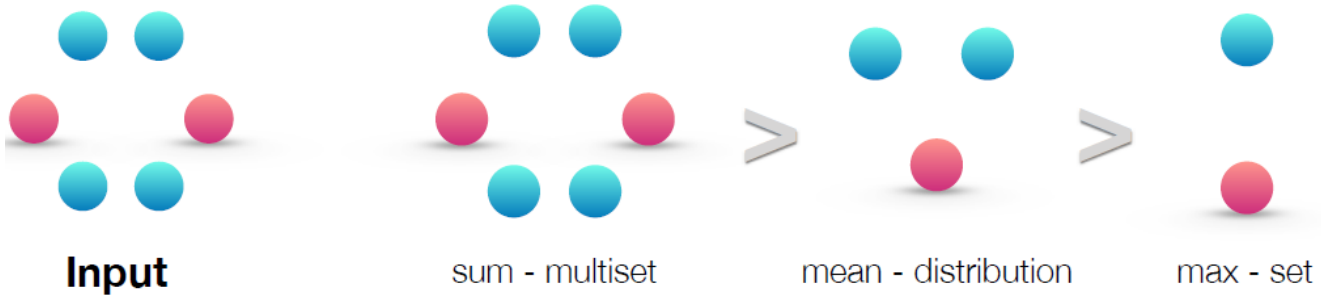

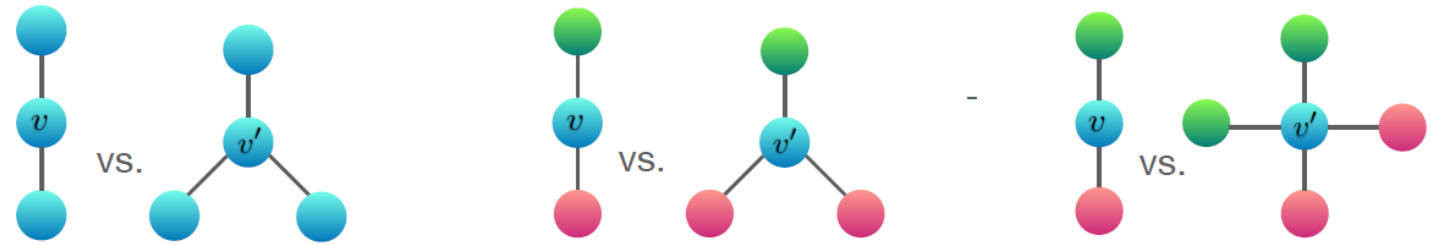

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Outline

Experiments

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- Training set performance: compare different GNN models based on their *representational power*
- Test set performance: quantifies *generalization ability*

Experiment Design

- 9 graph classification benchmarks were used[26]:
  - 4 bioinformatics datasets (*MUTAG*, *PTC*, *NCI1*, *PROTEINS*)
  - 5 social network datasets (*COLLAB*, *IMDB-BINARY*, *IMDB-MULTI*, *REDDIT-BINARY*, *REDDIT-MULTI5K*)

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  - Deep learning architectures i.e. DCNN, PATCHY-SAN, DGCNN
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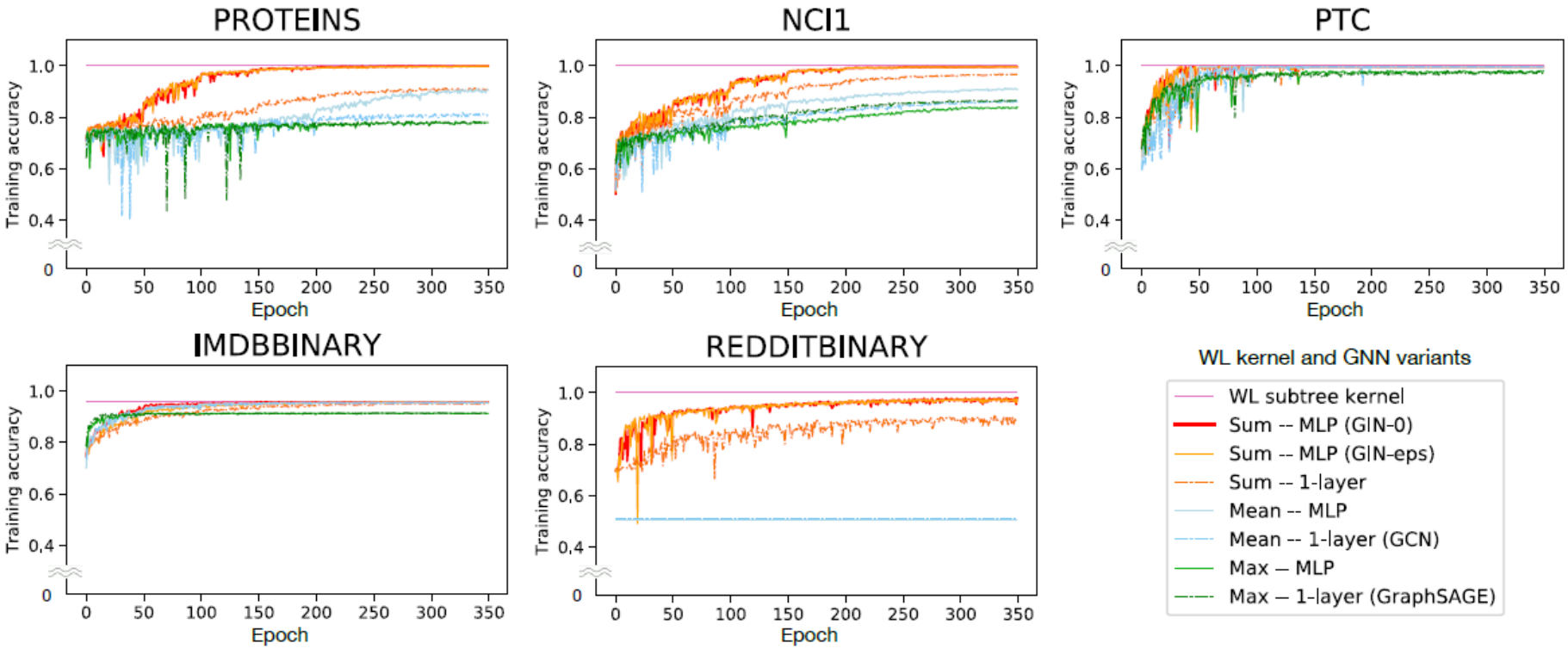
PROTEINS
NCI1
PTC
IMDBBINARY
REDDITBINARY
Training accuracy
Epoch
WL kernel and GNN variants
WL subtree kernel
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Sum -- MLP (GIN-eps)
Sum -- 1-layer
Mean -- MLP
Mean -- 1-layer (GCN)
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Max -- 1-layer (GraphSAGE)

Results

	Datasets	IMDB-B	IMDB-M	RDT-B	RDT-M5K	COLLAB	MUTAG	PROTEINS	PTC	NCI1
Datasets	# graphs	1000	1500	2000	5000	5000	188	1113	344	4110
	# classes	2	3	2	5	3	2	2	2	2
	Avg # nodes	19.8	13.0	429.6	508.5	74.5	17.9	39.1	25.5	29.8
Baselines	WL subtree	73.8 ± 3.9	50.9 ± 3.8	81.0 ± 3.1	52.5 ± 2.1	78.9 ± 1.9	90.4 ± 5.7	75.0 ± 3.1	59.9 ± 4.3	**86.0 ± 1.8** *
	DCNN	49.1	33.5	–	–	52.1	67.0	61.3	56.6	62.6
	PATCHYSAN	71.0 ± 2.2	45.2 ± 2.8	86.3 ± 1.6	49.1 ± 0.7	72.6 ± 2.2	**92.6 ± 4.2** *	75.9 ± 2.8	60.0 ± 4.8	78.6 ± 1.9
	DGCNN	70.0	47.8	–	–	73.7	85.8	75.5	58.6	74.4
	AWL	74.5 ± 5.9	51.5 ± 3.6	87.9 ± 2.5	54.7 ± 2.9	73.9 ± 1.9	87.9 ± 9.8	–	–	–
GNN variants	SUM–MLP (**GIN-0**)	**75.1 ± 5.1**	**52.3 ± 2.8**	**92.4 ± 2.5**	**57.5 ± 1.5**	**80.2 ± 1.9**	**89.4 ± 5.6**	**76.2 ± 2.8**	**64.6 ± 7.0**	**82.7 ± 1.7**
	SUM–MLP (**GIN-ϵ**)	**74.3 ± 5.1**	**52.1 ± 3.6**	**92.2 ± 2.3**	**57.0 ± 1.7**	**80.1 ± 1.9**	**89.0 ± 6.0**	**75.9 ± 3.8**	63.7 ± 8.2	**82.7 ± 1.6**
	SUM–1-LAYER	74.1 ± 5.0	**52.2 ± 2.4**	90.0 ± 2.7	55.1 ± 1.6	**80.6 ± 1.9**	**90.0 ± 8.8**	**76.2 ± 2.6**	63.1 ± 5.7	82.0 ± 1.5
	MEAN–MLP	73.7 ± 3.7	**52.3 ± 3.1**	50.0 ± 0.0	20.0 ± 0.0	79.2 ± 2.3	83.5 ± 6.3	75.5 ± 3.4	**66.6 ± 6.9**	80.9 ± 1.8
	MEAN–1-LAYER (GCN)	74.0 ± 3.4	51.9 ± 3.8	50.0 ± 0.0	20.0 ± 0.0	79.0 ± 1.8	85.6 ± 5.8	76.0 ± 3.2	64.2 ± 4.3	80.2 ± 2.0
	MAX–MLP	73.2 ± 5.8	51.1 ± 3.6	–	–	–	84.0 ± 6.1	76.0 ± 3.2	64.6 ± 10.2	77.8 ± 1.3
	MAX–1-LAYER (GraphSAGE)	72.3 ± 5.3	50.9 ± 2.2	–	–	–	85.1 ± 7.6	75.9 ± 3.2	63.9 ± 7.7	77.7 ± 1.5

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- Tight bounds on the representational capacity of popular GNN variants. (cf. WL test)
- Designed a provably maximally powerful GNN under the neighborhood aggregation framework (*Graph Isomorphism Network*)

Future research

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- Better understanding of the optimization landscape

Outline

Summary of GNNs

Here is a summary of "major" GNNs[27]: (next page)

[27] Zonghan Wu et al. "A Comprehensive Survey on Graph Neural Networks". In: *arXiv e-prints* (Jan. 2019). arXiv: 1901.00596 [cs.LG].

Summary of GNNs

(1: RecGNN, 2: Spectral-based ConvGNN, 3: Spatial-based ConvGNN)

Method	Category	Time Complexity	Features
GNN[18]	1	$O(m)$	Information diffusion mechanism, updates nodes' states until a stable equilibrium is reached.
Spectral CNN[4]	2	$O(n^3)$	Treats the filters as a set of learnable parameters.
ChebNet[6]	2	$O(m)$	Approximates the filger by Chebyshev polynomials of the diagonal matrix of eigenvalues.
GCN[13]	2	$O(m)$	First-order approximation of ChebNet
AGCN[15]	2	$O(n^2)$	Learns hidden structural relations by using the residual graph adjacency matrix through learnable metric.
DualGCN[30]	2	$O(m)$	Introduces dual graph convolutional architecture with two graph convolutional layers in parallel.
NN4G[16]	3	$O(m)$	Performs graph convolutions by summing up a node's neighborhood information directly.
DCNN[1]	3	$O(n^2)$	Treats graph convolutions as a diffusion process
MPNN[8]	3	$O(m)$	Treats graph convolutions as a message passing process.
GraphSAGE[9]	3	-	Sampling of fixed number of neighbors for each node.
GIN[24]	3	$O(m)$	This paper!

Outline

References I

[1] James Atwood and Don Towsley. "Diffusion-Convolutional Neural Networks". In: *Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain*. 2016, pp. 1993–2001.

[2] László Babai. "Graph isomorphism in quasipolynomial time [extended abstract]". In: *Proceedings of the 48th Annual ACM SIGACT Symposium on Theory of Computing, STOC 2016, Cambridge, MA, USA, June 18-21, 2016*. 2016, pp. 684–697.

[3] László Babai and Ludek Kucera. "Canonical Labelling of Graphs in Linear Average Time". In: *20th Annual Symposium on Foundations of Computer Science, San Juan, Puerto Rico, 29-31 October 1979*. 1979, pp. 39–46.

[4] Joan Bruna et al. "Spectral Networks and Locally Connected Networks on Graphs". In: *2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings*. 2014.

[5] Jin-yi Cai, Martin Fürer, and Neil Immerman. "An optimal lower bound on the number of variables for graph identifications". In: *Combinatorica* 12.4 (1992), pp. 389–410.

[6] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. "Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering". In: *Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain*. 2016, pp. 3837–3845.

[7] Thomas Gärtner, Peter A. Flach, and Stefan Wrobel. "On Graph Kernels: Hardness Results and Efficient Alternatives". In: *Computational Learning Theory and Kernel Machines, 16th Annual Conference on Computational Learning Theory and 7th Kernel Workshop, COLT/Kernel 2003, Washington, DC, USA, August 24-27, 2003, Proceedings*. 2003, pp. 129–143.

[8] Justin Gilmer et al. "Neural Message Passing for Quantum Chemistry". In: *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*. 2017, pp. 1263–1272.

[9] William L. Hamilton, Zhitao Ying, and Jure Leskovec. "Inductive Representation Learning on Large Graphs". In: *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA*. 2017, pp. 1024–1034.

References II

[10] Kurt Hornik. "Approximation capabilities of multilayer feedforward networks". In: *Neural Networks* 4.2 (1991), pp. 251–257.

[11] Kurt Hornik, Maxwell B. Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators". In: *Neural Networks* 2.5 (1989), pp. 359–366.

[12] Hisashi Kashima, Koji Tsuda, and Akihiro Inokuchi. "Marginalized Kernels Between Labeled Graphs". In: *Machine Learning, Proceedings of the Twentieth International Conference (ICML 2003), August 21-24, 2003, Washington, DC, USA*. 2003, pp. 321–328.

[13] Thomas N. Kipf and Max Welling. "Semi-Supervised Classification with Graph Convolutional Networks". In: *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*. 2017.

[14] Tao Lei et al. "Deriving Neural Architectures from Sequence and Graph Kernels". In: *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*. 2017, pp. 2024–2033.

[15] Ruoyu Li et al. "Adaptive Graph Convolutional Neural Networks". In: *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans, Louisiana, USA, February 2-7, 2018*. 2018, pp. 3546–3553.

[16] Alessio Micheli. "Neural Network for Graphs: A Contextual Constructive Approach". In: *IEEE Trans. Neural Networks* 20.3 (2009), pp. 498–511.

[17] Franco Scarselli et al. "Computational Capabilities of Graph Neural Networks". In: *IEEE Trans. Neural Networks* 20.1 (2009), pp. 81–102.

[18] Franco Scarselli et al. "The Graph Neural Network Model". In: *IEEE Trans. Neural Networks* 20.1 (2009), pp. 61–80.

References III

[19] Nino Shervashidze and Karsten M. Borgwardt. "Fast subtree kernels on graphs". In: *Advances in Neural Information Processing Systems 22: 23rd Annual Conference on Neural Information Processing Systems 2009. Proceedings of a meeting held 7-10 December 2009, Vancouver, British Columbia, Canada*. 2009, pp. 1660–1668.

[20] Nino Shervashidze et al. "Weisfeiler-Lehman Graph Kernels". In: *J. Mach. Learn. Res.* 12 (2011), pp. 2539–2561.

[21] S. V. N. Vishwanathan et al. "Graph Kernels". In: *J. Mach. Learn. Res.* 11 (2010), pp. 1201–1242.

[22] Boris Weisfeiler and Andrei A. Lehman. "A reduction of a graph to a canonical form and an algebra arising during this reduction". In: *Nauchno-Technicheskaya Informatsia* 2.9 (1968), pp. 12–16.

[23] Zonghan Wu et al. "A Comprehensive Survey on Graph Neural Networks". In: *arXiv e-prints* (Jan. 2019). arXiv: 1901.00596 [cs.LG].

[24] Keyulu Xu et al. "How Powerful are Graph Neural Networks?" In: *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. 2019.

[25] Keyulu Xu et al. "Representation Learning on Graphs with Jumping Knowledge Networks". In: *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*. 2018, pp. 5449–5458.

[26] Pinar Yanardag and S. V. N. Vishwanathan. "Deep Graph Kernels". In: *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Sydney, NSW, Australia, August 10-13, 2015*. 2015, pp. 1365–1374.

[27] Zhitao Ying et al. "Hierarchical Graph Representation Learning with Differentiable Pooling". In: *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, 3-8 December 2018, Montréal, Canada*. 2018, pp. 4805–4815.

[28] Manzil Zaheer et al. "Deep Sets". In: *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA*. 2017, pp. 3391–3401.

References IV

[29] Muhan Zhang et al. "An End-to-End Deep Learning Architecture for Graph Classification". In: *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans, Louisiana, USA, February 2-7, 2018*. 2018, pp. 4438–4445.

[30] Chenyi Zhuang and Qiang Ma. "Dual Graph Convolutional Networks for Graph-Based Semi-Supervised Classification". In: *Proceedings of the 2018 World Wide Web Conference*. WWW '18. Lyon, France: International World Wide Web Conferences Steering Committee, 2018, pp. 499–508. ISBN: 978-1-4503-5639-8.

Thank you for your attention! Any questions?