How Powerful are Graph Neural Networks?

(EE531 Final Project - Graph)

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

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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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A set of graphs $\{G_1, \ldots, G_N\} \subset \mathcal{G}$ is given, along with their labels $\{y_1, \ldots, y_N\} \subset \mathcal{Y}$.
Goal: Learn a representation vector h_G of G such that $y_G = f(h_G)$ i.e. such that G's label can be predicted.

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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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- GraphSAGE (Hamilton *et al.*, 2017):

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- Graph Convolutional Networks, or GCN (Kipf & Welling, 2017):

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

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- READOUT can be a simple permutation invariant function, or something more sophisticated (cf. Ying *et al.*, 2018; Zhang *et al.*, 2018)

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- This seemingly harmless problem has harassed researchers for decades!

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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 of graph isomorphism (Weisfeiler & Lehman, 1968), or simply WL test, is a combinatorial algorithm for GI.
- WL test is proved to be successful (and computationally efficient) in isomorphism testing for a broad class of graphs (Babai & Kucera, 1979)
- There are some cases (ex. regular graphs) when the WL test fails (Cai *et at.*, 1992)

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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

Let (G, l) be a labeled graph i.e. a graph G with an endowed node coloring $l : V(G) \to \Sigma$. (Σ: arbitrary codomain)

- At t-th iteration ($t \geq 0$), the 1-WL computes a node coloring $c_l^{(t)} : V(G) \to \Sigma$, which depends on the previous node coloring:

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

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

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- 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

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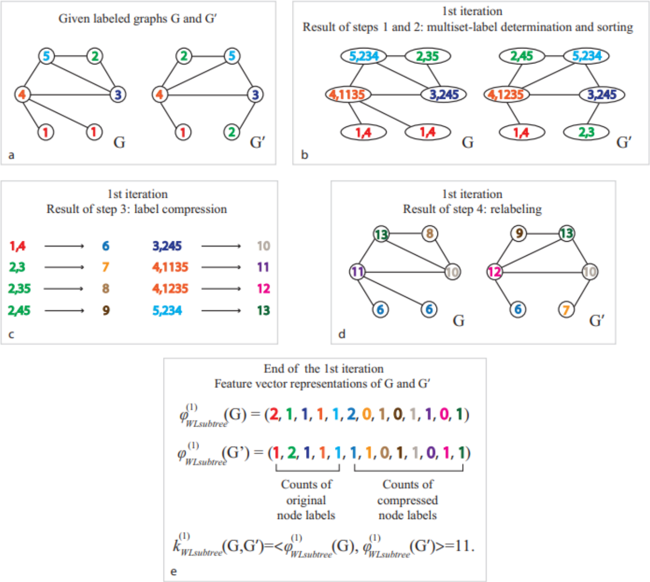
- Weisfeiler-Lehman subtree kernel (Shervashidze *et al.*, 2011): counts common *original and compressed labels* (resulting from 1-dim WL test) in two graphs.

WL subtree kernel



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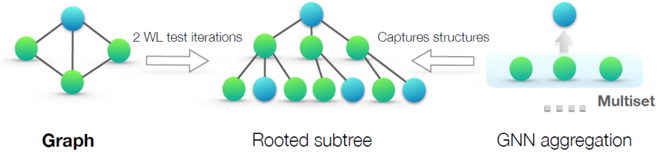
- The kernel uses the *counts of node labels* at different iterations of the WL test as the *feature vector* of a graph.
- Intuitively, a node's label at the k-th iteration of the 1-dim WL test represents a subtree structure of height k rooted at the node.



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

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

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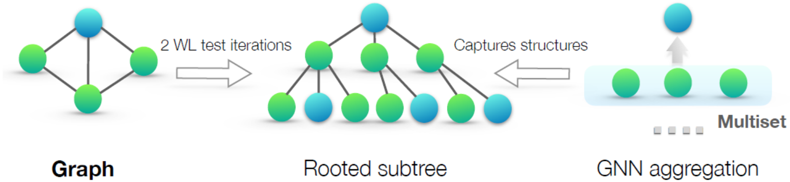

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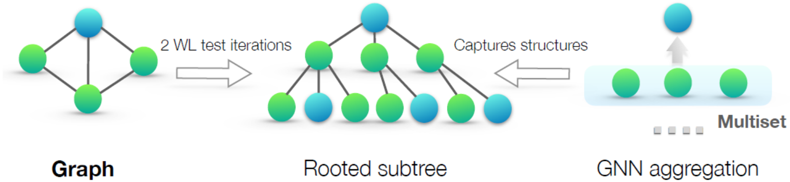

- GNN: recursive update of each node's feature vector *i.e.* its rooted subtree structure!
- Wl test: also results in rooted subtree! structure!
- Assign each feature vector a unique label from a countable universe.
- Then, feature vectors of a set of neighboring nodes form a *multiset*

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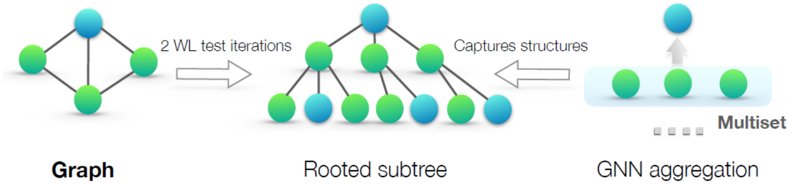

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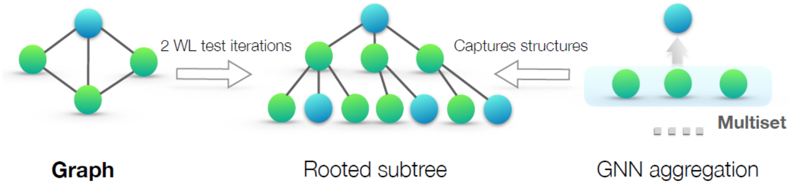

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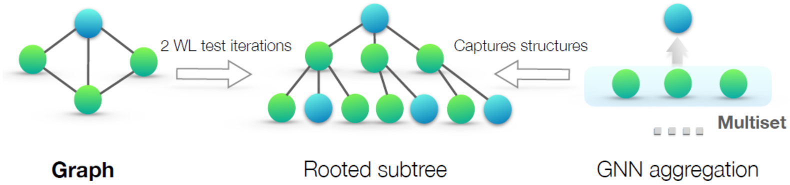

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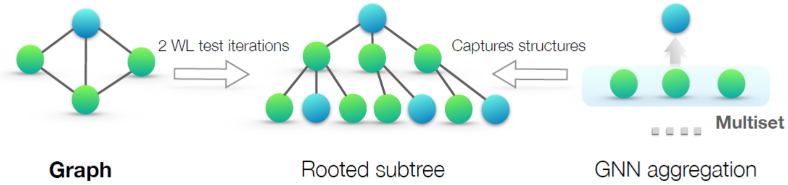

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- GNN's aggregation scheme: class of functions over multisets that their neural networks can represent

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Lemma 2

Let G_1 and G_2 be any two non-isomorphic graphs.
If a graph neural network $\mathcal{A} : \mathcal{G} \to \mathbb{R}^d$ maps G_1 and G_2 to different embeddings, the Weisfeiler-Lehman graph isomorphism test also decides G_1 and G_2 are not isomorphic.

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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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- GNNs can not only discriminate different structures, but can also learn to map similar graph structures to similar embeddings and capture dependencies between graph structures.
- Especially useful when co-occurence of subtrees is sparse across different graphs, or there are noisy edges and node features.

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- Let us develop a simple architecture, GIN!

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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!

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- 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.
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- We can use MLPs to model and learn f and φ. (also, make ϵ a learnable parameter, or a fixed scalar)
- Then, GIN updates node representations as:

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

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- To do that, let us use information from all depths/iterations of the model (inspired by Jumping Knowledge Networks (Xu *et al.*, 2018)):

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

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- 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.

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- What if the sum $h(X) = \sum_{x \in X} f(x)$ is replaced by mean/max pooling?

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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 $\mathscr{C}(X)$ for all compact subsets X of $\mathbb{R}^k$.*

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- Every continuous function can be approximated arbitrarily closely by a multi-layer perceptron with just one hidden layer.
- 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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Lemma 7

There exist finite multisets $X_1 \neq X_2$ so that for any linear mapping W, $\sum_{x \in X_1} \mathrm{ReLU}(Wx) = \sum_{x \in X_2} \mathrm{ReLU}(Wx)$

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- 1-layer perceptrons can behave much like linear mappings, so the GNN layers degenerate into simply summing over neighborhood features.
- Proof idea: bias term is lacking in the linear mapping.
- Unlike models using MLPs, 1-layer perceptron (even with the bias term) is *not a universal approximator* of multiset functions.
- Even if GNNs with 1-layer perceptrons can be injective to some degree, such embeddings may not adequately capture structural similarity. (may be difficult for simple classifiers to fit)

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- As described previously, Graph Convolutional Network (GCN; Kipf & Welling, 2017) takes the form:

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

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- How can we characterize the structures that GCN can or cannot capture?

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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*.

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Summary

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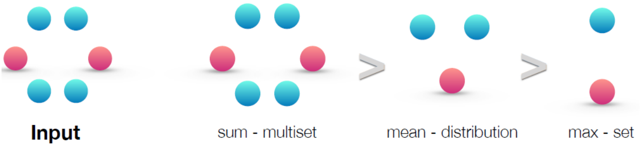

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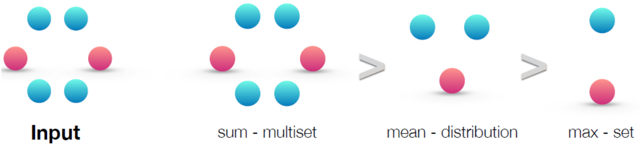

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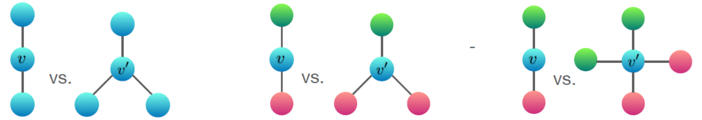

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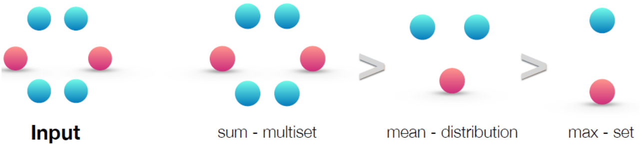

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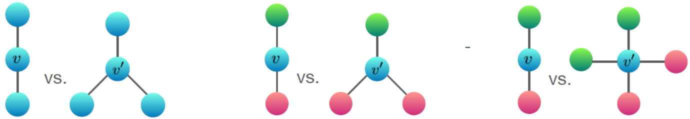

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- Mean aggregator (as in GCN) captures the statistical and distributional information of the graph.
- Max-pooling aggregator (as in GraphSAGE) captures the representative elements of the graph, or its skeleton

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Experiments

The goal of the experiment is to compare the training and test performance of GIN and less powerful GNN variants.

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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 (Yanardag & Vishwanathan, 2015):
  - 4 bioinformatics datasets (*MUTAG, PTC, NCI1, PROTEINS*)
  - 5 social network datasets (*COLLAB, IMDB-BINARY, IMDB-MULTI, REDDIT-BINARY, REDDIT-MULTI5K*)

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- The baselines used were:
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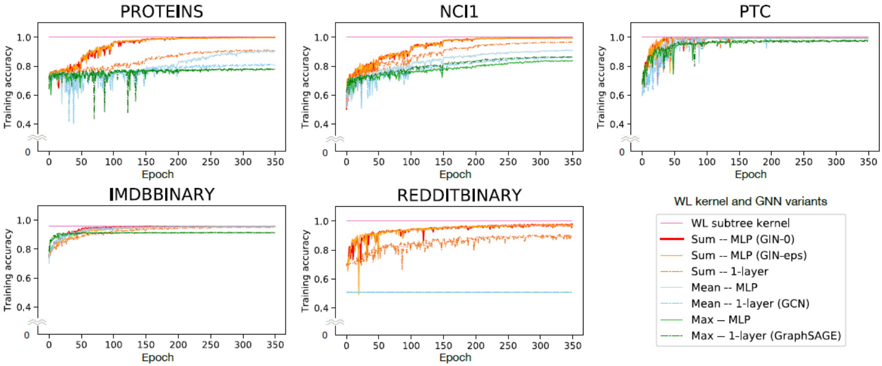
  - Deep learning architectures i.e. DCNN, PATCHY-SAN, DGCNN
  - AWL

Results


PROTEINS
NCI1
PTC
IMDBBINARY
REDDITBINARY
Training accuracy
Epoch
WL kernel and GNN variants
WL subtree kernel
Sum -- MLP (GIN-0)
Sum -- MLP (GIN-eps)
Sum -- 1-layer
Mean -- MLP
Mean -- 1-layer (GCN)
Max – MLP
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	$\mathbf{86.0 \pm 1.8}$ *
	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	$\mathbf{92.6 \pm 4.2}$ *	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**)	$\mathbf{75.1 \pm 5.1}$	$\mathbf{52.3 \pm 2.8}$	$\mathbf{92.4 \pm 2.5}$	$\mathbf{57.5 \pm 1.5}$	$\mathbf{80.2 \pm 1.9}$	$\mathbf{89.4 \pm 5.6}$	$\mathbf{76.2 \pm 2.8}$	$\mathbf{64.6 \pm 7.0}$	$\mathbf{82.7 \pm 1.7}$
	Sum–MLP (**GIN-ϵ**)	$\mathbf{74.3 \pm 5.1}$	$\mathbf{52.1 \pm 3.6}$	$\mathbf{92.2 \pm 2.3}$	$\mathbf{57.0 \pm 1.7}$	$\mathbf{80.1 \pm 1.9}$	$\mathbf{89.0 \pm 6.0}$	$\mathbf{75.9 \pm 3.8}$	63.7 ± 8.2	$\mathbf{82.7 \pm 1.6}$
	Sum–1-Layer	74.1 ± 5.0	$\mathbf{52.2 \pm 2.4}$	90.0 ± 2.7	55.1 ± 1.6	$\mathbf{80.6 \pm 1.9}$	$\mathbf{90.0 \pm 8.8}$	$\mathbf{76.2 \pm 2.6}$	63.1 ± 5.7	82.0 ± 1.5
	Mean–MLP	73.7 ± 3.7	$\mathbf{52.3 \pm 3.1}$	50.0 ± 0.0	20.0 ± 0.0	79.2 ± 2.3	83.5 ± 6.3	75.5 ± 3.4	$\mathbf{66.6 \pm 6.9}$	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

Outline

1 Introduction
2 Preliminaries
- GNNs
- WL test
- (Overview of) Theoretical Framework

3 Representational capacity of GNNs
4 Graph Isomorphism Network (GIN)
5 Less powerful, but still interesting GNNs
- 1-Layer Perceptrons
- GCN
- GraphSAGE

6 Experiments
7 Summary
8 Future Research
9 Roles and Responsibilities

Summary

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- Tight bounds on the representational capacity of popular GNN variants. (cf. WL test)

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- Theoretical foundations for reasoning about the expressive power of GNNS
- 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*)

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- Go beyond neighborhood aggregation
- Understand/improve the generalization properties of GNNs
- What if the node features are continuous (uncountable)?
- Better understanding of the optimization landscape

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Roles and Responsibilities

- Junghyun Lee prepared all the materials.

Roles and Responsibilities

- Junghyun Lee prepared all the materials.
- And as requested, here is a picture of myself:

Thank you for your attention! Any questions?