Graph Neural Networks

Johannes Lutzeyer

Advanced Deep Learning: Lecture 3

January 21, 2025

Overview of Today's Lecture

1) A Brief Review of Graph Representation Learning;

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2) Graph Neural Networks;

3) Different Approaches to Message Passing Including Recent Research;

4) Recent Advances on the Robustness of Graph Neural Networks.

Graph Representation Learning

Overall Goal: Learn "informative" representations of graph structured data

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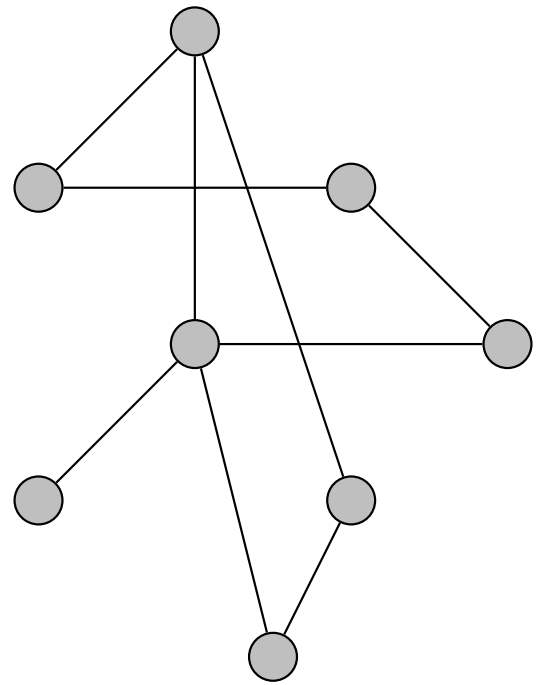

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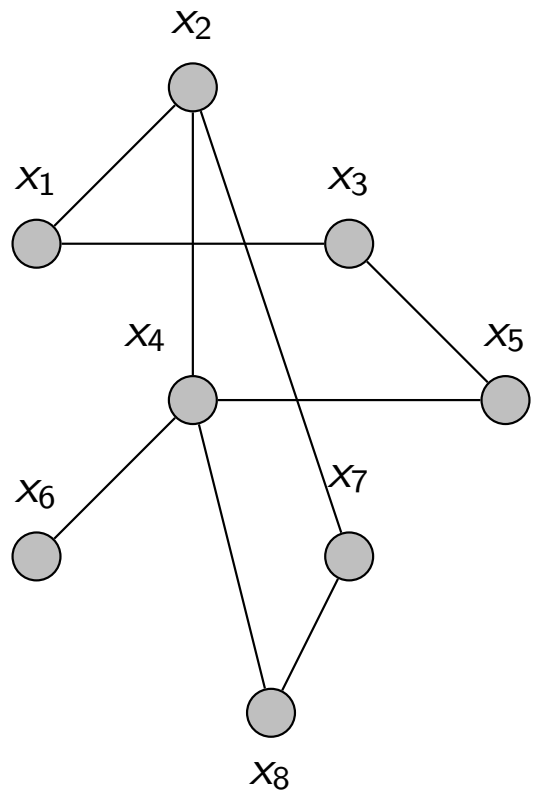

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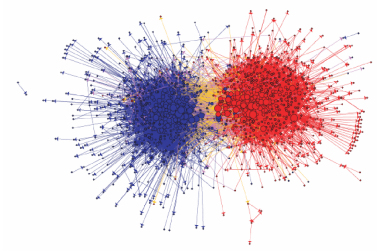

US political weblogs
(Adamic & Glance, 2005)

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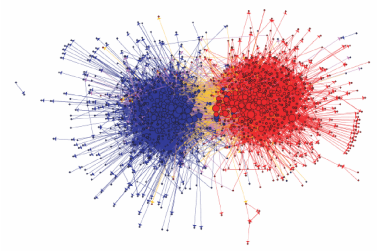

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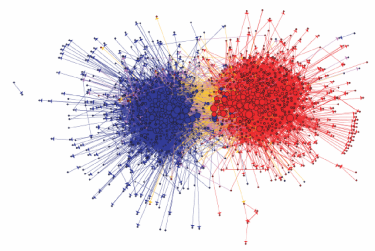

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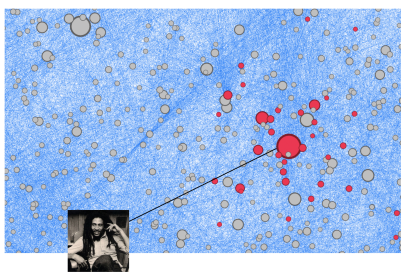

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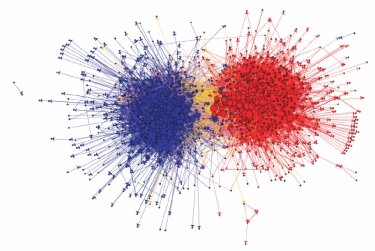

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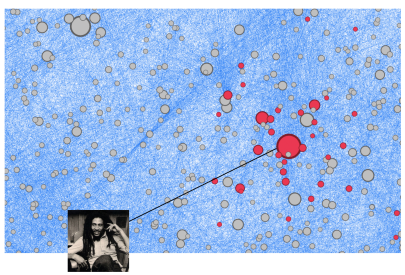

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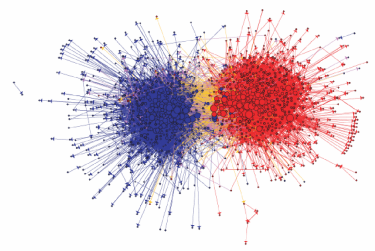

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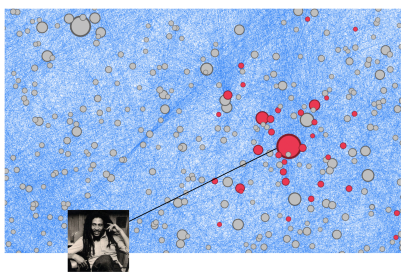

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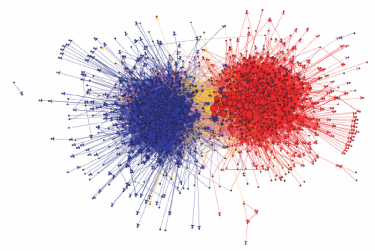

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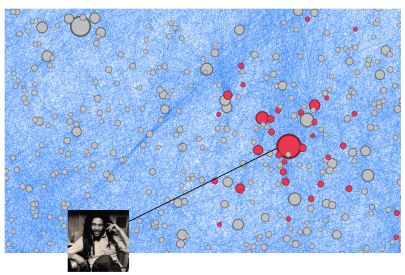

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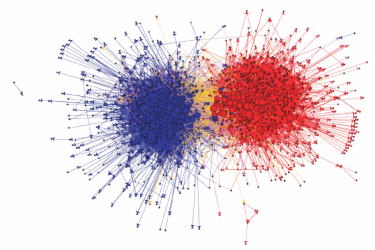

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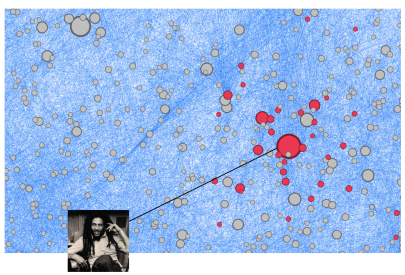

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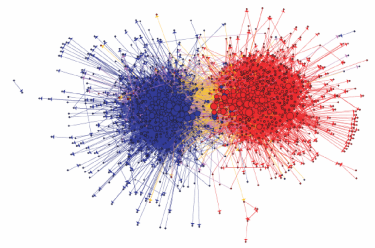

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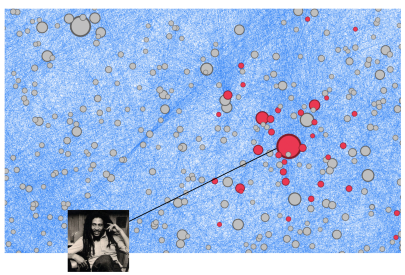

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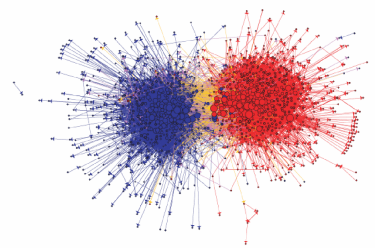

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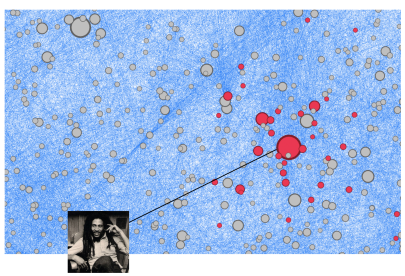
- Node and Graph Regression
- Link Prediction
- Can you think of another?



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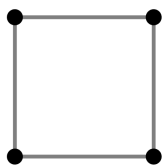
Graph Shift Operators

Definition

Graphs $G = (V, E)$ can be represented using:

- *adjacency matrix* $A \in \{0,1\}^{n \times n}$ where $A_{ij} = 1$ iff $(i,j) \in E$.



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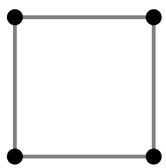

$$A = \begin{pmatrix} 0&1&0&1 \\ 1&0&1&0 \\ 0&1&0&1 \\ 1&0&1&0 \end{pmatrix} \qquad L = \begin{pmatrix} 2&-1&0&-1 \\ -1&2&-1&0 \\ 0&-1&2&-1 \\ -1&0&-1&2 \end{pmatrix}$$

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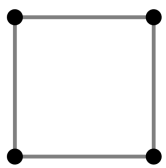

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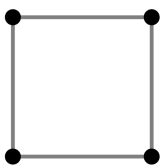

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Definition (Sandryhaila and Moura, 2013)

A matrix $S \in \mathbb{R}^{n \times n}$ is called a *Graph Shift Operator* (GSO) if it satisfies: $S_{ij} = 0$ for $i \neq j$ and $(i,j) \notin E$.

Multi Layer Perceptrons

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Here is an example of a three-layer MLP,

$$\hat{y} = \sigma\left(\mathrm{ReLU}\left(\mathrm{ReLU}\left(XW^{(1)}\right)W^{(2)}\right)W^{(3)}\right).$$

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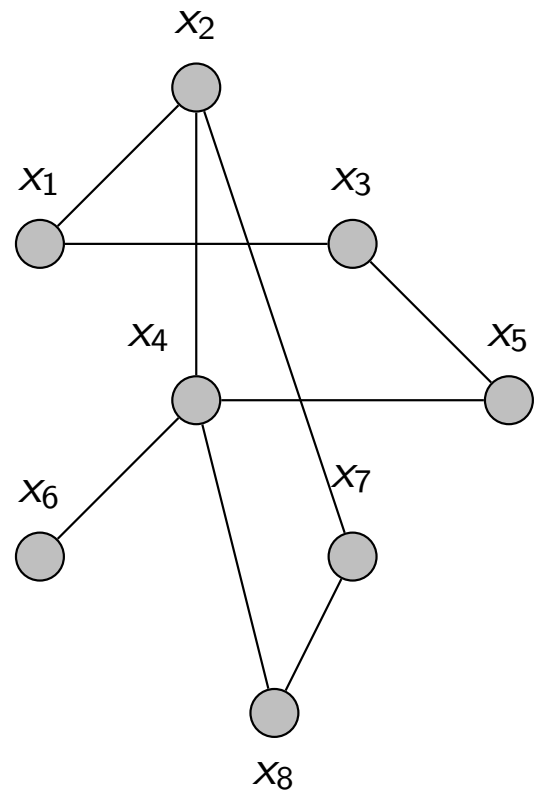

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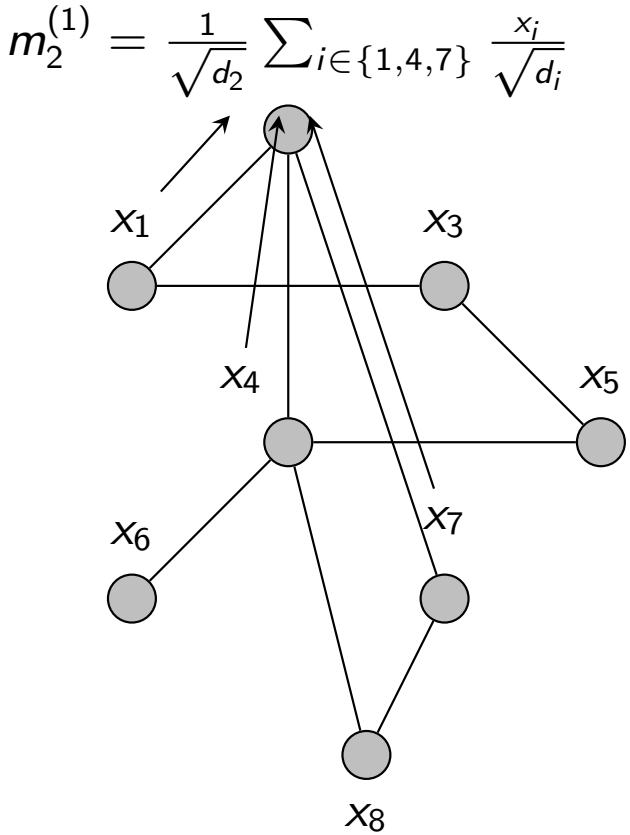
$$m_v^{(k)} = M^{(k)}\left(\left\{h_u^{(k-1)} : u \in \mathcal{N}(v)\right\}\right),$$

where

- $\mathcal{N}(v) = \{u : (u, v) \in E\}$ denotes the neighbourhood of a node v in $G = (V, E)$,
- $m_v^{(k)} \in \mathbb{R}^d$ denotes the representation of the messages received by neighbours of the node v,
- $M^{(k)}$ is a permutation-invariant function operating on sets.



E.g., the Graph Convolutional Network (GCN, Kipf and Welling, 2017)

$$\tilde{A}X,$$

where $\tilde{A} \in \mathbb{R}^{n \times n}$ and $X \in \mathbf{R}^{n \times d_0}$.

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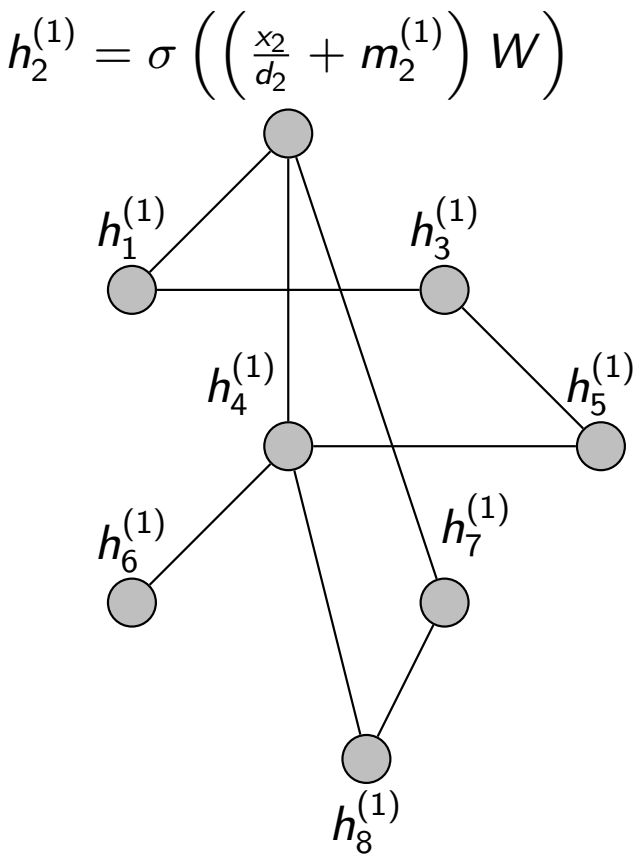
where

- $U^{(k)}$ is an often trainable update function combining $m_v^{(k)}$ and the representation of node v at the previous layer $h_v^{(k-1)}$.

E.g., the Graph Convolutional Network (GCN, Kipf and Welling, 2017)

$$H^{(1)} = \mathrm{ReLU}\left(\tilde{A}XW^{(1)}\right),$$

where $\tilde{A} \in \mathbb{R}^{n \times n}$, $X \in \mathbb{R}^{n \times d_0}$ and $W^{(1)} \in \mathbb{R}^{d_0 \times d_1}$.



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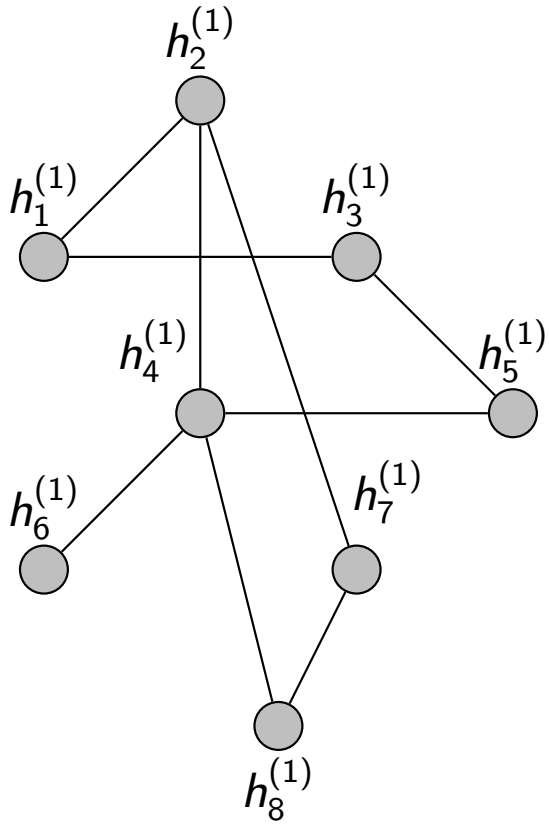


E.g., the Graph Convolutional Network (GCN, Kipf and Welling, 2017)

$$H^{(1)} = \mathrm{ReLU}\left(\tilde{A}XW^{(1)}\right),$$

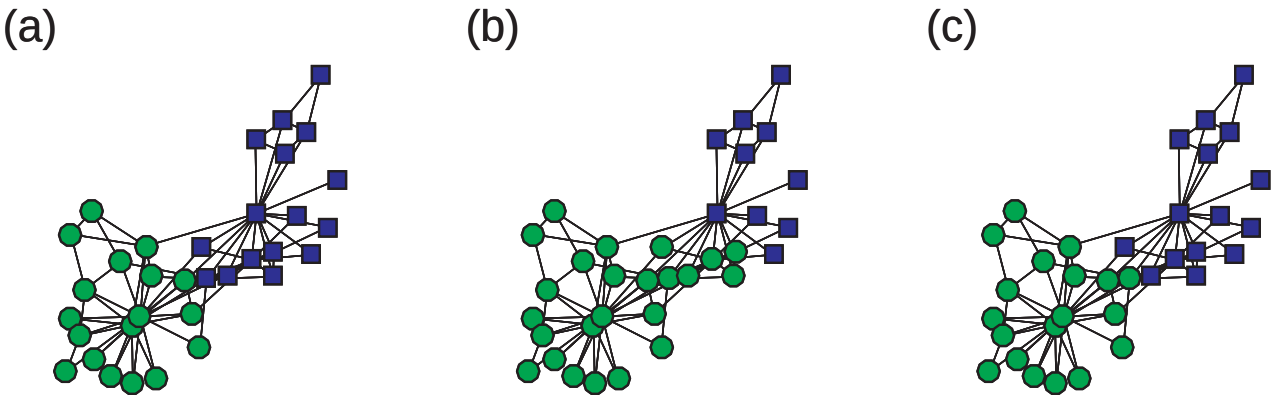
where $\tilde{A} \in \mathbb{R}^{n\times n}$, $X \in \mathbb{R}^{n\times d_0}$ and $W^{(1)} \in \mathbb{R}^{d_0\times d_1}$.

Iteratively performing the message-passing and update computations allows us to build 'deep' learning models, e.g., a 3-layer GCN

$$\hat{y} = \sigma\left(\tilde{A}\,\mathrm{ReLU}\left(\tilde{A}\,\mathrm{ReLU}\left(\tilde{A}XW^{(1)}\right)W^{(2)}\right)W^{(3)}\right).$$

GSOs in Graph Representation Learning

- Spectral clustering:



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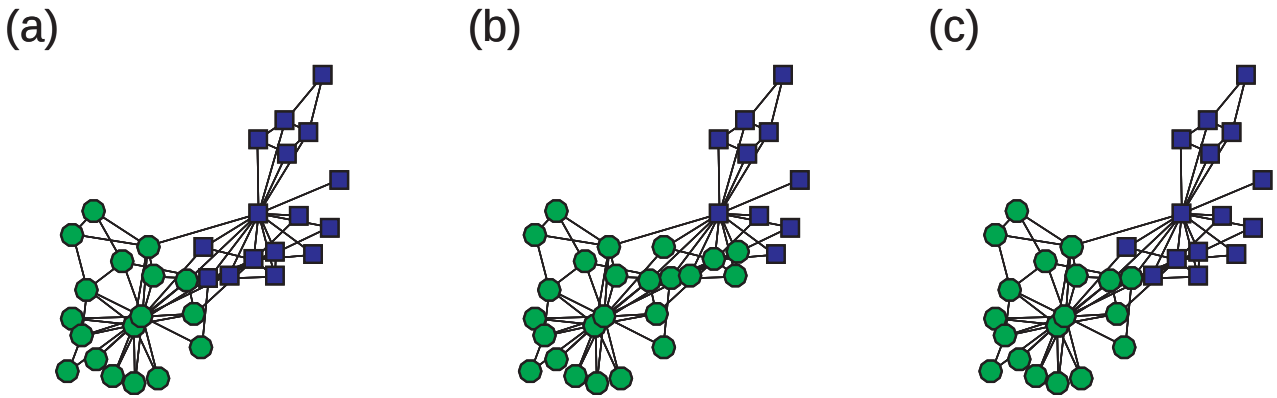

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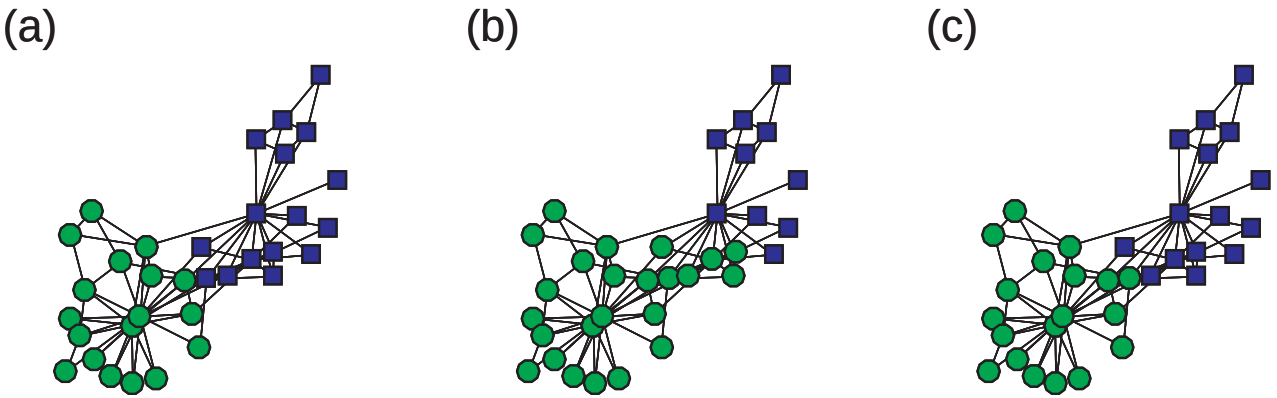

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In Message Passing Neural Networks, the choice of message passing function corresponds to a choice of GSO.

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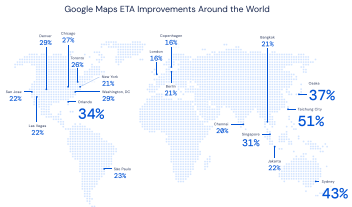

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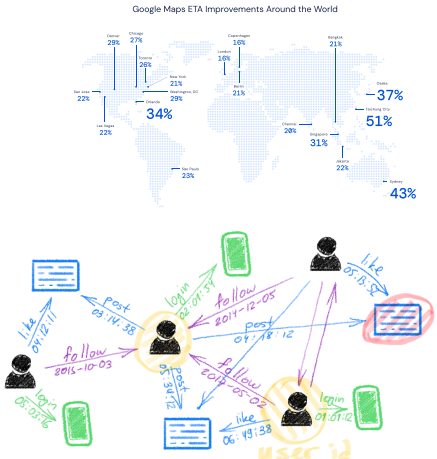

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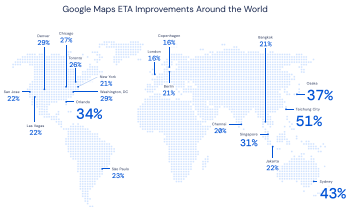

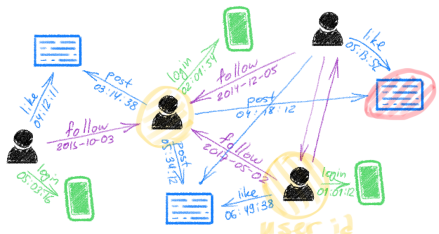

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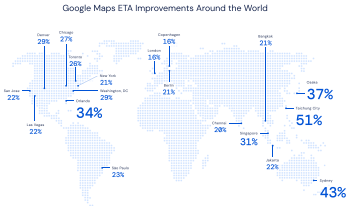

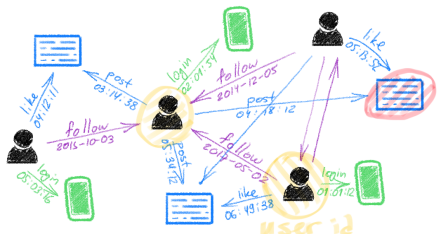

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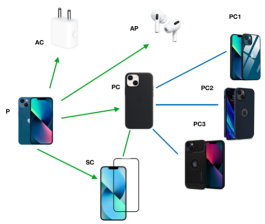

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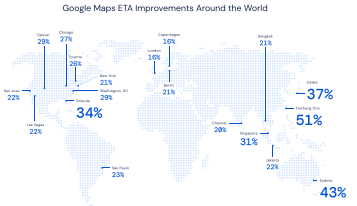

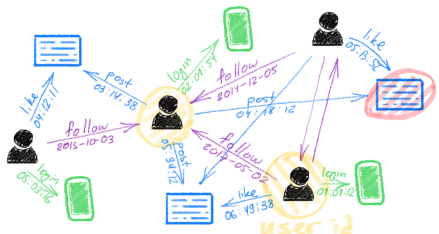

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The message passing step is a defining component of GNNs.

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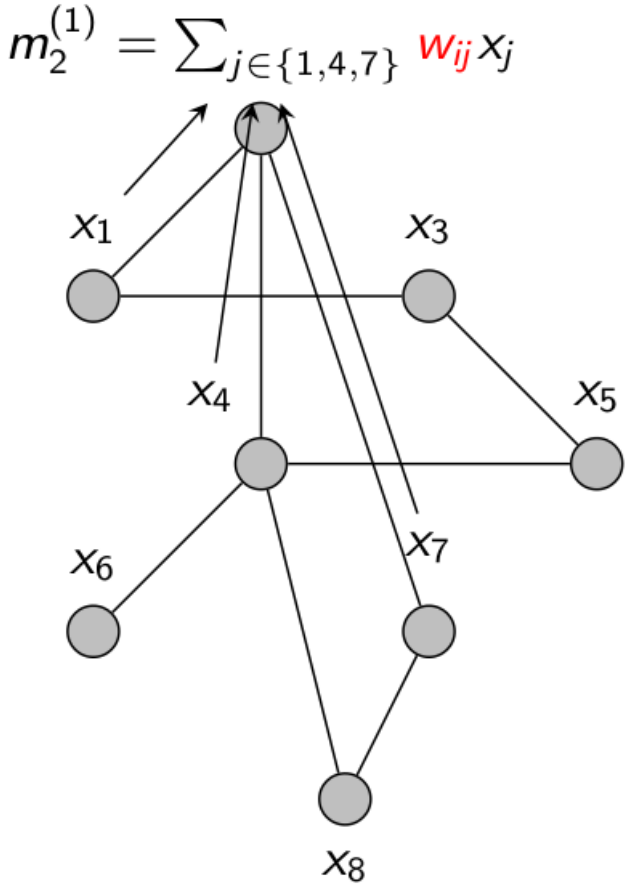
Topic for the Upcoming Segment of Today's Lecture

Categorise several existing GNNs by their message passing step.

Different Approaches to Message Passing

- Fixed Graph



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  - PGSO-GNN (Dasoulas et al., 2021, ICLR)

    Message-Passing Operation:
    $\gamma(A, \mathcal{S}) = (m_1 D_a^{e_1} + m_2 D_a^{e_2} A_a D_a^{e_3} + m_3 I_n) X,$
    where $A_a = A + aI_n$, $D_a = \text{Diag}(A_a \mathbf{1}_n)$ and
    $(m_1, m_2, m_3, e_1, e_2, e_3, a)$ are scalar, *trainable* parameters.

$\mathcal{S} = (m_1, m_2, m_3, e_1, e_2, e_3, a)$	**Operator**	**Description**
$(0, 1, 0, 0, 0, 0, 0)$	A	Adjacency matrix and Summation Aggregation Operator of GNNs
$(1, -1, 0, 1, 0, 0, 0)$	$D - A$	Unnormalised Laplacian matrix L
$(1, 1, 0, 1, 0, 0, 0)$	$D + A$	Signless Laplacian matrix Q (Cvetkovic et al., 1997)
$(0, -1, 1, 0, -1, 0, 0)$	$I_n - D^{-1}A$	Random-walk Normalised Laplacian L_{rw}
$(0, -1, 1, 0, -\frac{1}{2}, -\frac{1}{2}, 0)$	$I_n - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$	Symmetric Normalised Laplacian L_{sym}
$(0, 1, 0, 0, -\frac{1}{2}, -\frac{1}{2}, 1)$	$D_1^{-\frac{1}{2}} A_1 D_1^{-\frac{1}{2}}$	Normalised Adjacency matrix of GCNs (Kipf and Welling, 2017)
$(0, 1, 0, 0, -1, 0, 0)$	$D^{-1}A$	Mean Aggregation Operator of GNNs (Xu et al., 2019)

PGSO in Graph Neural Networks

Notation:

- $\phi(A) : [0,1]^{n \times n} \to \mathbb{R}^{n \times n}$ denotes a non-parametrised function of A.
- $\mathcal{M}(\phi(A), X)$ denotes a GNN model.

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Utilization of PGSO in GNNs

1. **GNN-PGSO**: $\mathcal{M}(\phi(A), X) \to \mathcal{M}'(\gamma(A, \mathcal{S}), X)$.
2. **GNN-mPGSO (multi-PGSO)**: $\mathcal{M}(\phi(A), X) \to \mathcal{M}''(\gamma^{[K]}(A, \mathcal{S}^{[K]}), X)$, where $\gamma^{[K]}(A, \mathcal{S}^{[K]}) = [\gamma(A, \mathcal{S}^1), \ldots, \gamma(A, \mathcal{S}^K)]$.

- Put simply, we **replace** the GSO used in a GNN model by $\gamma(A, \mathcal{S})$.

Convolutions and Message-Passing

- Examples of utilisation of GNN-PGSO models

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where $W^{(l)}$ is a weight matrix and σ is a non-linear activation function. The GCN-PGSO and GCN-mPGSO models are defined, respectively, as

$$H^{(l+1)} = \sigma\big(\gamma(A, \mathcal{S}) H^{(l)} W^{(l)}\big) \text{ and } H^{(l+1)} = \sigma\big(\gamma(A, \mathcal{S}^l) H^{(l)} W^{(l)}\big).$$

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where ϵ_{ij} are edge weights defined as $\epsilon_{ij} = m_2 \left(D_a\right)_i^{e_2} \left(D_a\right)_j^{e_3}$.

Results on Real-world Datasets

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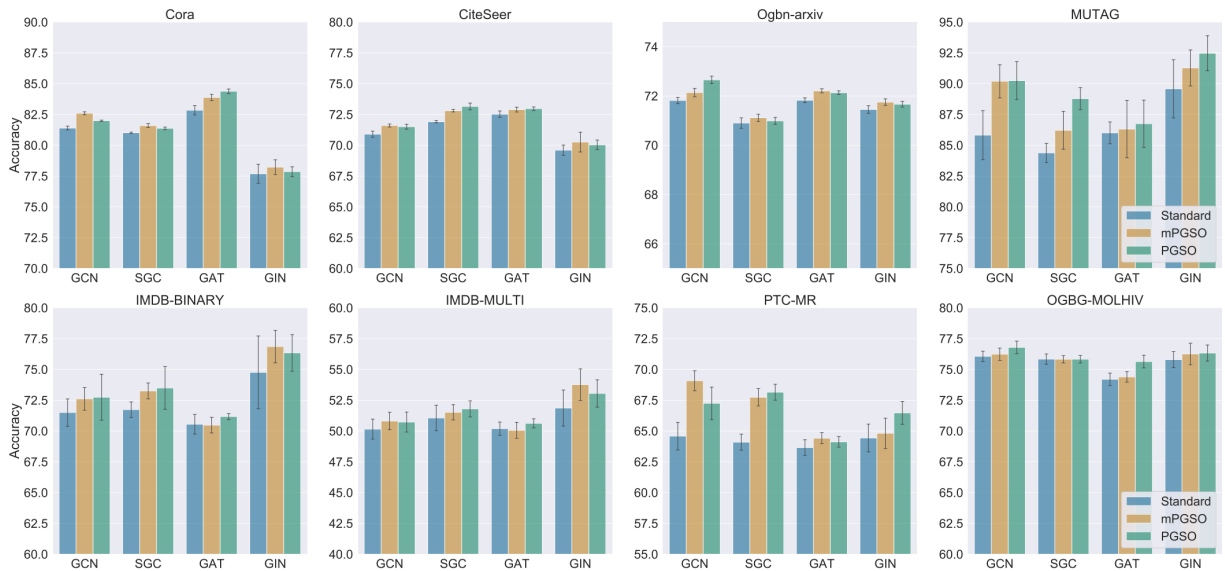

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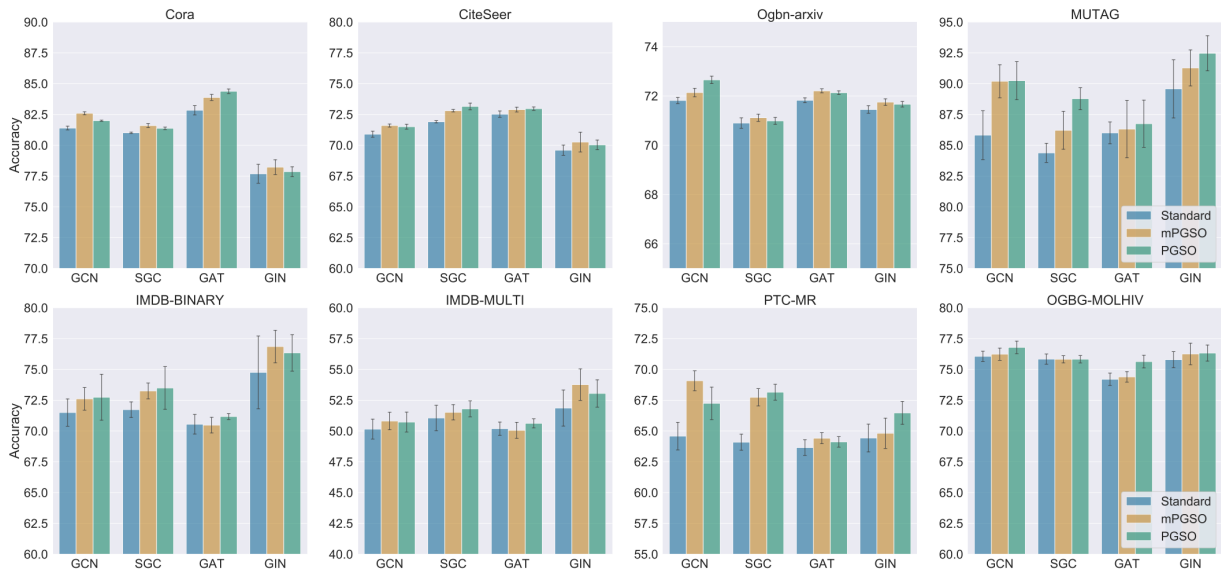

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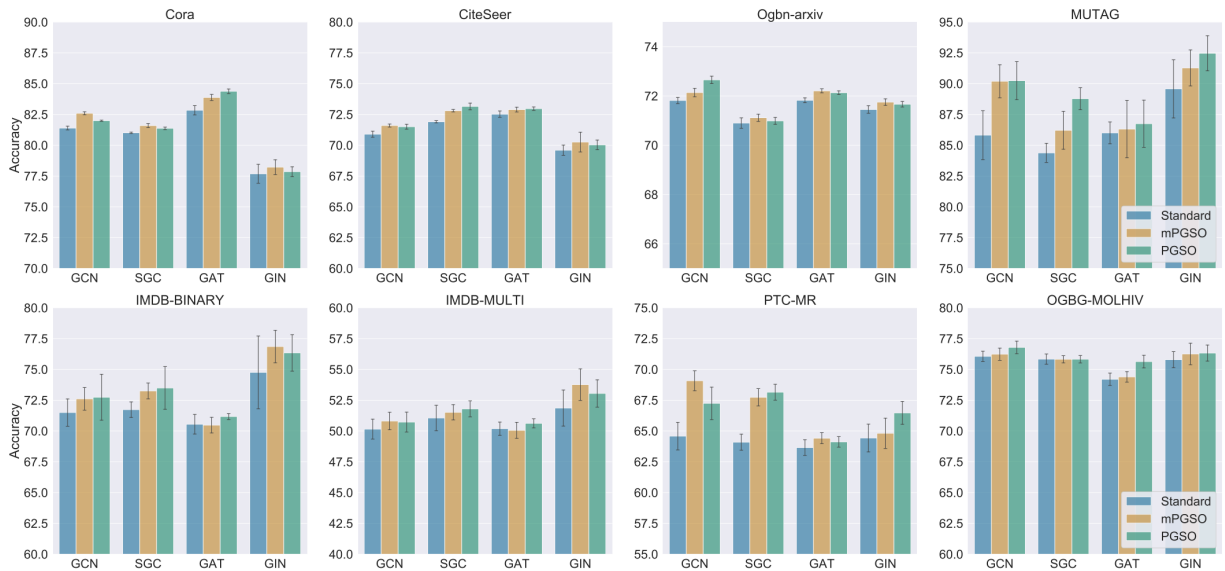

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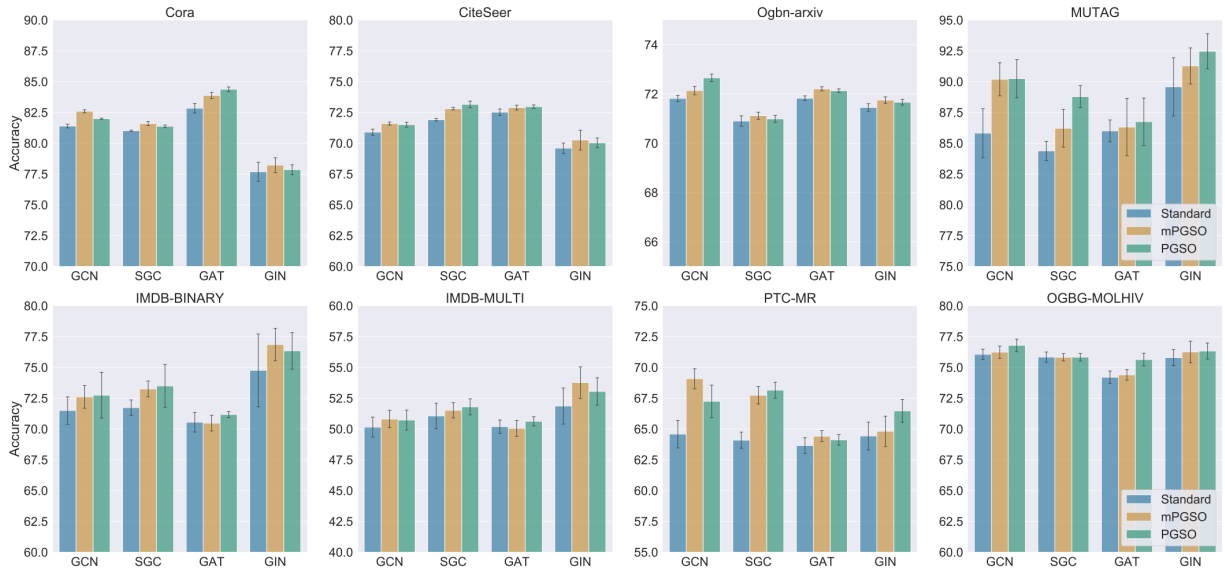

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- Our code is publicly available: https://github.com/gdasoulas/PGSO.

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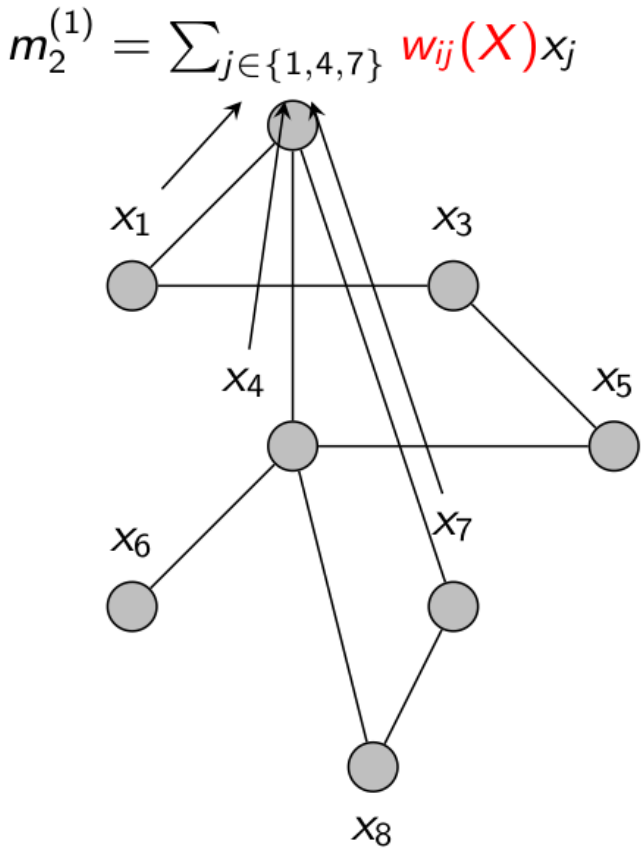
- Feature-Dependent Reweighting of Edges



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    Do you notice something in the arrangement of the weight matrices?

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    where $(K)_{ij} = \begin{cases} 0, & \text{for } A_{ij} = 0; \\ x_i^T x_j, & \text{for } A_{ij} \neq 0. \end{cases}$

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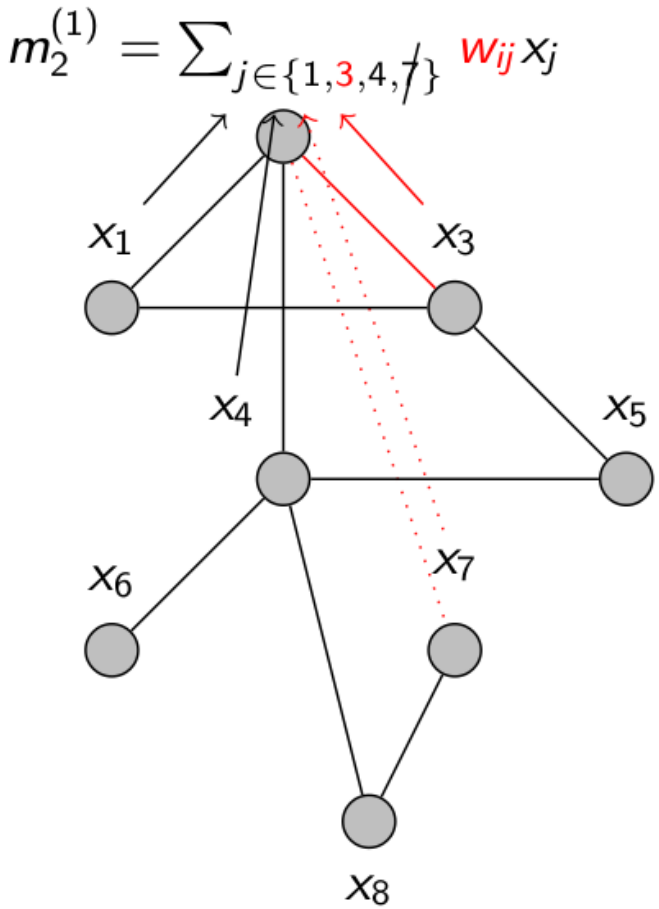

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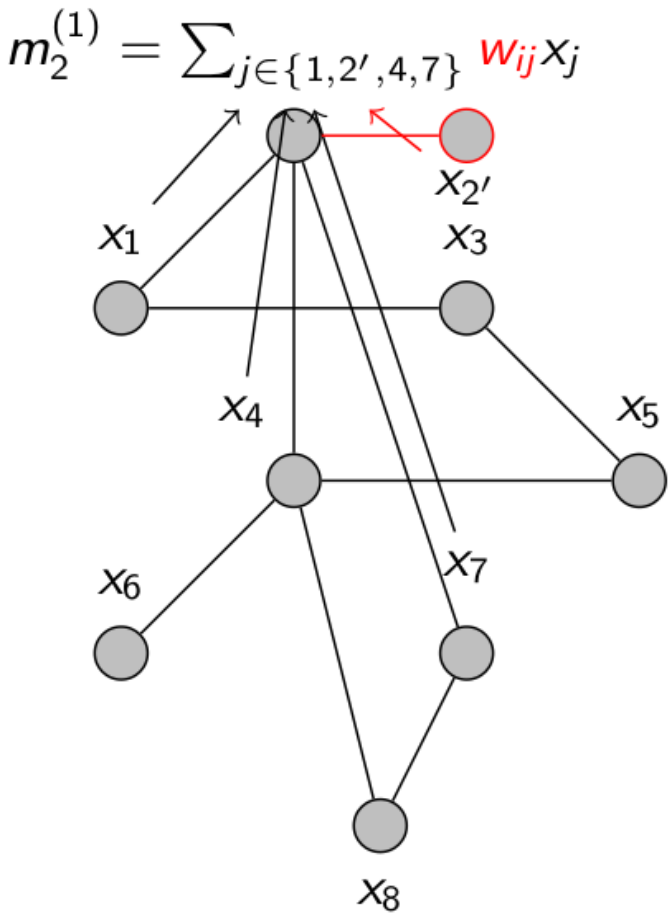

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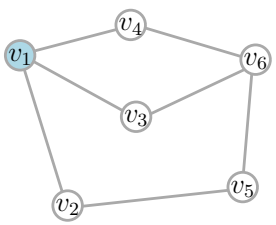

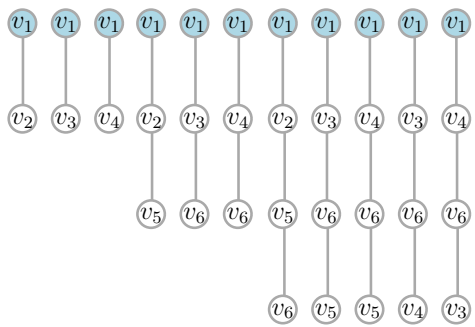

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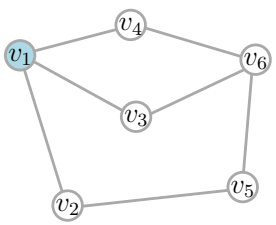

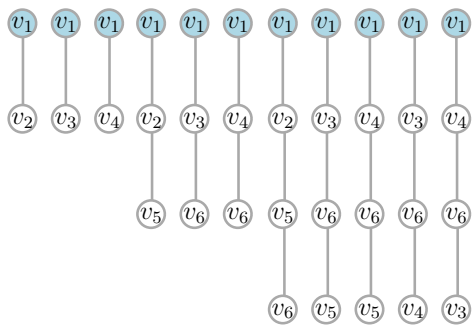

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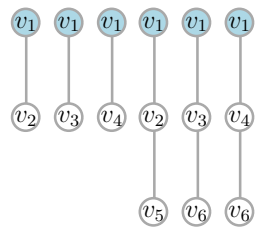

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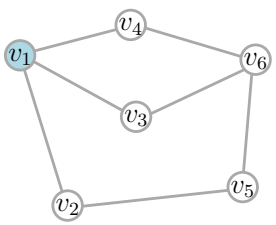

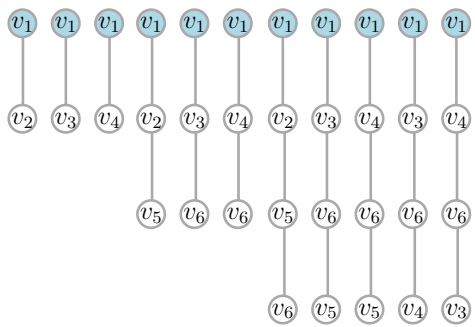

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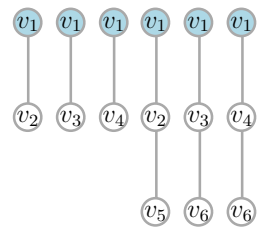

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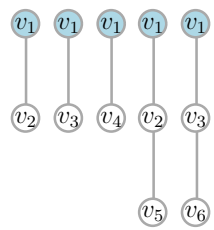

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Path Neural Networks

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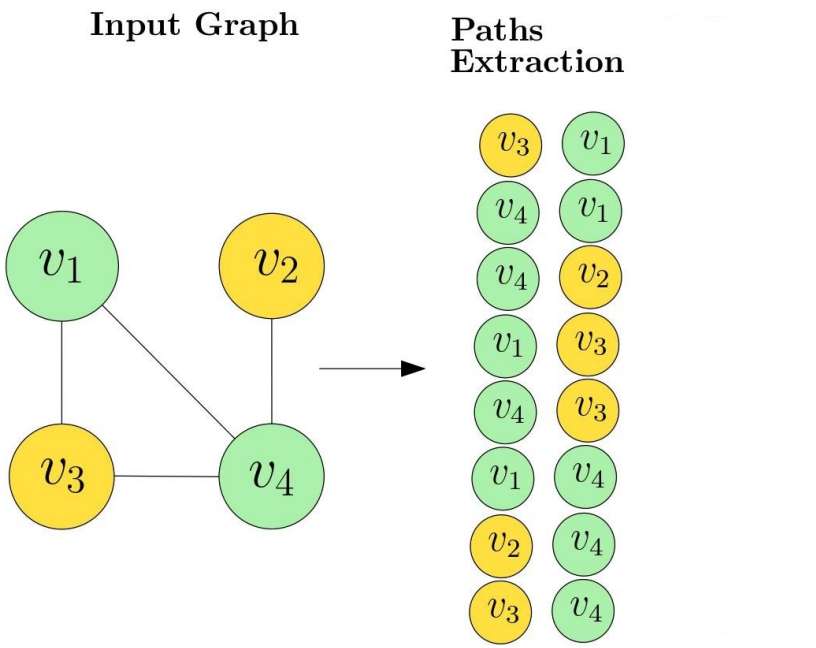
At layer ℓ of the model we process paths of length ℓ, e.g., $\ell = 2$.



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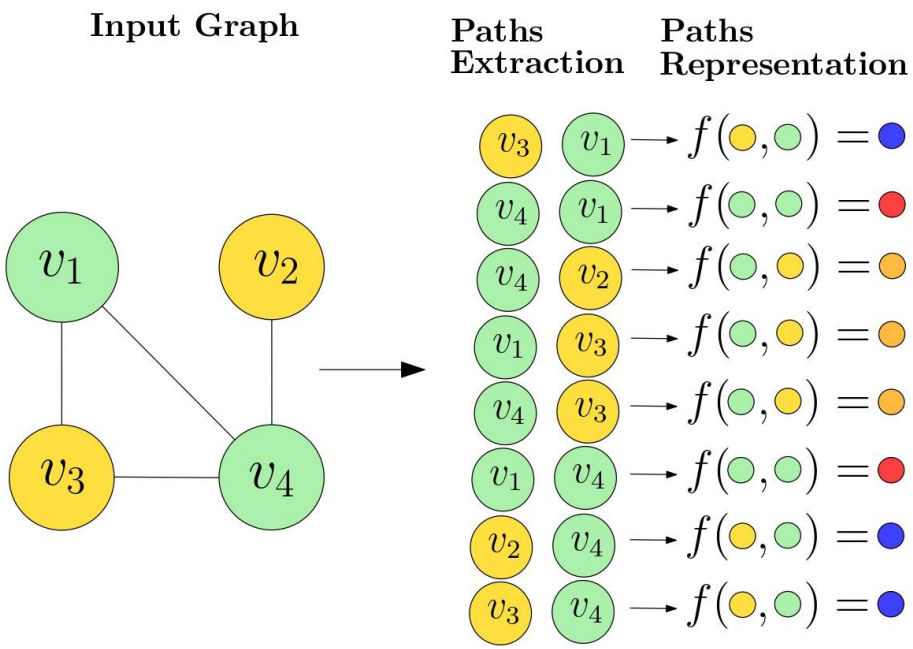

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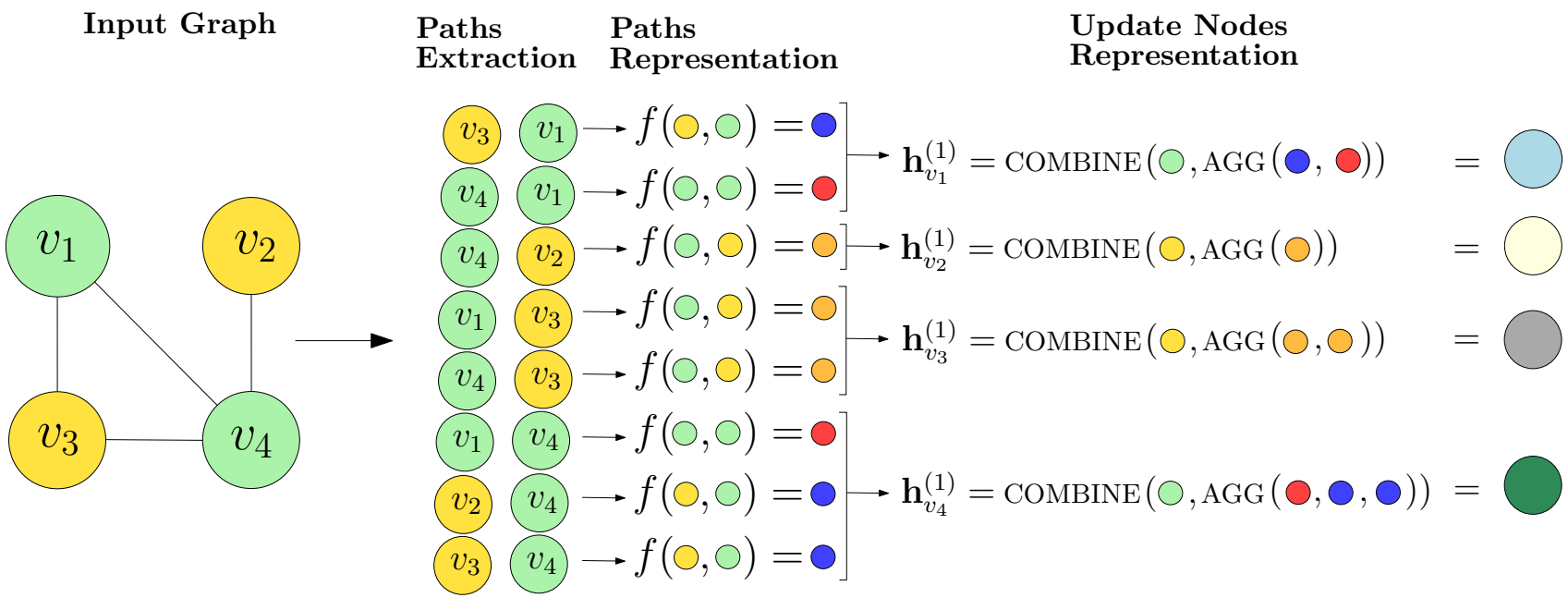

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PathNN-$\mathcal{SP}$ also **distinguishes any two graphs distinguished by the WL test**. But in the presence of multiple shortest paths between two vertices a particular sampling of these shortest paths could lead to the PathNN-$\mathcal{SP}$ distinguishing even structurally equivalent nodes.

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- **6 Real-World Graph Classification Datasets**

	DD	PROTEINS	NCI1	ENZYMES	IMDB-B	IMDB-M
GIN	75.3 ± 2.9	73.3 ± 4.0	80.0 ± 1.4	59.6 ± 4.5	71.2 ± 3.9	48.5 ± 3.3
GraphSAGE	72.9 ± 2.0	73.0 ± 4.5	76.0 ± 1.8	58.2 ± 6.0	68.8 ± 4.5	47.6 ± 3.5
GAT	73.9 ± 3.4	70.9 ± 2.7	77.3 ± 2.5	49.5 ± 8.9	69.2 ± 4.8	48.2 ± 4.9
SPN ($K = 1$)	72.7 ± 2.6	71.0 ± 3.7	80.0 ± 1.5	67.5 ± 5.5	NA	NA
SPN ($K = 5$)	77.4 ± 3.8	74.2 ± 2.7	78.6 ± 3.8	69.4 ± 6.2	NA	NA
PathNet ($N = 10, K = 2$)	OOM	70.5 ± 3.9	64.1 ± 2.3	69.3 ± 5.4	70.4 ± 3.8	49.1 ± 3.6
Nested GNN	**77.8** ± 3.9	74.2 ± 3.7	NA	31.2 ± 6.7	NA	NA
PathNN-$\mathcal{P}$ ($K = 1$)	76.9 ± 3.7	**75.2** ± 3.9	77.5 ± 1.6	**73.0** ± 5.2	**72.6** ± 3.3	**50.8** ± 4.5
PathNN-$\mathcal{SP}$ ($K = 2$)	75.3 ± 2.7	73.1 ± 3.1	82.0 ± 1.6	71.6 ± 6.4	70.8 ± 3.5	50.0 ± 4.1
PathNN-$\mathcal{SP}$ ($K = 3$)	77.0 ± 3.1	72.2 ± 2.7	82.2 ± 1.7	69.2 ± 4.7	-	-
PathNN-$\mathcal{SP}^+$ ($K = 2$)	74.7 ± 3.0	73.1 ± 3.7	81.0 ± 1.4	72.5 ± 5.3	70.5 ± 3.4	50.7 ± 4.5
PathNN-$\mathcal{SP}^+$ ($K = 3$)	76.5 ± 4.6	73.2 ± 3.3	**82.3** ± 1.9	70.4 ± 3.1	-	-
PathNN-$\mathcal{AP}$ ($K = 2$)	75.0 ± 4.4	73.1 ± 4.9	81.3 ± 1.8	71.8 ± 4.8	71.7 ± 3.6	49.8 ± 4.2
PathNN-$\mathcal{AP}$ ($K = 3$)	OOM	73.1 ± 4.0	82.3 ± 1.7	69.0 ± 5.3	OOM	OOM

- Our code is publicly available: https://github.com/gasmichel/PathNNs_expressive

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1) Bounding the Expected Robustness of Graph Neural Networks Subject to Node Feature Attacks

Abbahaddou*, et al. (2024, ICLR)

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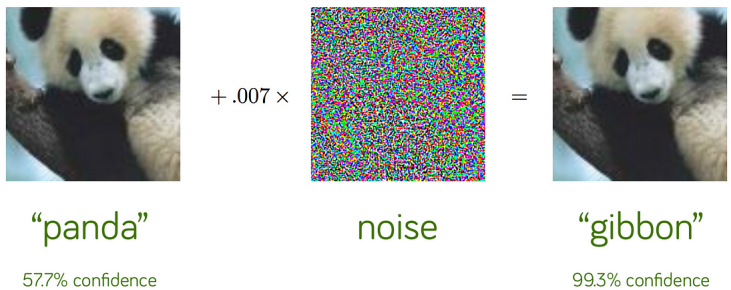
Goal: Adversarial attacks apply a *small* change to the input to achieve a *large* change in the output of our model.



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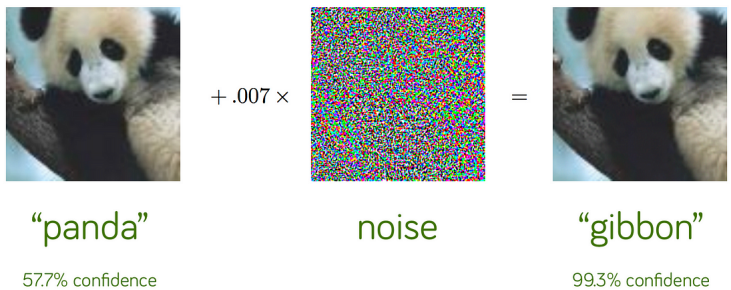

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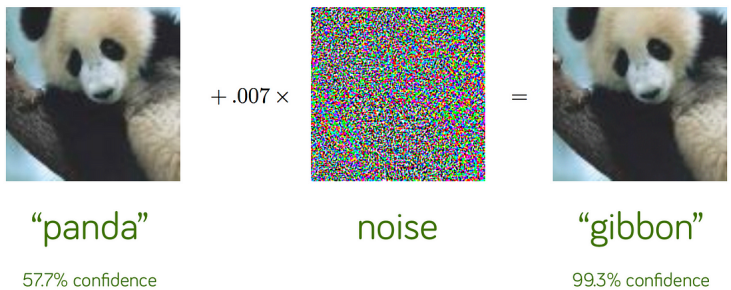

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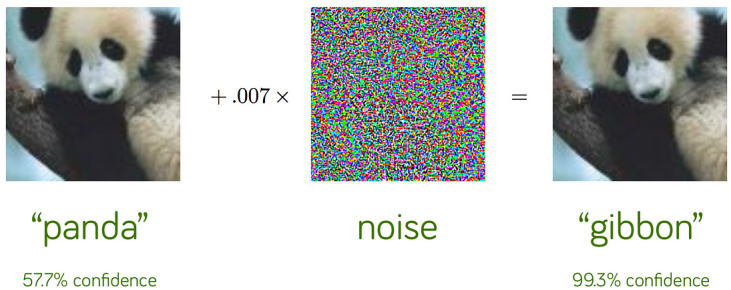

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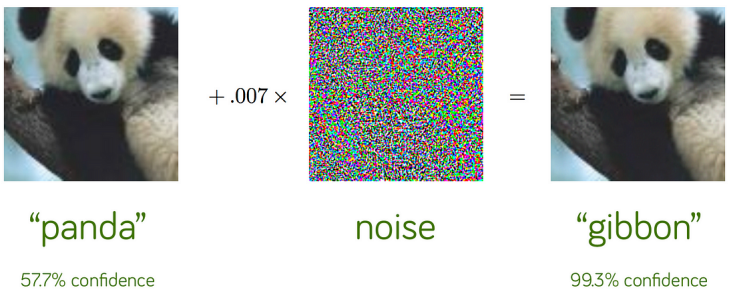

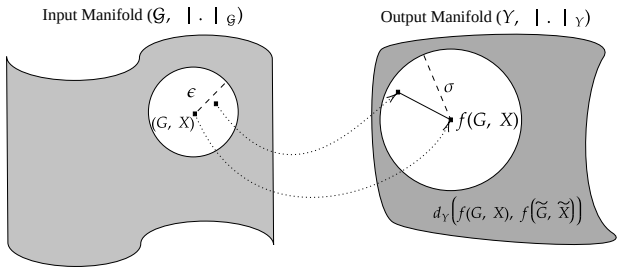

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Then, a graph function $f : (\mathcal{G}, \mathcal{X}) \to \mathcal{Y}$ is $((d^{\alpha,\beta}, \epsilon), (d_{\mathcal{Y}}, \gamma))$–*robust* if its vulnerability $Adv_\epsilon^{\alpha,\beta}[f]$ can be upper-bounded by γ, i.e., $Adv_\epsilon^{\alpha,\beta}[f] \leq \gamma$.

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Then, the vulnerability of GCNs is upper bounded by

$$\gamma = \prod_{i=1}^{L} \|W^{(i)}\|_1 \frac{\epsilon \sum_{u \in \mathcal{V}} \hat{w}_u}{\sigma},$$

with $\hat{w}_u$ denoting the sum of normalized walks of length $(L-1)$ starting from node u.

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$$\gamma = \prod_{i=1}^{L} \|W^{(i)}\|_1 \frac{\epsilon \sum_{u \in \mathcal{V}} \hat{w}_u}{\sigma},$$

with $\hat{w}_u$ denoting the sum of normalized walks of length $(L-1)$ starting from node u.

Insight: Our upper bound on the vulnerability of a GCN is **smaller for small** $\prod_{i=1}^{L} \|W^{(i)}\|_1$ yielding a **more robust GCN.**

Methodology

Fact: Orthonormal matrices have norm 1.

$\Rightarrow$ According to our bound a GNN with orthonormal weight matrices should be more robust.

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Björk Orthonormalisation Algorithm

Given a weight matrix W we iteratively alter it to approximate the closest orthonormal matrix $\hat{W}$. When $\hat{W}_0 = W$, we recursively compute

$$\hat{W}_{k+1} = \hat{W}_k \left(I + \tfrac{1}{2} \left(I - \hat{W}_k^T \hat{W}_k \right) + \ldots + (-1)^p \binom{-1/2}{p} \left(I - \hat{W}_k^T \hat{W}_k \right)^p \right).$$

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Proposed Solution: In our *GCORN* model we propose the inclusion of several Björk Orthonormalisation iterations in each forward pass during the training of a GCN, **yielding weight matrices that approach orthonormality and thereby a more robust GNN**.

Results

Table: Node classification accuracy ($\pm$ standard deviation) for feature-based attacks.

Attack	Dataset	GCN	GCN-k	AirGNN	RGCN	ParsevalR	GCORN
Random ($\psi = 0.5$)	Cora	68.4 $\pm$ 1.9	69.2 $\pm$ 2.6	73.5 $\pm$ 1.9	71.6 $\pm$ 0.3	72.9 $\pm$ 0.9	**77.1 $\pm$ 1.8**
	CiteSeer	57.8 $\pm$ 1.5	62.3 $\pm$ 1.2	64.6 $\pm$ 1.6	63.7 $\pm$ 0.6	65.1 $\pm$ 0.8	**67.8 $\pm$ 1.4**
	PubMed	68.3 $\pm$ 1.2	71.2 $\pm$ 1.1	70.9 $\pm$ 1.3	71.4 $\pm$ 0.5	71.8 $\pm$ 0.8	**73.1 $\pm$ 1.1**
	CS	85.3 $\pm$ 1.1	86.7 $\pm$ 1.1	87.5 $\pm$ 1.6	88.2 $\pm$ 0.9	87.6 $\pm$ 0.6	**89.8 $\pm$ 1.2**
	OGBN-Arxiv	68.2 $\pm$ 1.5	52.8 $\pm$ 0.5	66.5 $\pm$ 1.3	63.8 $\pm$ 1.9	68.3 $\pm$ 1.9	**69.1 $\pm$ 1.8**
Random ($\psi = 1.0$)	Cora	41.7 $\pm$ 2.1	46.3 $\pm$ 2.8	53.7 $\pm$ 2.2	52.8 $\pm$ 1.6	55.3 $\pm$ 1.2	**57.6 $\pm$ 1.9**
	CiteSeer	38.2 $\pm$ 1.3	45.3 $\pm$ 1.4	49.8 $\pm$ 2.1	43.7 $\pm$ 2.2	51.2 $\pm$ 1.2	**57.3 $\pm$ 1.7**
	PubMed	60.1 $\pm$ 1.7	62.3 $\pm$ 1.3	62.4 $\pm$ 1.2	61.9 $\pm$ 1.2	61.3 $\pm$ 1.7	**65.8 $\pm$ 1.4**
	CS	69.9 $\pm$ 1.3	73.2 $\pm$ 0.9	76.7 $\pm$ 2.8	76.2 $\pm$ 1.4	78.7 $\pm$ 1.2	**81.3 $\pm$ 1.6**
	OGBN-Arxiv	66.4 $\pm$ 1.9	46.6 $\pm$ 0.6	62.7 $\pm$ 1.6	63.0 $\pm$ 2.4	66.1 $\pm$ 0.7	**67.3 $\pm$ 2.1**
PGD	Cora	54.1 $\pm$ 2.4	58.3 $\pm$ 1.6	68.2 $\pm$ 1.8	62.5 $\pm$ 1.2	68.6 $\pm$ 1.7	**71.1 $\pm$ 1.4**
	CiteSeer	52.3 $\pm$ 1.1	59.6 $\pm$ 1.6	59.3 $\pm$ 2.1	61.9 $\pm$ 1.1	62.1 $\pm$ 1.5	**65.6 $\pm$ 1.4**
	PubMed	66.1 $\pm$ 2.1	67.3 $\pm$ 1.3	70.8 $\pm$ 1.7	69.5 $\pm$ 0.9	68.9 $\pm$ 2.1	**72.3 $\pm$ 1.3**
	CS	71.3 $\pm$ 1.1	74.1 $\pm$ 0.8	76.3 $\pm$ 2.1	76.6 $\pm$ 1.2	77.3 $\pm$ 0.6	**79.6 $\pm$ 1.2**
	OGBN-Arxiv	67.5 $\pm$ 0.9	49.9 $\pm$ 0.7	55.7 $\pm$ 0.9	63.6 $\pm$ 0.7	67.6 $\pm$ 1.2	**68.1 $\pm$ 1.1**
Nettack	Cora	60.9 $\pm$ 2.5	64.2 $\pm$ 5.2	66.7 $\pm$ 3.8	63.4 $\pm$ 3.8	67.5 $\pm$ 2.5	**68.3 $\pm$ 1.4**
	CiteSeer	55.8 $\pm$ 1.4	71.7 $\pm$ 1.4	67.5 $\pm$ 2.5	70.8 $\pm$ 3.8	69.2 $\pm$ 3.8	**77.5 $\pm$ 2.5**
	PubMed	60.0 $\pm$ 2.5	65.8 $\pm$ 2.9	69.2 $\pm$ 1.4	**71.7 $\pm$ 3.8**	68.3 $\pm$ 1.4	70.8 $\pm$ 1.4
	CS	55.8 $\pm$ 1.4	71.6 $\pm$ 1.4	76.7 $\pm$ 1.4	71.7 $\pm$ 2.9	75.8 $\pm$ 2.8	**78.3 $\pm$ 1.4**
	OGBN-Arxiv	49.2 $\pm$ 2.9	53.3 $\pm$ 1.4	**56.7 $\pm$ 1.4**	52.6 $\pm$ 2.5	55.8 $\pm$ 1.4	55.8 $\pm$ 1.4

- Our **GCORN model often outperforms** existing defense approaches when subject to feature based attacks.

Results

Table: Node classification accuracy (± standard deviation) for structure-based attacks.

Attack	Dataset	GCN	GCN-Jaccard	RGCN	GNN-SVD	GNN-Guard	ParsevalR	GCORN
Mettack	Cora	73.0 ± 0.7	75.4 ± 1.8	69.2 ± 0.3	73.6 ± 0.9	74.4 ± 0.8	71.9 ± 0.7	**77.3 ± 0.5**
	CiteSeer	63.2 ± 0.9	69.5 ± 1.9	68.9 ± 0.6	65.8 ± 0.6	68.8 ± 1.5	68.3 ± 0.8	**73.7 ± 0.3**
	PubMed	60.7 ± 0.7	62.9 ± 1.8	65.1 ± 0.4	82.1 ± 0.8	**84.8 ± 0.3**	69.5 ± 1.1	71.8 ± 0.4
	CoraML	73.1 ± 0.6	75.4 ± 0.4	77.1 ± 1.1	71.3 ± 1.0	76.5 ± 0.7	76.9 ± 1.3	**79.2 ± 0.6**
PGD	Cora	76.7 ± 0.9	78.3 ± 1.1	72.0 ± 0.3	71.6 ± 0.4	75.0 ± 2.0	78.4 ± 1.2	**79.9 ± 0.4**
	CiteSeer	67.8 ± 0.8	70.9 ± 1.0	62.2 ± 1.8	60.3 ± 2.4	68.9 ± 2.2	70.6 ± 1.0	**73.1 ± 0.5**
	PubMed	75.3 ± 1.6	73.8 ± 1.3	78.6 ± 0.4	81.9 ± 0.4	**84.3 ± 0.4**	77.3 ± 0.7	77.4 ± 0.4
	CoraML	76.9 ± 1.2	75.0 ± 2.4	77.5 ± 0.3	73.1 ± 0.5	75.5 ± 0.8	81.3 ± 0.4	**84.1 ± 0.2**
DICE	Cora	74.9 ± 0.8	76.9 ± 0.9	79.6 ± 0.3	72.2 ± 1.4	75.6 ± 1.1	**79.7 ± 0.8**	78.9 ± 0.4
	CiteSeer	64.1 ± 0.5	66.0 ± 0.6	68.7 ± 0.5	62.6 ± 1.2	65.5 ± 1.1	68.9 ± 0.4	**74.6 ± 0.4**
	PubMed	79.4 ± 0.4	78.3 ± 0.2	**79.8 ± 0.4**	76.6 ± 0.5	77.8 ± 0.7	79.2 ± 0.3	78.1 ± 0.6
	CoraML	78.3 ± 0.6	77.5 ± 0.3	80.1 ± 0.4	58.7 ± 0.4	77.5 ± 0.2	80.5 ± 1.3	**81.1 ± 0.8**

- Our **GCORN model often outperforms** existing defense approaches when subject to feature based attacks.
- GCORN is also effective against **structure-based, as well as combined structure and feature attacks**.

2) A Simple and Yet Fairly Effective Defense for Graph Neural Networks

Ennadir, et al. (2024, AAAI)

Problem Set-Up

Problem: Available defense methods often have high computational complexity and training time (often increasing with increasing graph size).

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Solution Approach: We propose a GNN, called the *NoisyGNN*, in which **hidden states are perturbed** by random noise following a normal distribution $N \sim \mathcal{N}(0, \beta I)$, i.e., our GNNs are of the form

$$\hat{y} = \sigma\left(\tilde{A}\,\mathrm{ReLU}\left(\tilde{A}XW^{(1)} + N\right)W^{(2)}\right).$$

Theoretical Results

Upper Bounds on GNN Vulnerability

We consider structural perturbations of the input graph (A, X), with a budget ϵ and 2-layer GNNs with 1-Lipschitz continuous activation functions and weight matrices $W^{(1)}, W^{(2)}$.

- Then, the vulnerability of GCNs is upper bounded by

$$\frac{2(\|W^{(2)}\|\|W^{(1)}\|\|X\|\epsilon)^2}{\beta};$$

- Then, the vulnerability of GINs is upper bounded by

$$\frac{(\|W^{(2)}\|\|W^{(1)}\|\|X\|\epsilon(2\|A\|+\epsilon))^2}{2\beta}.$$

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Insight: Our upper bound on the vulnerability of a GNN is **smaller for large** β yielding a **more robust GNN.**

Experimental Results

Dataset	Attack Budget	GCNGuard	GCN-Jaccard	GCN-SVD	RGNN	NoisyGCN
Cora	Clean	77.5 ± 0.7	80.9 ± 0.7	80.6 ± 0.4	**83.5 ± 0.3**	83.2 ± 0.4
	Budget (5%)	75.8 ± 0.6	78.9 ± 0.8	78.4 ± 0.6	78.3 ± 0.6	**81.2 ± 0.7**
	Budget (10%)	74.7 ± 0.4	**76.7 ± 0.7**	71.5 ± 0.8	70.7 ± 0.8	74.5 ± 0.6
CiteSeer	Clean	70.1 ± 1.5	71.2 ± 0.7	70.7 ± 0.4	**72.3 ± 0.5**	71.9 ± 0.4
	Budget (5%)	69.9 ± 1.1	70.3 ± 2.3	68.9 ± 0.7	70.6 ± 0.7	**72.3 ± 0.6**
	Budget (10%)	70.0 ± 1.5	67.5 ± 2.1	68.8 ± 0.6	68.7 ± 1.2	**70.4 ± 0.8**
PubMed	Clean	84.5 ± 0.6	85.0 ± 0.5	82.7 ± 0.3	**85.1 ± 0.8**	85.0 ± 0.6
	Budget (5%)	**84.3 ± 0.9**	79.6 ± 0.3	81.3 ± 0.6	81.1 ± 0.7	81.8 ± 0.4
	Budget (10%)	**84.1 ± 0.3**	67.4 ± 1.1	81.1 ± 0.7	65.2 ± 0.4	73.3 ± 0.6
PolBlogs	Clean	93.1 ± 0.6	-	86.5 ± 0.8	94.9 ± 0.3	**95.2 ± 0.4**
	Budget (5%)	72.8 ± 0.8	-	**85.1 ± 1.6**	76.0 ± 0.8	79.7 ± 0.6
	Budget (10%)	68.7 ± 1.0	-	**84.8 ± 2.3**	69.2 ± 1.2	73.4 ± 0.5

Table: Node classification accuracy (± standard deviation) when subject to Mettack.

- Our NoisyGCNs **sometimes outperform** other defense methods.

Experimental Results

Table: Mean training time analysis (in s) of the NoisyGNN in comparison to other baselines for both the GCN and GIN instances.

Dataset	GCNGuard	GCN-Jaccard	RGCN	GCN-SVD	NoisyGCN
Cora	28.52	1.93	1.16	1.39	1.29
CiteSeer	36.04	1.58	1.23	1.12	1.24
PubMed	731.26	12.27	34.19	4.60	2.41
PolBlogs	18.17	5.17	0.96	0.80	0.65

Dataset	GINGuard	GIN-Jaccard	RGCN	GIN-SVD	NoisyGIN
Cora	48.93	3.12	1.31	1.51	1.93
CiteSeer	58.45	3.78	1.44	2.20	2.76
PubMed	963.58	16.28	41.09	6.33	7.86
PolBlogs	43.7	5.52	0.95	3.71	3.16

- Our NoisyGCNs **sometimes outperform** other defense methods.
- NoisyGNNs are **faster to train** than most other defense methods.

Experimental Results

Table: Classification accuracy (± standard deviation) of combining defense methods with the proposed noise injection on different benchmark datasets.

Method	Cora	CiteSeer	PolBlogs
GINGuard	61.8±0.5	55.6±1.8	82.7±0.6
+ Noisy	**66.2±1.3**	**58.3±1.9**	**83.6±0.8**
GIN-Jaccard	70.4±1.1	61.2±2.3	-
+ Noisy	**72.9±0.8**	**64.9±1.8**	-
GCNGuard	69.5±0.7	66.2±0.6	64.7±0.8
+ Noisy	**72.4±1.2**	**68.9±0.9**	**65.8±1.3**
GCN-Jaccard	66.7±0.5	61.2±1.1	-
+ Noisy	**69.6±0.9**	**63.1±0.6**	-

- Our NoisyGCNs **sometimes outperform** other defense methods.
- NoisyGNNs are **faster to train** than most other defense methods.
- When **combined with other defense methods**, best performance is achieved.

Conclusions

- Graph Representation Learning is a highly active area of research at the moment gaining both academic and industrial interest.

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- If the graph structure is insufficient for the learning task, e.g., necessary information presents itself as a long-range effect on the original graph, then we should pick a criterion to limit the search space of n^2 node pairs and rewire accordingly.

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- If the graph structure is insufficient for the learning task, e.g., necessary information presents itself as a long-range effect on the original graph, then we should pick a criterion to limit the search space of n^2 node pairs and rewire accordingly.
- If we are aware of certain substructures of particular relevance to our learning task or require a highly expressive model, then we should explicitly represent these substructures in the message passing scheme.

Thank you for your attention!

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References

Y. Abbahaddou, S. Ennadir, J. F. Lutzeyer, M. Vazirgiannis & H. Boström, "Bounding the Expected Robustness of Graph Neural Networks Subject to Node Feature Attacks," *International Conference on Learning Representations(ICLR),* 2024.

L. A. Adamic & N. Glance, "The political blogosphere and the 2004 US election: divided they blog," *In Proceedings of the 3rd International Workshop on Link Discovery*, pp. 36–43, 2005.

U. Alon & E. Yahav, "On the Bottleneck of Graph Neural Networks and its Practical Implications," In: *International Conference on Learning Representations (ICLR)*, 2020.

A. Bojchevski, J. Gasteiger, B. Perozzi, A. Kapoor, M. Blais, B. Rózemberczki, M. Lukasik & S. Günnemann, "Scaling graph neural networks with approximate pagerank," *Proceedings of the 26th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD)*, pp. 2464-2473, 2020.

F. Borisyuk, S. He, Y. Ouyang, M. Ramezani, P. Du, X. Hou, C. Jiang, N. Pasumarthy, P. Bannur, B. Tiwana, P. Liu, "LiGNN: Graph Neural Networks at LinkedIn," *arXiv:2402.11139*, 2024.

S. Brody, U. Alon & E. Yahav, "How Attentive Are Graph Attention Networks?," In: *International Conference on Learning Representations (ICLR)*, 2022.

M. Bronstein, "Graph ML at Twitter," *Twitter Engineering Blog Post*, `https://blog.twitter.com/engineering/en_us/topics/insights/2020/graph-ml-at-twitter`, 2020.

M. Bronstein, "Geometric Deep Learning: The Erlangen Programme of ML," *Keynote Talk at The International Conference on Learning Representations*, 2021.

S. Butler & F. Chung, "Spectral graph theory," In: L. Hogben (ed) *Handbook of linear algebra (2nd edition)*, Boca Raton, FL: CRC Press, pp. 47/1—47/14, 2017.

M. Chatzianastasis, J. F. Lutzeyer, G. Dasoulas & M. Vazirgiannis, "Graph Ordering Attention Networks," *Thirty-Sixth AAAI Conference on Artificial Intelligence (AAAI),* 2023.

D. Cvetkovic, R. Rowlinson & S. Simic, *Eigenspaces of graphs*, Cambridge, UK: Cambridge University Press, 1997.

L. Dall'Amico, R. Couillet & N. Tremblay, "Optimal Laplacian regularization for sparse spectral community detection," *ICASSP*, 2020.

G. Dasoulas, J. F. Lutzeyer & M. Vazirgiannis, "Learning Parametrised Graph Shift Operators," In: *International Conference on Learning Representations (ICLR)*, 2021.

A. Deac, M. Lackenby & P. Veličković, "Expander Graph Propagation," *arXiv:2210.02997*, 2022.

J. A. Deri & J. M. F. Moura, "Spectral projector-based graph Fourier transforms," *IEEE Journal of Selected Topics in Signal Processing*, vol. 11, pp. 785–795, 2017.

V.P. Dwivedi & X. Bresson, "A Generalization of Transformer Networks to Graphs," *AAAI Workshop on Deep Learning on Graphs: Methods and Applications*, 2021.

S. Ennadir, Y. Abbahaddou, J. F. Lutzeyer, M. Vazirgiannis & H. Boström, "A Simple and Yet Fairly Effective Defense for Graph Neural Networks," *Thirty-Seventh AAAI Conference on Artificial Intelligence (AAAI),* 2024.

F. Frasca, B. Bevilacqua, M. Bronstein & H. Maron, "Understanding and Extending Subgraph GNNs by Rethinking Their Symmetries," *Proceedings of the 36st International Conference on Neural Information Processing Systems (NeurIPS),* 2022.

F. Geerts & J. L. Reutter, "Expressiveness and Approximation Properties of Graph Neural Networks," *International Conference on Learning Representations (ICLR)*, 2022.

I. J. Goodfellow, J. Shlens, & C. Szegedy, "Explaining and harnessing adversarial examples," International Conference of Learning Representations (ICLR), 2015.

J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals & G. E. Dahl, "Neural message passing for Quantum chemistry," *Proceedings of the 34th International Conference on Machine Learning (ICML)*, 2017.

S. Günnemann, "Graph Neural Networks: Adversarial Robustness," *Graph Neural Networks: Foundations, Frontiers, and Applications*, pp. 149–176, 2022.

B. Hammer, "On the approximation capability of recurrent neural networks," *Neurocomputing*, pp. 107–123, 2000.

A. Jain, I. Liu, A. Sarda & P. Molino, "Food Discovery with Uber Eats: Using Graph Learning to Power Recommendations," *Uber Engineering Blog Post*, `https://eng.uber.com/uber-eats-graph-learning/`, 2019.

Thomas N. Kipf & M. Welling, "Variational Graph Auto-Encoders" *NeurIPS Workshop on Bayesian Deep Learning*, 2016.

Thomas N. Kipf & M. Welling, "Semi-supervised classification with graph convolutional networks," *International Conference on Learning Representations (ICLR)*, 2017.

O. Lange & L. Perez, "Traffic prediction with advanced Graph Neural Networks," *DeepMind Research Blog Post*, `https://deepmind.com/blog/article/traffic-prediction-with-advanced-graph-neural-networks`, 2020.

G. Liu, D. B. Catacutan, K. Rathod, K. Swanson, W. Jin, J. C. Mohammed, A. Chiappino-Pepe, S. A. Syed, M. Fragis, K. Rachwalski, J. Magolan, M. G. Surette, B. K. Coombes, T. Jaakkola, R. Barzilay, J. J. Collins, J. M. Stokes, "Deep learning-guided discovery of an antibiotic targeting Acinetobacter baumannii," *Nature Chemical Biology*, pp. 1–9, 2023.

J. Lutzeyer, *Network Representation Matrices and their Eigenproperties: A Comparative Study,* PhD thesis: Imperial College London, 2020.

J. Lutzeyer, C. Wu & M. Vazirgiannis, "Graph Neural Network Simplification: Sparsifying the Update Step," *ICLR Workshop on Geometrical and Topological Representation Learning*, 2022.

G. Michel, G. Nikolentzos, J. Lutzeyer & M. Vazirgiannis, "Path Neural Networks: Expressive and Accurate Graph Neural Networks," *Proceedings of the 40th International Conference on Machine Learning (ICML)*, 2023.

C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J.E Lenssen, G. Rattan & M. Grohe, "Weisfeiler and Lehman Go Neural: Higher-order Graph Neural Networks," *Proceedings of the AAAI Conference on Artificial Intelligence*, pp. 4602–4609, 2019.

A. Ortega, P. Frossard, J. Kovacevic, J. M. F. Moura & P. Vandergheynst, "Graph signal processing: Overview, challenges, and applications," *Proceedings of the IEEE*, vol. 106, pp. 808–828, 2018.

T. Qin & K. Rohe, "Regularized Spectral Clustering under the Degree-Corrected Stochastic Blockmodel," *Advances in neural information processing systems (NIPS)*, pp. 3120–3128, 2013.

A. R. Ramos Vela, J. F. Lutzeyer, A. Giovanidis & M. Vazirgiannis, "Improving Graph Neural Networks at Scale: Combining Approximate PageRank and CoreRank," *NeurIPS New Frontiers in Graph Learning Workshop*, 2022.

G. Salha-Galvan, J. F. Lutzeyer, G. Dasoulas, R. Hennequin & M. Vazirgiannis, "Modularity-Aware Graph Autoencoders for Joint Community Detection and Link Prediction," *arxiv:2202.00961*, 2022.

G. Salha-Galvan, *Contributions to Representation Learning with Graph Autoencoders and Applications to Music Recommendation,* PhD thesis: École Polytechnique, Institut Polytechnique de Paris, 2022.

A. Sandryhaila & J. M. F. Moura "Discrete signal processing on graphs," *IEEE Transactions on Signal Processing*, vol. 61, pp. 1644–1656, 2013.

M. E. A. Seddik, C. Wu, J. F. Lutzeyer & M. Vazirgiannis, "Node Feature Kernels Increase Graph Convolutional Network Robustness," *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2022.

P. Sen, G. Namata, M. Bilgic, L. Getoor, B. Galligher & T. Eliassi-Rad, *AI Magazine*, p. 93, 2008.

J. M. Stokes, K. Yang, K. Swanson, W. Jin, A. Cubillos-Ruiz, N. M. Donghia, C. R. MacNair, S. French, L. A. Carfrae, Z. Bloom-Ackermann, V. M. Tran, A. Chiappino-Pepe, A. H. Badran, I. W. Andrews, E. J. Chory, G. M. Church, E. D. Brown, T. S. Jaakkola, R. Barzilay & J. J. Collins, "A Deep Learning Approach to Antibiotic Discovery," *Cell*, pp. 688–702, 2020.

L. Sun, Y. Dou, C. Yang, J. Wang, P. S. Yu & B. Li, "Adversarial attack and defense on graph data: A survey," *arXiv:1812.10528*, 2020.

J. Topping, F. Di Giovanni, B. P. Chamberlain, X. Dong & M. M. Bronstein, "Understanding Over-Squashing and Bottlenecks on Graphs via Curvature," *International Conference on Learning Representations (ICLR)*, 2022.

P. Veličković, G. Cucurull, A. Casanova, A. Romero, P. Liò & Y. Bengio, "Graph Attention Networks," *6th International Conference on Learning Representations (ICLR),* 2018.

P. Veličković, "Message Passing All the Way Up," *ICLR Workshop on Geometrical and Topological Representation Learning,* 2022.

S. Virinchi, A. Saladi & A. Mondal, "Recommending Related Products Using Graph Neural Networks in Directed Graphs," In: *European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML PKDD)*, 2022.

P. L. Williams & R. D. Beer, "Nonnegative decomposition of multivariate information," *arXiv:1004.2515*, 2010.

J. Wang, P. Huang, H. Zhao, Z. Zhang, B. Zhao & Dik Lun Lee, "Billion-scale Commodity Embedding for E-Commerce Recommendation in Alibaba," In Proceedings of the *24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (KDD)*, pp. 839–848, 2018.

K. Xu, W. Hu, J. Leskovec & S. Jegelka."How powerful are graph neural networks?", *International Conference on Learning Representations (ICLR)*, 2019.

R. Ying, R. He, K. Chen, P. Eksombatchai, W. L. Hamilton & J. Leskovec, "Graph Convolutional Neural Networks for Web-Scale Recommender Systems," In Proceedings of the *24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (KDD)*, pp. 974–983, 2018.

Y. Zhou, H. Zheng & X. Huang, "Graph Neural Networks: Taxonomy, Advances and Trends," *arXiv:2012.08752*, 2020.