



UNIVERSITAT DE
BARCELONA

Graph neural networks

Meysam Madadi

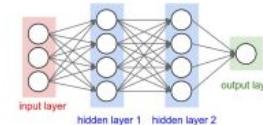
Slides credit: Lulia Duta and Andrei Nicolicioiu

Choose your model

UNSTRUCTURED



Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	Iris setosa
4.9	3.0	1.4	0.2	Iris setosa
7.0	3.2	4.7	1.4	Iris versicolor
6.4	3.2	4.5	1.5	Iris versicolor
6.3	3.3	6.0	2.5	Iris virginica
5.8	3.3	6.0	2.5	Iris virginica

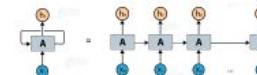


MLP

SEQUENTIAL

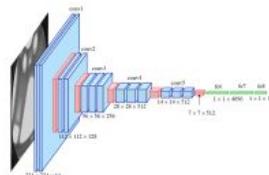
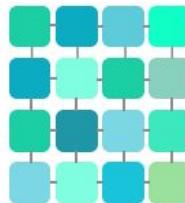


Have a nice day! :)



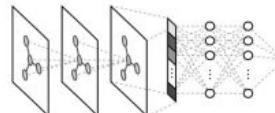
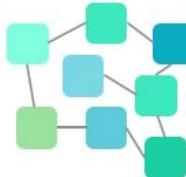
RNN

GRID



CNN

RELATIONAL STRUCTURE



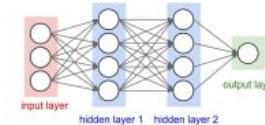
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MLP

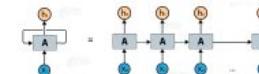
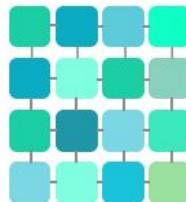
SEQUENTIAL



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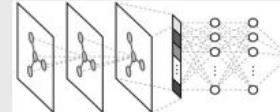
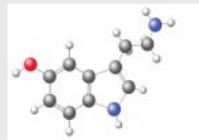
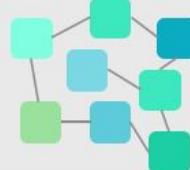
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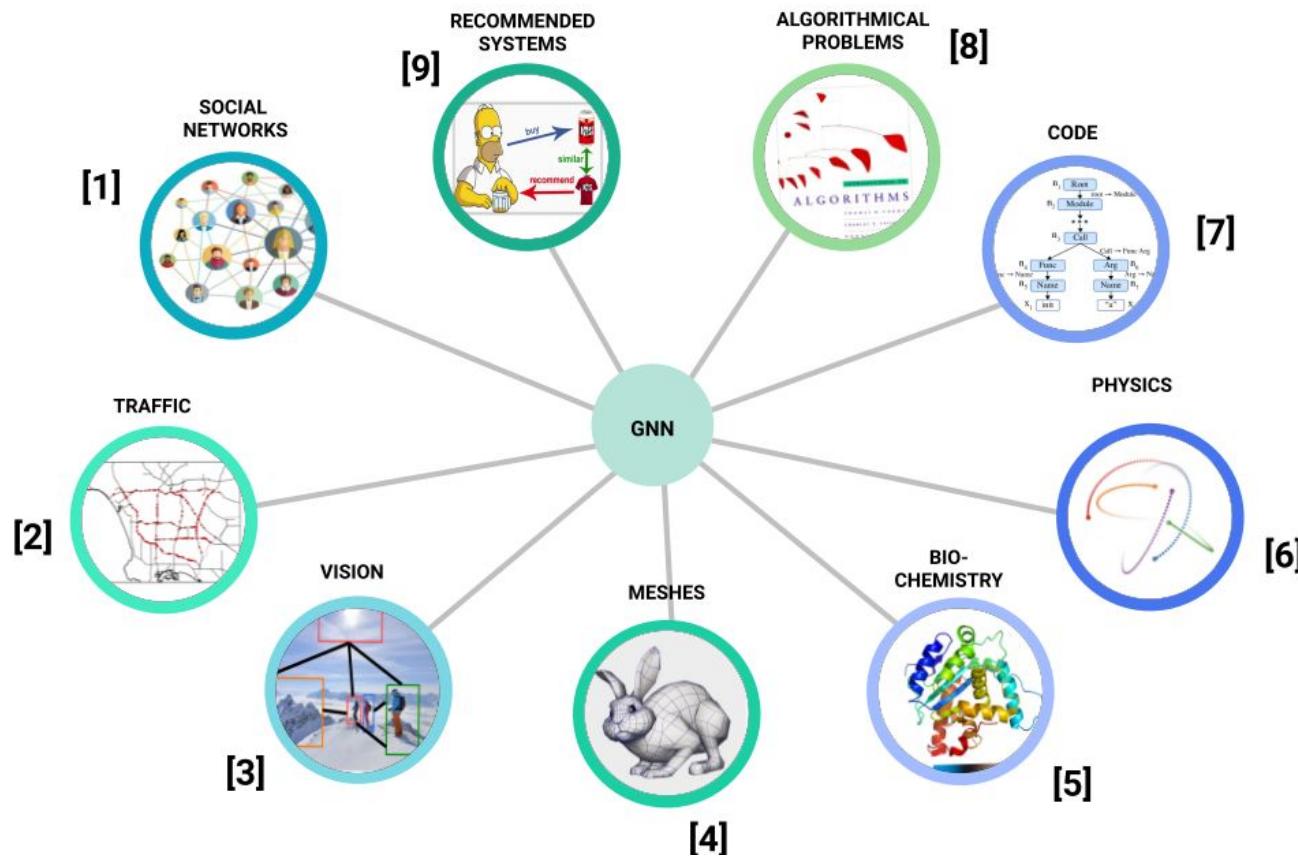
CNN

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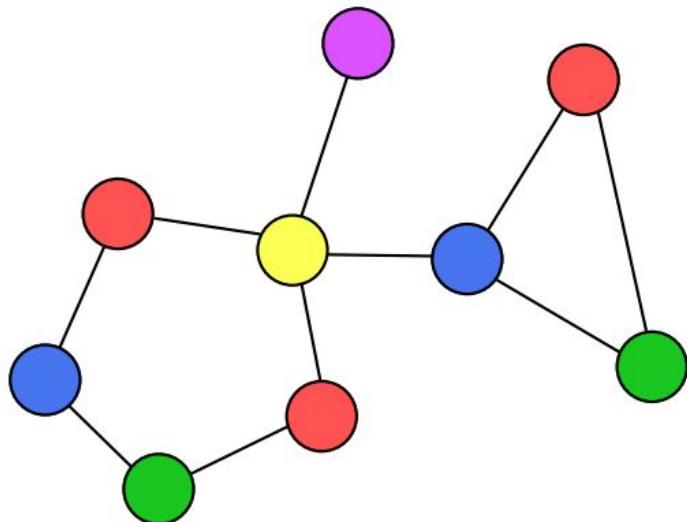


GNN

Tasks



Data: Graph Structure

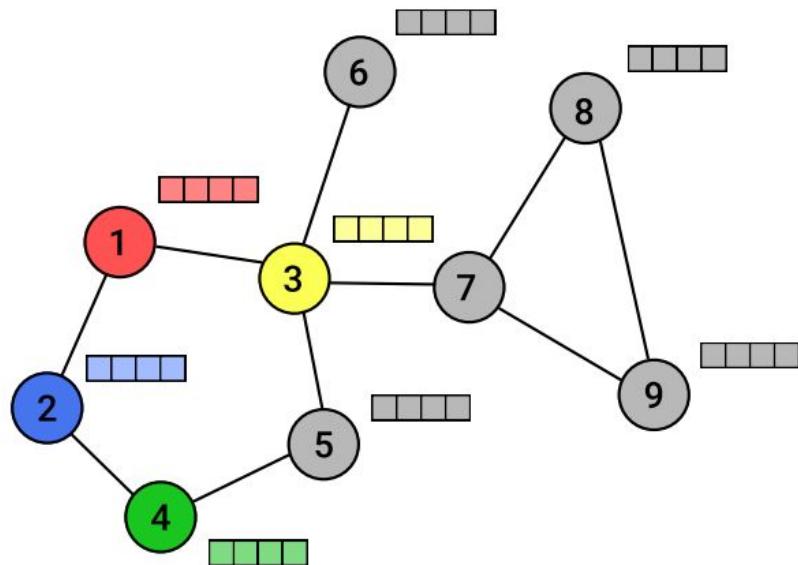


Tasks where we have access or we can create a graph structure.

A graph G is characterized by:

- a set of **nodes**
 $X = \{x_i | i \in 1..N\}$
- connected by **edges**
 $\mathcal{E} = \{e_{ij} | i, j \in 1..N\}$

Data: Graph Structure



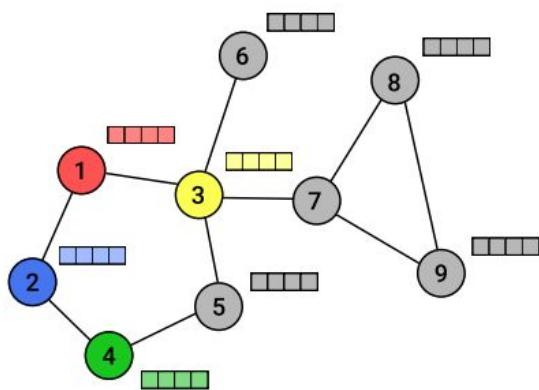
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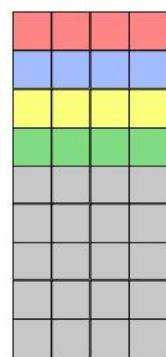
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Each node i is characterized by a set of features $x_i \in \mathbb{R}^D$

Data: Graph Structure - Nodes

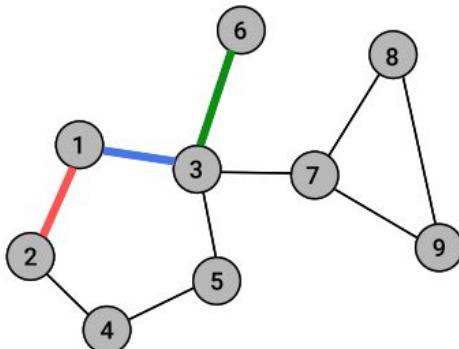


$$X \in \mathbb{R}^{N \times D}$$



- all the nodes $x_i \in \mathbb{R}^D$ are stacked into a matrix $X \in \mathbb{R}^{N \times D}$
- each row corresponds to a node $x_i \in \mathbb{R}^D$

Data: Graph Structure - Edges

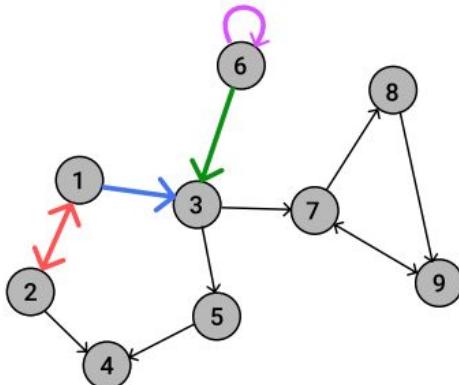


$$A \in \mathbb{R}^{N \times N}$$

	1	2	3	4	5	6	7	8	9
1	0	1	1	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	1	1	1	0	0
4	0	1	0	0	1	0	0	0	0
5	0	0	1	1	0	0	0	0	0
6	0	0	1	0	0	0	0	0	0
7	0	0	1	0	0	0	0	1	1
8	0	0	0	0	0	0	1	0	1
9	0	0	0	0	0	0	1	1	0

- the edges \mathcal{E} could be represented by an adjacency matrix $A \in \mathbb{R}^{N \times N}$
- $a_{ij} \neq 0$ if there is an edge between node i and node j

Data: Graph Structure - Edges



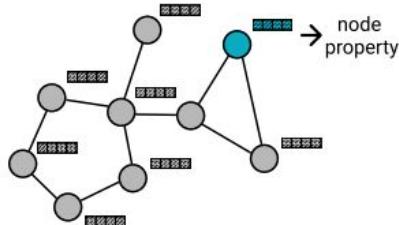
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	1	2	3	4	5	6	7	8	9
1	0	1	0	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	0	1	0	0	0
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5	0	0	1	1	0	0	0	0	0
6	0	0	0	0	0	1	0	0	0
7	0	0	1	0	0	0	0	0	1
8	0	0	0	0	0	0	1	0	0
9	0	0	0	0	0	0	1	1	0

- un-directed graph: adjacency matrix is symmetric
- directed graph: adjacency matrix is **not** symmetric
- $a_{ij} \neq 0$ if there is an edge **from j to i**
- a graph could contain *self-loops*

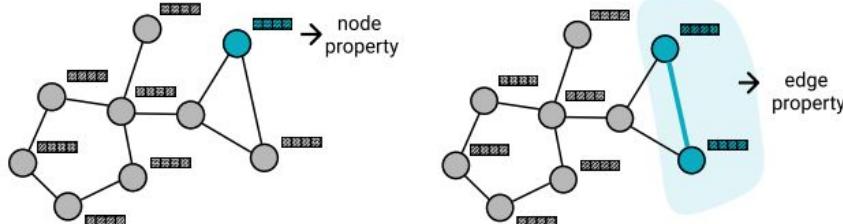
GNNs Goal

- Based on the node features (X) and the graph structure (A), we want to learn a representation of the graph.
- Depending on the task, the representation could be:
 1. node level: $Y \in \mathbb{R}^{N \times K}$



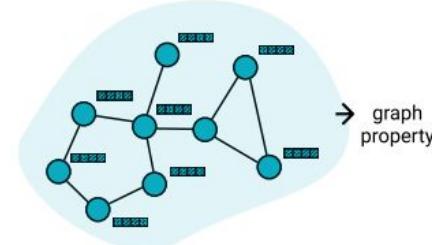
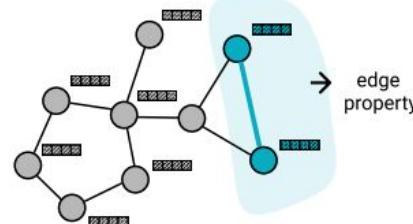
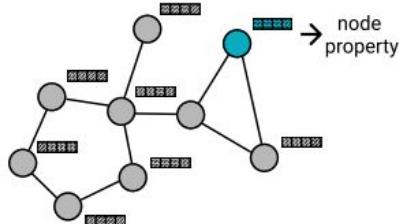
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GNNs Goal

- Based on the node features (X) and the graph structure (A), we want to learn a representation of the graph.
- Depending on the task, the representation could be:
 1. node level: $Y \in \mathbb{R}^{N \times K}$
 2. edge level: $Y \in \mathbb{R}^{M \times K}$
 3. graph level: $Y \in \mathbb{R}^K$



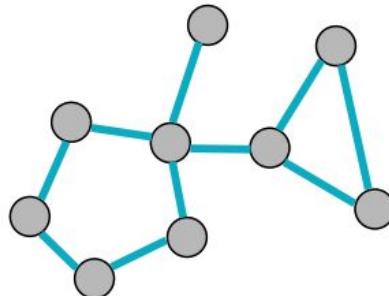
Properties: structure

Structure - dependent

the processing should take into account the structure of the graphs

1. the processing should take into account how nodes are connected

CONNECTIVITY



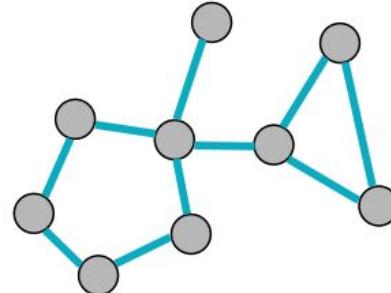
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Structure - dependent

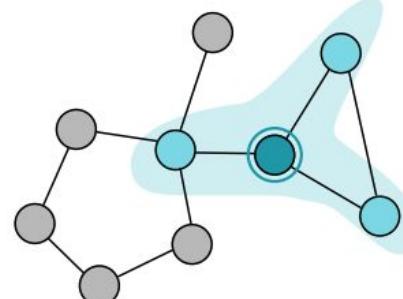
the processing should take into account the structure of the graphs

1. the processing should take into account how nodes are connected
2. a node should be influenced more by its neighbours

CONNECTIVITY



NEIGHBOURHOOD



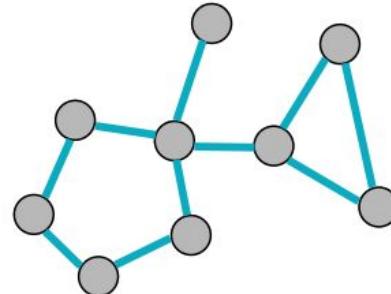
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Structure - dependent

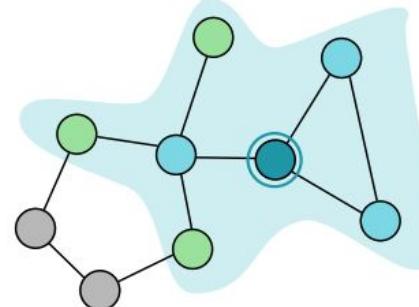
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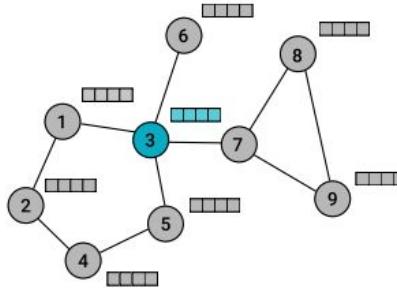
Properties: permutation invariance and equivariance

There is no canonical order for the nodes of the graph.

Permutation invariance

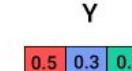
The global output of the graph processing should be invariant to the order of the nodes.

$$f(PX, PAP') = f(X, A)$$



X	1	2	3	4	5	6	7	8	9
1	0	1	1	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	1	1	1	0	0
4	0	1	0	0	1	0	0	0	0
5	0	0	1	1	0	0	0	0	0
6	0	0	1	0	0	0	0	0	0
7	0	0	1	0	0	0	0	1	1
8	0	0	0	0	0	0	1	0	1
9	0	0	0	0	0	0	1	1	0

A	1	2	3	4	5	6	7	8	9
1	0	1	1	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	1	1	1	0	0
4	0	1	0	0	1	0	0	0	0
5	0	0	1	1	0	0	0	0	0
6	0	0	1	0	0	0	0	0	0
7	0	0	1	0	0	0	0	1	1
8	0	0	0	0	0	0	1	0	1
9	0	0	0	0	0	0	1	1	0



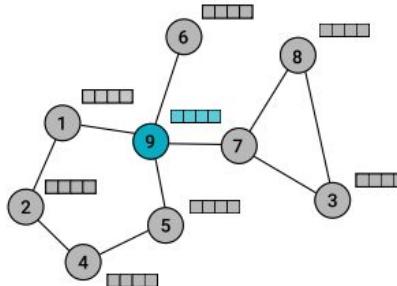
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X	1	2	3	4	5	6	7	8	9
1	0	1	0	0	0	0	0	0	1
2	1	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	1	1	0
4	0	1	0	0	1	0	0	0	0
5	0	0	0	1	0	0	0	0	1
6	0	0	0	0	0	0	0	0	1
7	0	0	1	0	0	0	0	1	0
8	0	0	1	0	0	0	1	0	0
9	1	0	0	0	1	1	1	0	0

A	1	2	3	4	5	6	7	8	9
1	0	1	0	0	0	0	0	0	1
2	1	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	1	1	0
4	0	1	0	0	1	0	0	0	0
5	0	0	0	1	0	0	0	0	1
6	0	0	0	0	0	0	0	0	1
7	0	0	1	0	0	0	0	1	0
8	0	0	1	0	0	0	1	0	0
9	1	0	0	0	1	1	1	0	0

Y	0.5	0.3	0.2
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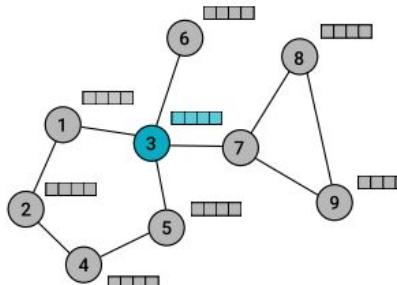
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There is no canonical order for the nodes of the graph.

Permutation equivariance

If we permute the input nodes of the graph, the nodes' output should be permuted in the same way.

$$f(PX, PAP') = Pf(X, A)$$



	X
1	
2	
3	
4	
5	
6	
7	
8	
9	

	1	2	3	4	5	6	7	8	9
1	0	1	1	0	0	0	0	0	0
2	1	0	0	0	0	0	0	0	0
3	1	0	0	0	1	1	1	0	0
4	0	1	0	0	1	0	0	0	0
5	0	0	1	1	0	0	0	0	0
6	0	0	1	0	0	0	0	0	0
7	0	0	1	0	0	0	0	1	1
8	0	0	0	0	0	0	1	0	1
9	0	0	0	0	0	0	1	1	0

1			
2			
3			
4			
5			
6			
7			
8			
9			

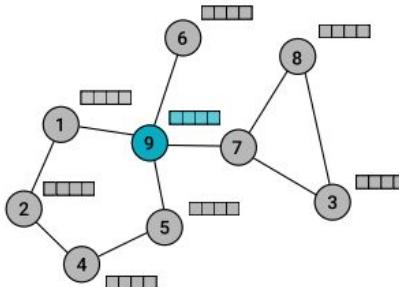
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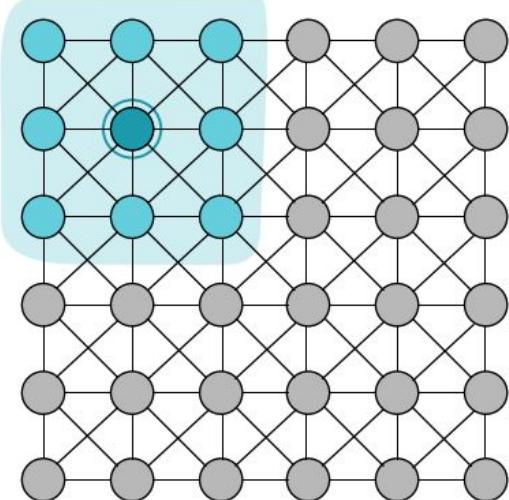


X	
1	2
2	3
3	4
4	5
5	6
6	7
7	8
8	9
9	1

A								
1	2	3	4	5	6	7	8	9
1	0	1	0	0	0	0	0	1
2	1	0	0	0	0	0	0	0
3	0	0	0	0	0	0	1	1
4	0	1	0	0	1	0	0	0
5	0	0	0	1	0	0	0	1
6	0	0	0	0	0	0	0	1
7	0	0	1	0	0	0	1	1
8	0	0	1	0	0	0	1	0
9	1	0	0	0	1	1	1	0

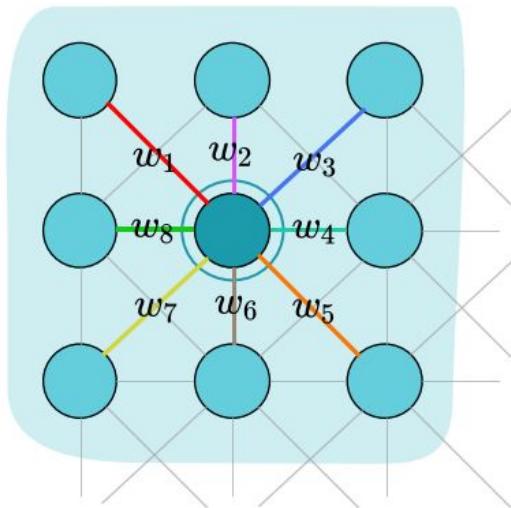
Y	
1	2
2	3
3	4
4	5
5	6
6	7
7	8
8	9
9	1

Convolutional Network



- takes into account a **neighbourhood**
- the **structure is fixed**: a grid for 2D Conv or a sequence for 1D Conv
- the model is invariant to translations

Convolutional Network



$$y_i = \sum_{j \in \mathcal{N}_i} w_j x_j$$

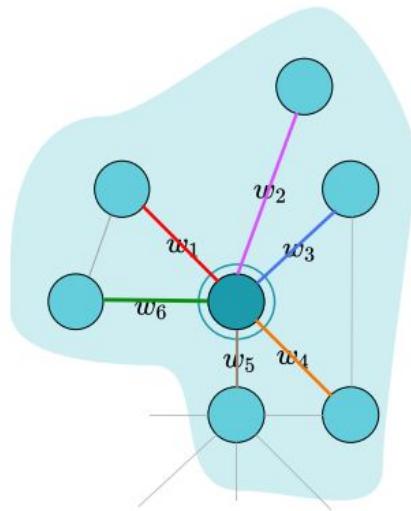
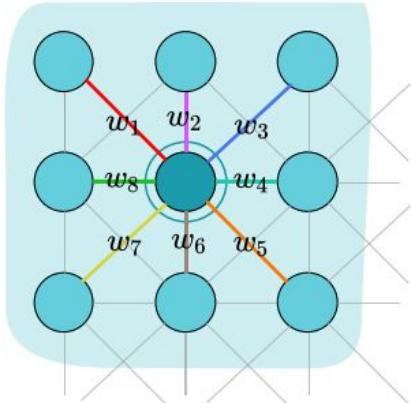
For a convolutional network the neighbourhood is

- **fixed:** for a $K \times K$ convolutional filter we combine exactly K^2 neighbours
- **ordered:** we can impose a canonical order among neighbours (left, right, up, down)

Convolutional Network

$$y_i = \sum_{j \in \mathcal{N}_i} w_j x_j$$

Can we do the same for graphs?

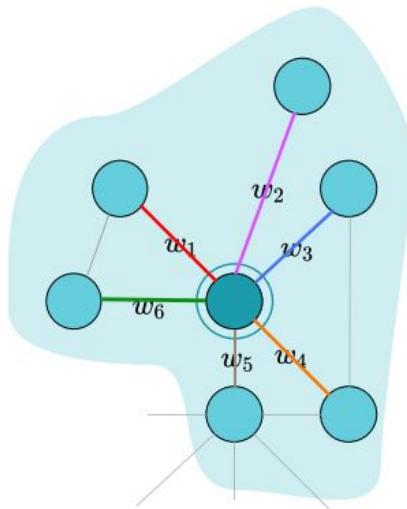
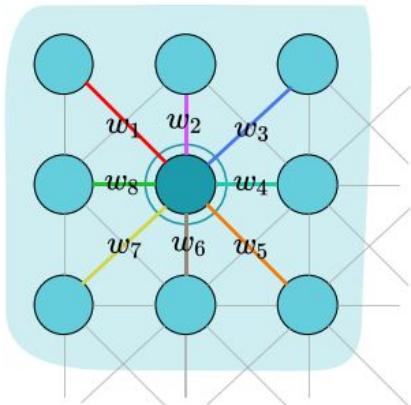


Convolutional Network

$$y_i = \sum_{j \in \mathcal{N}_i} w_j x_j$$

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- can't have variable number of weights
- have to establish an order

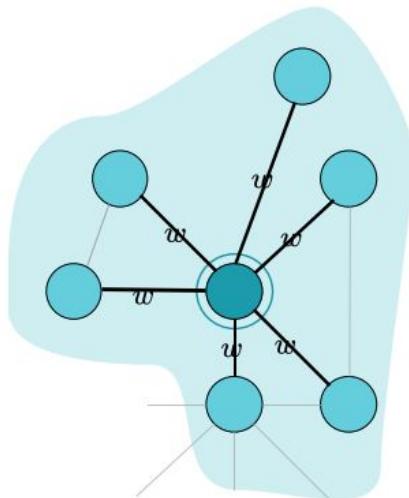
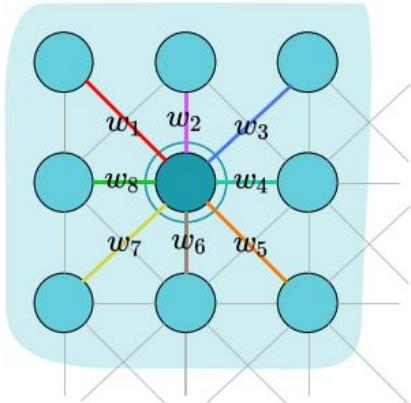


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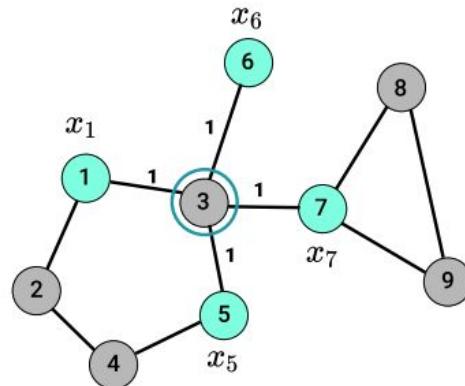
$$y_i = \sum_{j \in \mathcal{N}_i} w x_j$$

- Solution: same w for all nodes



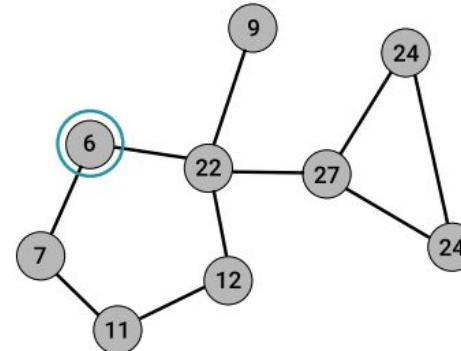
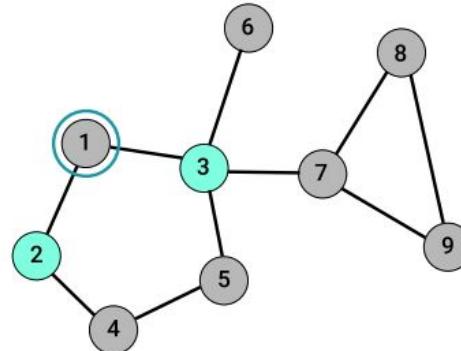
Graph Propagation

Simple graph representation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



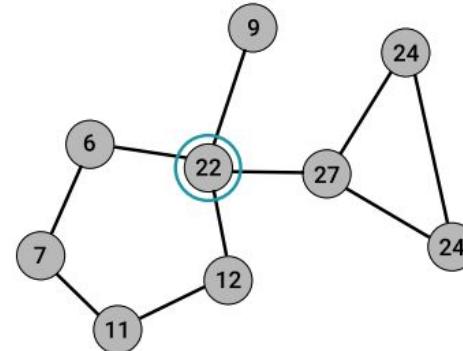
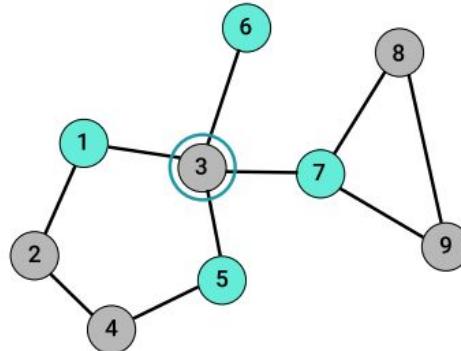
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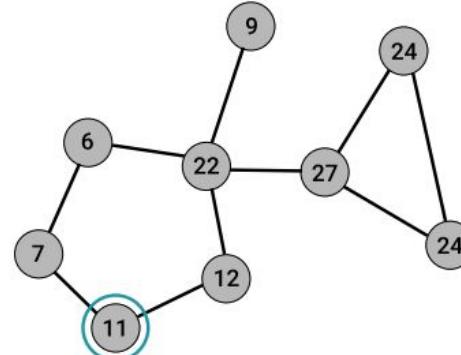
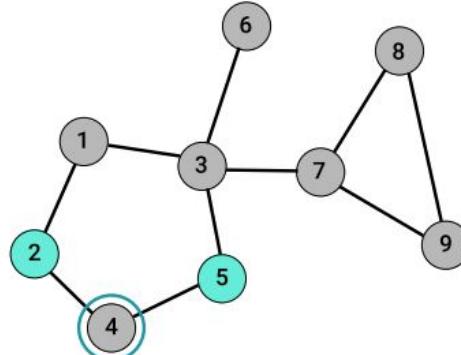
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Simple graph representation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



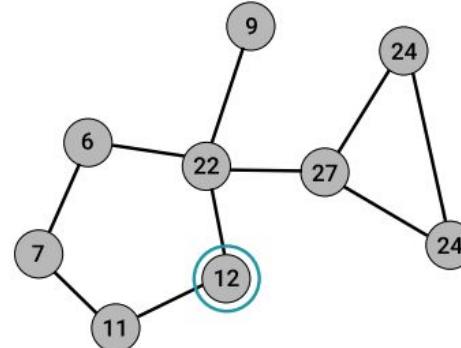
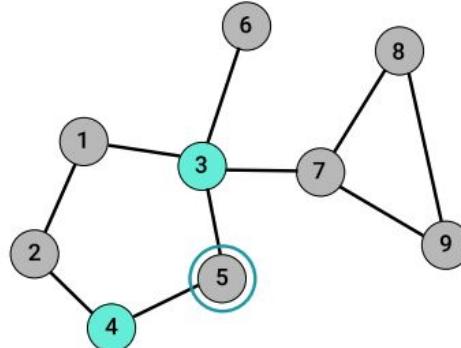
Graph Propagation

Simple graph representation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



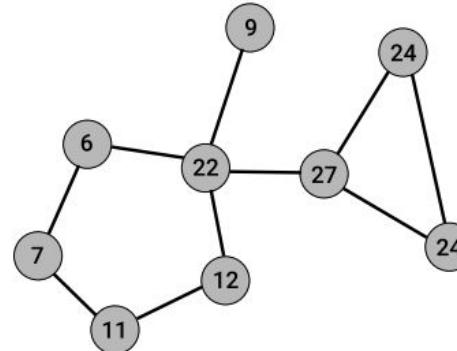
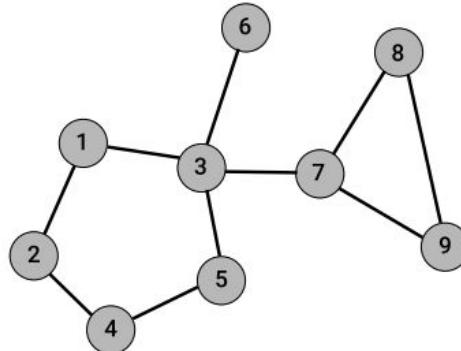
Graph Propagation

Simple graph representation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



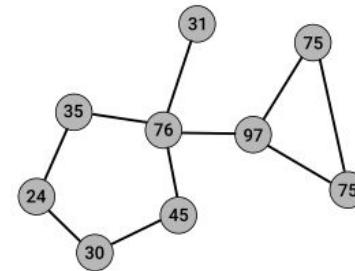
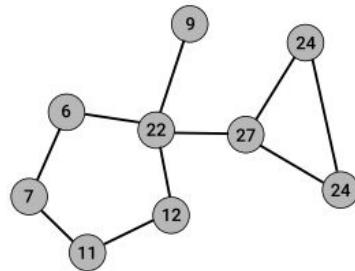
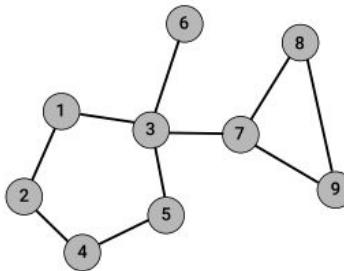
Graph Propagation

Simple graph representation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



Graph Propagation

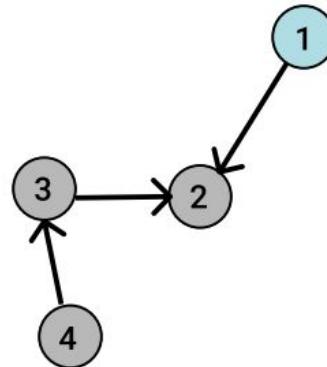
Simple graph propagation (set $w = 1$): $y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j$



- if applied iteratively, it takes into account the structure

Simplest Graph Propagation

$y_i = \sum_{j \in \mathcal{N}_i} x_j$ can be rewritten in a compact, matrix form as $Y = AX$



$$A \in \mathbb{R}^{N \times N} \quad X \in \mathbb{R}^N \quad Y \in \mathbb{R}^N$$

0	0	0	0
1	0	1	0
0	0	0	1
0	0	0	0

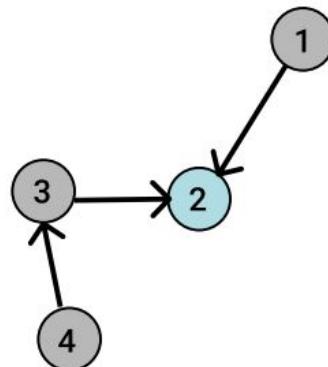
1
2
3
4

=

0

Simplest Graph Propagation

$y_i = \sum_{j \in \mathcal{N}_i} x_j$ can be rewritten in a compact, matrix form as $Y = AX$



$$A \in \mathbb{R}^{N \times N} \quad X \in \mathbb{R}^N \quad Y \in \mathbb{R}^N$$

0	0	0	0
1	0	1	0
0	0	0	1
0	0	0	0

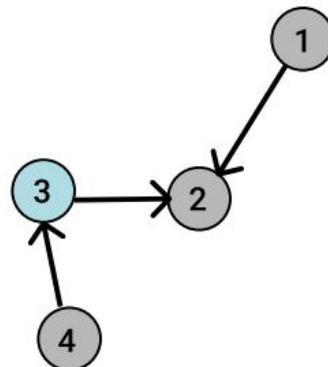
1
2
3
4

 $=$

0
1+3

Simplest Graph Propagation

$y_i = \sum_{j \in \mathcal{N}_i} x_j$ can be rewritten in a compact, matrix form as $Y = AX$



$$A \in \mathbb{R}^{N \times N} \quad X \in \mathbb{R}^N \quad Y \in \mathbb{R}^N$$

0	0	0	0
1	0	1	0
0	0	0	1
0	0	0	0

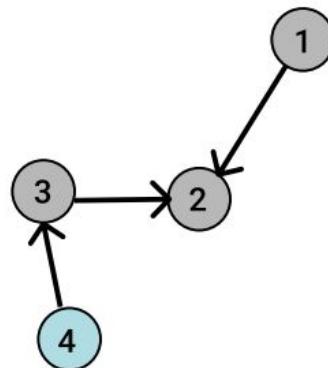
1
2
3
4

 $=$

0
1+3
4

Simplest Graph Propagation

$y_i = \sum_{j \in \mathcal{N}_i} x_j$ can be rewritten in a compact, matrix form as $Y = AX$



$$A \in \mathbb{R}^{N \times N} \quad X \in \mathbb{R}^N \quad Y \in \mathbb{R}^N$$

0	0	0	0
1	0	1	0
0	0	0	1
0	0	0	0

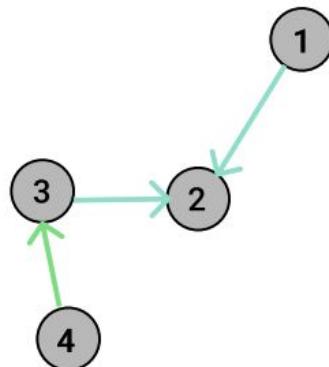
1
2
3
4

 $=$

0
1+3
4
0

Simplest Graph Propagation

$y_i = \sum_{j \in \mathcal{N}_i} x_j$ Nodes could have high-dimensional representation $X \in \mathbb{R}^{N \times D}$



$$A \in \mathbb{R}^{N \times N}$$

0	0	0	0
1	0	1	0
0	0	0	1
0	0	0	0

$$X \in \mathbb{R}^{N \times D}$$

x_1
x_2
x_3
x_4

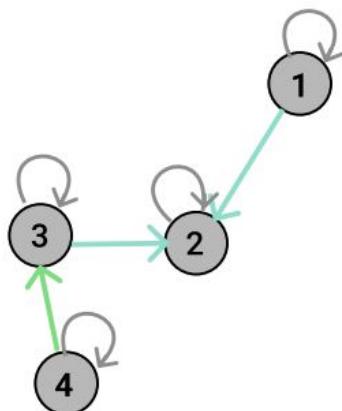
$$Y \in \mathbb{R}^{N \times D}$$

0
$x_1 + x_3$
x_4
0

 $=$

Simplest Graph Propagation

$y_i = \boxed{x_i} + \sum_{j \in \mathcal{N}_i} x_j$ We should take into account also the current node - self-loops.



$$A \in \mathbb{R}^{N \times N}$$

1	0	0	0
1	1	1	0
0	0	1	1
0	0	0	1

$$X \in \mathbb{R}^{N \times D} \quad Y \in \mathbb{R}^{N \times D}$$

x_1
x_2
x_3
x_4

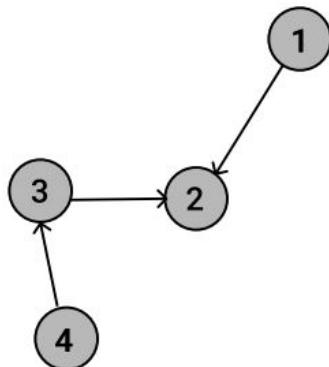
 $=$

x_1
$x_1 + x_2 + x_3$
$x_3 + x_4$
x_4

Simplest Graph Propagation

To combine more complex representations:

$$y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j \quad \rightarrow \quad y_i = x_i W + \sum_{j \in \mathcal{N}_i} x_j W$$



$$X \in \mathbb{R}^{N \times D} \quad W \in \mathbb{R}^{D \times C} \quad Y \in \mathbb{R}^{N \times C}$$

x_1
x_2
x_3
x_4



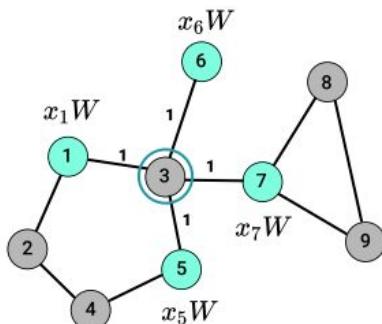
$x_1 W$
$x_2 W$
$x_3 W$
$x_4 W$

Simplest Graph Propagation

To combine more complex representations:

$$y_i = x_i + \sum_{j \in \mathcal{N}_i} x_j \quad \rightarrow \quad y_i = x_i W + \sum_{j \in \mathcal{N}_i} x_j W$$

The operations performed in the graph could be rewritten as:



$$Y = AXW$$

Iteratively, for more layers:

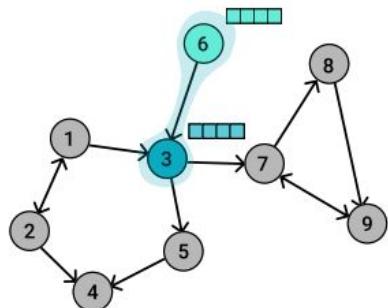
$$Y = A\sigma(AXW_1)W_2$$

$$Y = A\sigma \dots A\sigma(AXW_1)W_2 \dots W_n$$

GNNs: Message Passing Framework - Send

Send Function

- for each pair of 2 connected nodes, create a **message**



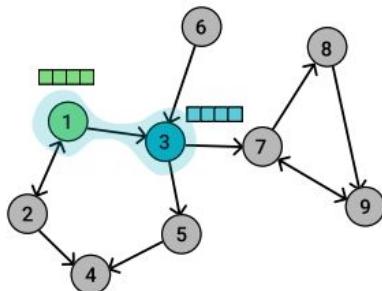
$$m_{ij} = f_{msg}(x_i, x_j) \in \mathbb{R}^C \quad \forall (i, j) \in \mathcal{E}$$

$$m_{3,6} = f_{msg}(\text{[] } , \text{[] })$$

GNNs: Message Passing Framework - Send

Send Function

- for each pair of 2 connected nodes, create a **message**



$$m_{ij} = f_{msg}(x_i, x_j) \in \mathbb{R}^C \quad \forall (i, j) \in \mathcal{E}$$

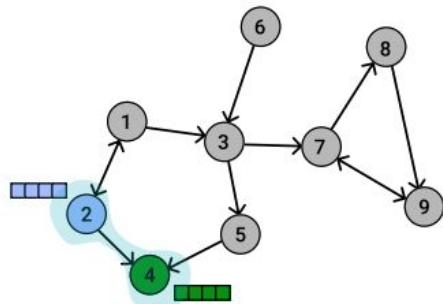
$$m_{3,6} = f_{msg}(\text{cyan bar}, \text{cyan bar})$$

$$m_{3,1} = f_{msg}(\text{cyan bar}, \text{green bar})$$

GNNs: Message Passing Framework - Send

Send Function

- for each pair of 2 connected nodes, create a **message**



$$m_{ij} = f_{msg}(x_i, x_j) \in \mathbb{R}^C \quad \forall (i, j) \in \mathcal{E}$$

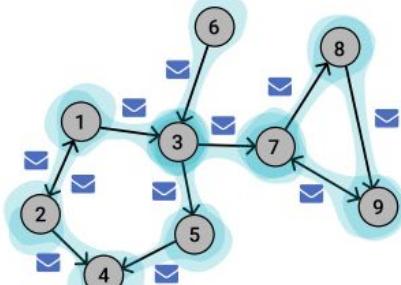
$$m_{3,6} = f_{msg}(\text{blue}, \text{blue})$$

$$m_{3,1} = f_{msg}(\text{blue}, \text{green})$$

$$m_{4,2} = f_{msg}(\text{green}, \text{blue})$$

GNNs: Message Passing Framework - Send

- f_{msg} is a learnable function (e.g. an MLP)
- its parameters are shared between each pair of nodes



Learnable function

$$m_{ij} = \overbrace{f_{msg}(x_i, x_j)}^{\text{Learnable function}} \in \mathbb{R}^C \quad \forall (i, j) \in \mathcal{E}$$

$$m_{3,6} = f_{msg}(\text{[red box]}, \text{[green box]})$$
$$m_{3,1} = f_{msg}(\text{[red box]}, \text{[blue box]})$$

...

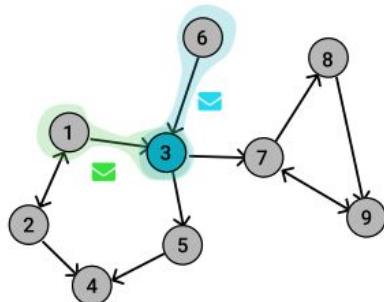
$$m_{4,2} = f_{msg}(\text{[green box]}, \text{[blue box]})$$

Same parameters

GNNs: Message Passing Framework - Aggregation

Aggregation Function

For each node i , **aggregate** the incoming messages from all its neighbours.



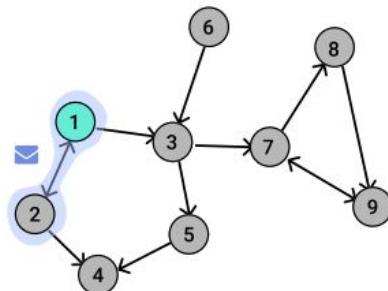
$$h_i = f_{agg}(\{m_{ij} | \forall j \in \mathcal{N}_i\})$$

$$h_3 = f_{agg}(\{ \text{green message}, \text{blue message} \})$$

GNNS: Message Passing Framework - Aggregation

Aggregation Function

For each node i , **aggregate** the incoming messages from all its neighbours.



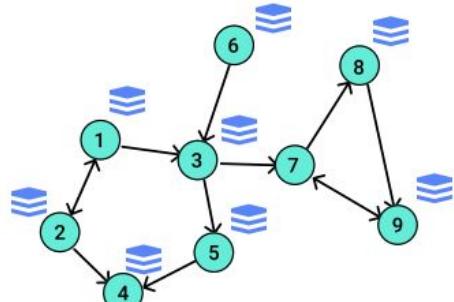
$$h_i = f_{agg}(\{m_{ij} \mid \forall j \in \mathcal{N}_i\})$$

$$h_3 = f_{agg}(\{ \text{green}, \text{blue}, \text{green} \})$$

$$h_1 = f_{agg}(\{ \text{blue} \})$$

GNNs: Message Passing Framework - Aggregation

- aggregate incoming messages with the function f_{agg} :
eg. sum, mean, max, min
- it should be **invariant to the order** of the nodes and
should **allow a variable number** of messages



operator
$$h_i = \overbrace{f_{agg}}^{\text{operator}} (\{m_{ij} | \forall j \in \mathcal{N}_i\}) \in \mathbb{R}^C$$

$$h_3 = f_{agg}(\{ \text{✉}, \text{✉} \})$$

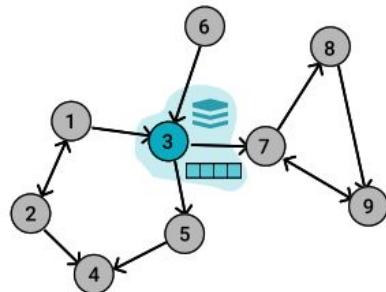
...

$$h_1 = f_{agg}(\{ \text{✉} \})$$

GNNs: Message Passing Framework - Update

Update Function

For each node i , **update** its representation using the aggregated message.



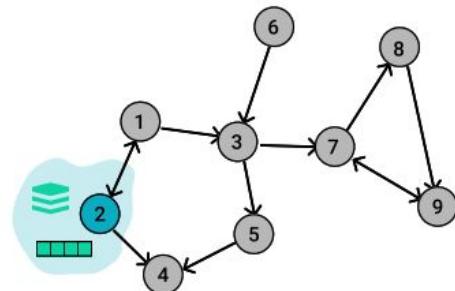
$$\tilde{x}_i = f_{upd}(x_i, h_i)$$

$$\tilde{x}_3 = f_{upd}(\text{█ , █})$$

GNNs: Message Passing Framework - Update

Update Function

For each node i , **update** its representation using the aggregated message.



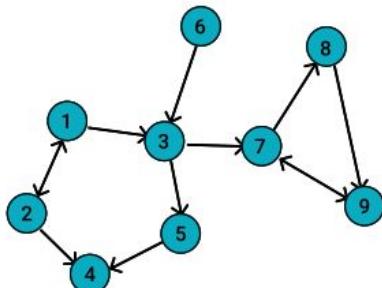
$$\tilde{x}_i = f_{upd}(x_i, h_i)$$

$$\tilde{x}_3 = f_{upd}(\text{[] } , \text{[] })$$

$$\tilde{x}_2 = f_{upd}(\text{[] } , \text{[] })$$

GNNs: Message Passing Framework - Update

- f_{upd} is a learnable function (e.g. an MLP)
- its parameters are shared between all the nodes



Learnable function

$$\tilde{x}_i = \overbrace{f_{upd}(x_i, h_i)}^{\text{Learnable function}} \in \mathbb{R}^C$$

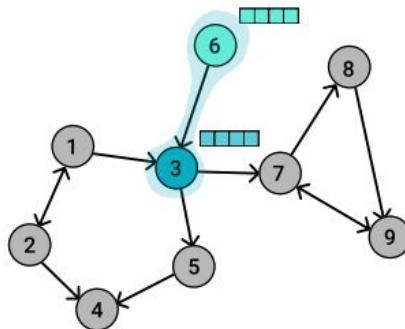
$$\begin{aligned}\tilde{x}_3 &= f_{upd}(\text{---}, \text{---}) \\ &\dots \\ \tilde{x}_2 &= f_{upd}(\text{---}, \text{---})\end{aligned}$$

Same parameters

GNNs - Overview

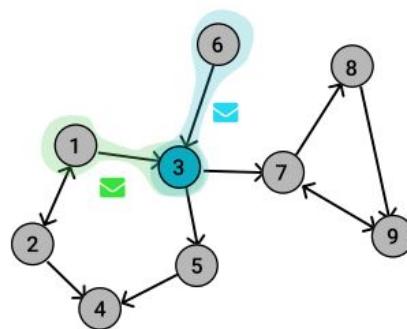
1. Send

$$m_{ij} = f_{msg}(x_i, x_j)$$



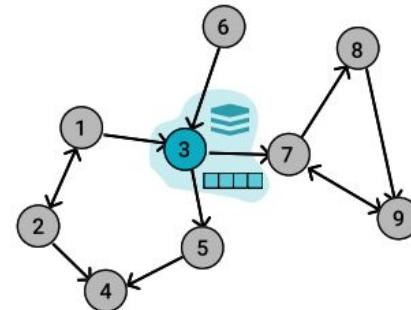
2. Aggregate

$$H_i = f_{agg}(\{m_{ij} | \forall j \in \mathcal{N}_i\})$$



3. Update

$$\tilde{x}_i = f_{upd}(x_i, H_i)$$



General GNN framework

$$f_{upd}\{x_i, \ f_{agg}\{ f_{msg}(x_i, x_j) \mid \forall j \in \mathcal{N}_i \} \}$$

Depending on how the 3 functions are instantiated, different architectures could be obtained:

Convolutional GNNs

$$f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\phi(x_j)\})$$

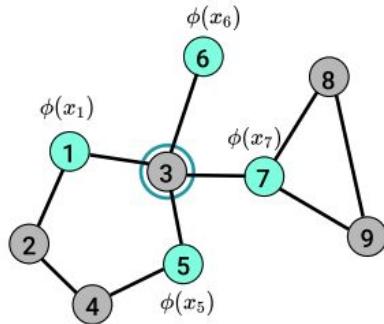
Attention GNNs

$$f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\alpha(x_i, x_j)\phi(x_j)\})$$

Message Passing

$$f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\phi(x_i, x_j)\})$$

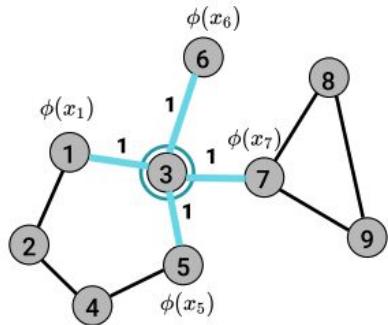
Graph Convolutional Network



$$y_i = f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{ \phi(x_j) \})$$

- messages depend only on the source nodes

Graph Convolutional Network



$$y_i = f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\phi(x_j)\})$$

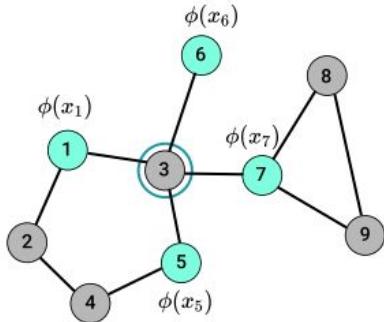
- messages depend only on the source nodes
- aggregation function is implemented as a sum/mean operation
- aggregation could be normalized according to the nodes' degree: $\frac{1}{\sqrt{deg(i)deg(j)}}$

Matrix form: $Y = \sigma(\tilde{A}XW)$

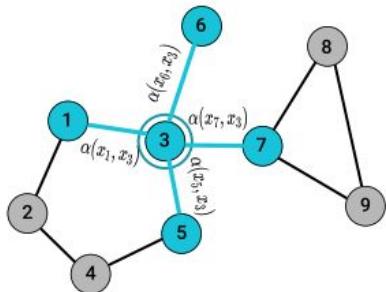
Graph Attention Network

$$y_i = f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\alpha(x_i, x_j) \{ \phi(x_j) \} \})$$

- messages depend only on the source nodes



Graph Attention Network



$$y_i = f_{upd}(x_i, \{ \bigoplus_{\forall j \in \mathcal{N}_i} \{ \alpha(x_i, x_j) \phi(x_j) \} \})$$

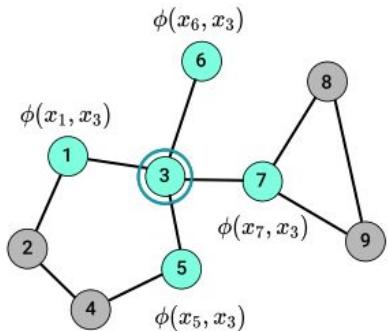
- messages depend only on the source nodes
- aggregation function is based on attention mechanism

GAT: $\alpha(x_i, x_j) \propto \text{ReLU}(a[x_i W_1, x_j W_2]^T) \in \mathbb{R}$

Self-Attention: $\alpha(x_i, x_j) \propto x_i W_1 (x_j W_2)^T \in \mathbb{R}$

- the model is able to learn the desired structure

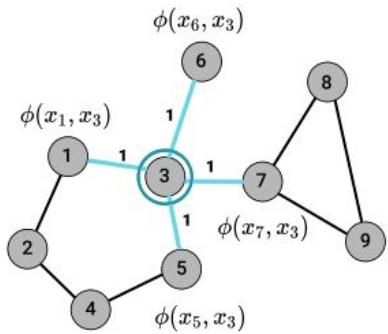
Message Passing Neural Network



$$y_i = f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{ \phi(x_i, x_j) \})$$

- messages depend on both source and destination
- if edge features are available, the message could also take them into account

Message Passing Neural Network

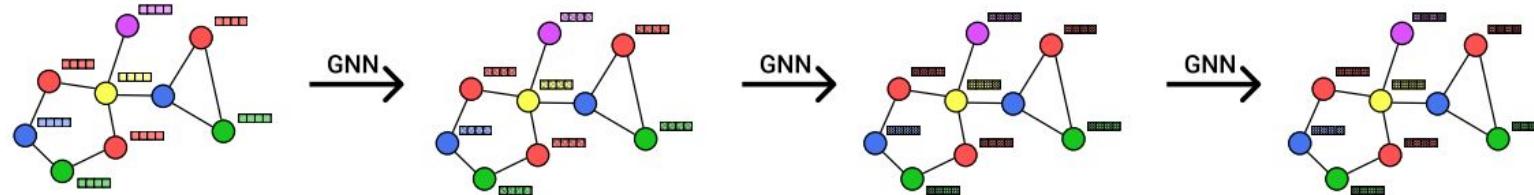


$$y_i = f_{upd}(x_i, \bigoplus_{\forall j \in \mathcal{N}_i} \{\phi(x_i, x_j)\})$$

- messages depend on both source and destination
- if edge features are available, the message could also take them into account
- aggregation function is implemented as a sum/mean operation

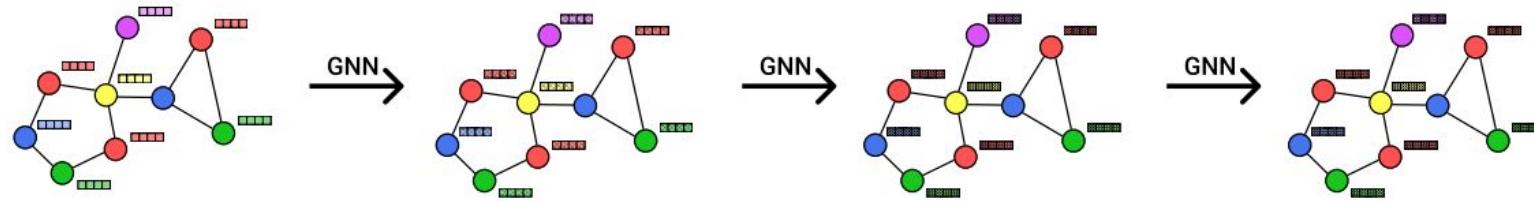
Multiple Layers

- for a more powerful representation, we can stack multiple layers

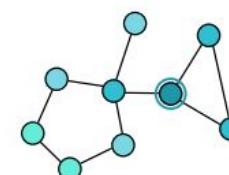
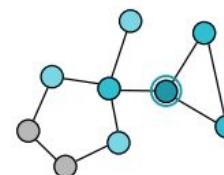
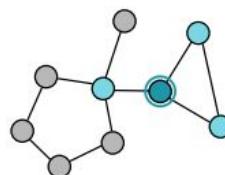
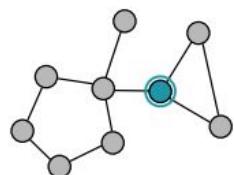


Multiple Layers

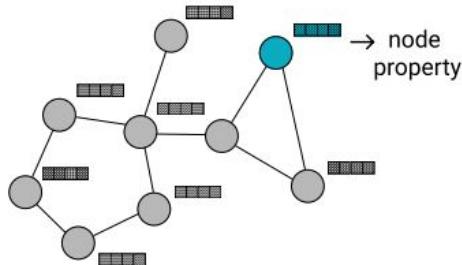
- for a more powerful representation, we can stack multiple layers
- each layer increases the receptive field of each node



RECEPTIVE FIELD:



Graph Output - Node Level



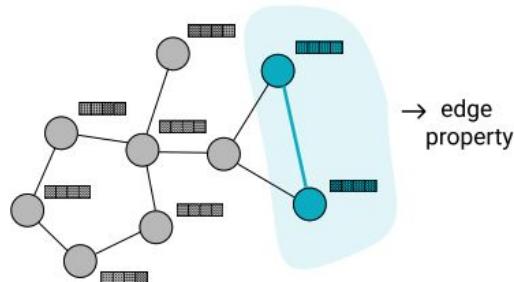
- predict an output y_i from each node

$$y_i = f_{output}(\tilde{x}_i) \in \mathbb{R}^K$$

- the loss function is applied for each node in the graph

$$\mathcal{L} = \sum_{i \in \mathcal{V}} \mathcal{L}_i(y_i, l_i)$$

Graph Output - Edge Level

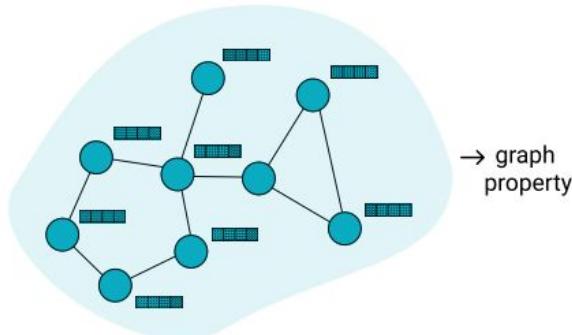


- predict an output y_{ij} from each pair of nodes
$$y_{ij} = f_{output}(\tilde{x}_i, \tilde{x}_j) \in \mathbb{R}^K$$

- the loss function is applied for each edge in the graph

$$\mathcal{L} = \sum_{(i,j) \in \mathcal{E}} \mathcal{L}_i(y_{ij}, l_{ij})$$

Graph Output - Graph Level



- predict a single output y for the whole graph

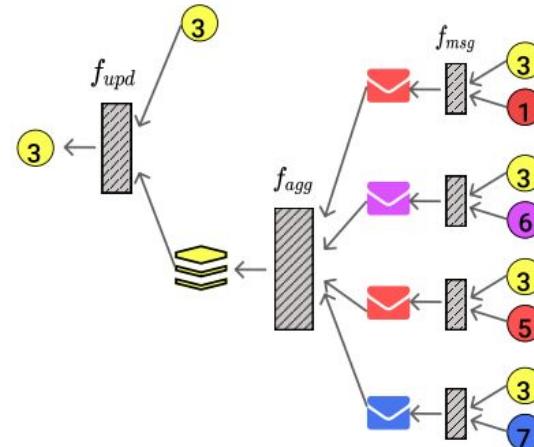
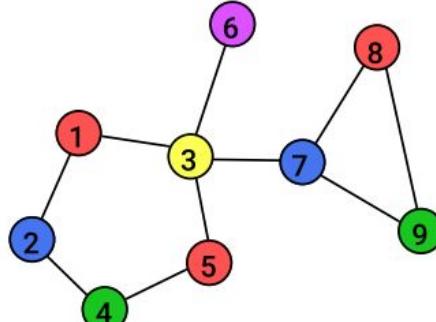
$$y = f_{readout}(\{\tilde{x}_i | \forall i \in \mathcal{V}\}) \in \mathbb{R}^K$$

- $f_{readout}$ could be a simple order-invariant aggregator (e.g. sum, mean), or more complex graph pooling mechanisms
- the loss function is applied for each graph in the dataset

$$\mathcal{L} = \mathcal{L}_i(y, l)$$

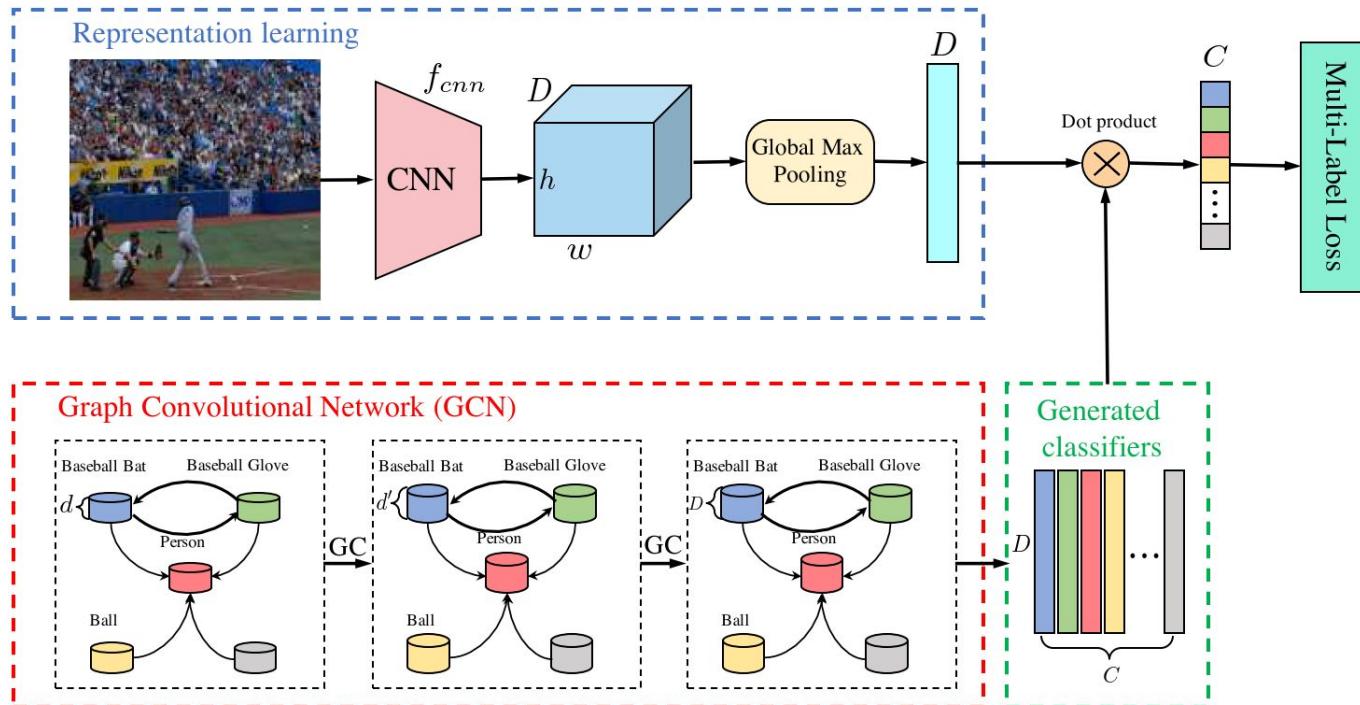
Learning

- the output of a GNN for a node i is obtained by applying a **sequence of operations** on the initial nodes
- all the operations along the sequence should be **differentiable**



GNN applications in vision

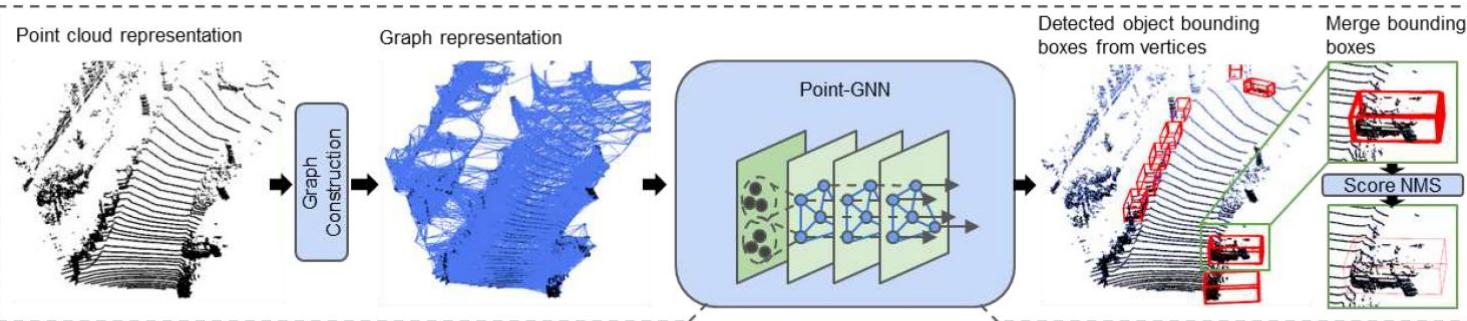
Multi-label image classification



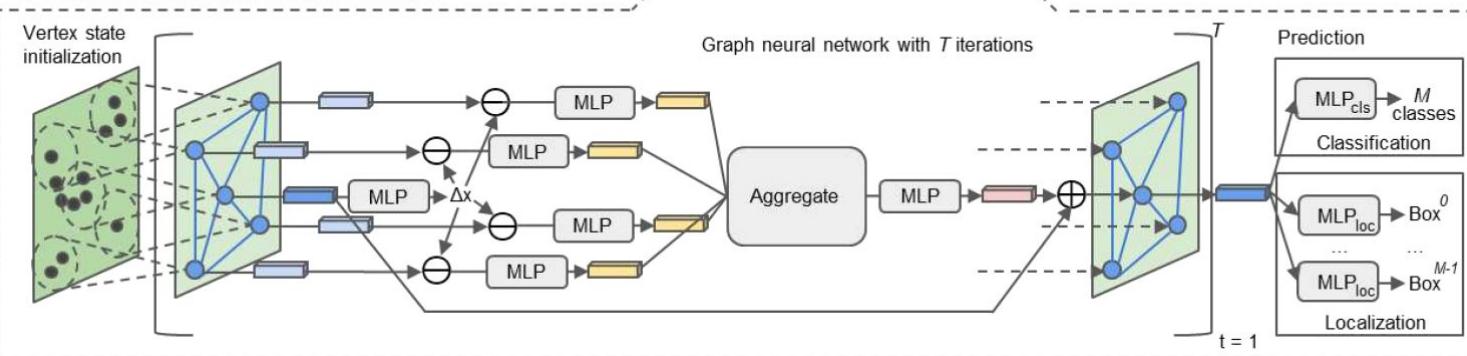
Chen, Zhao-Min, Xiu-Shen Wei, Peng Wang, and Yanwen Guo. "Multi-label image recognition with graph convolutional networks." In Proceedings of the IEEE/CVF conference on computer vision and pattern recognition, pp. 5177-5186. 2019.

Object detection from 3D point clouds

a: Graph Construction from a Point Cloud

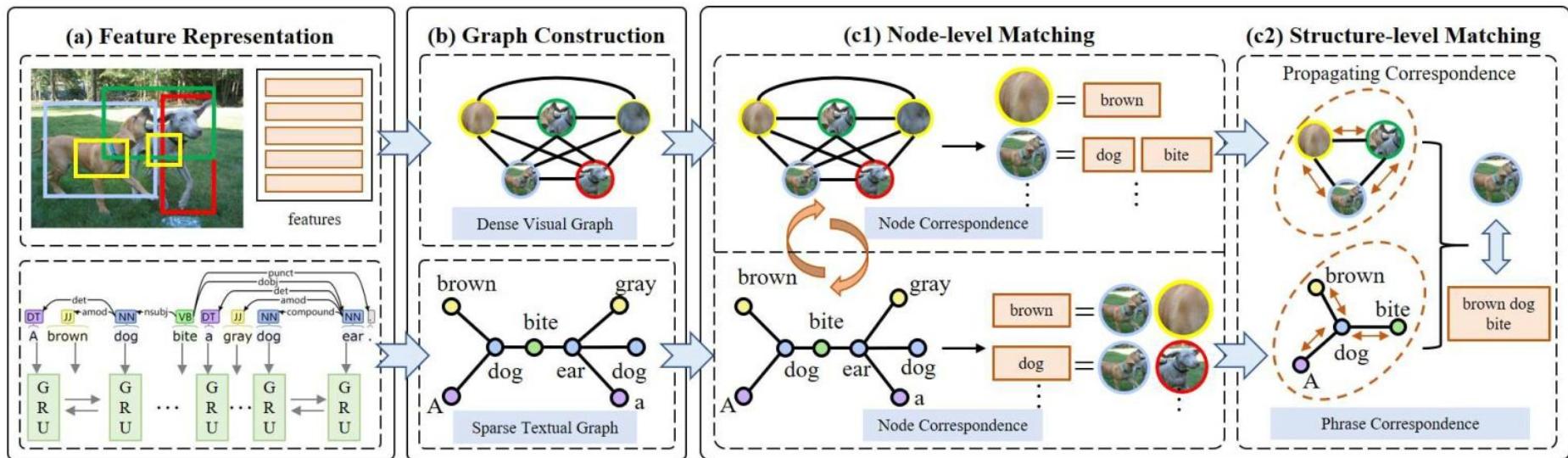


b: Graph Neural Network for Object Detection

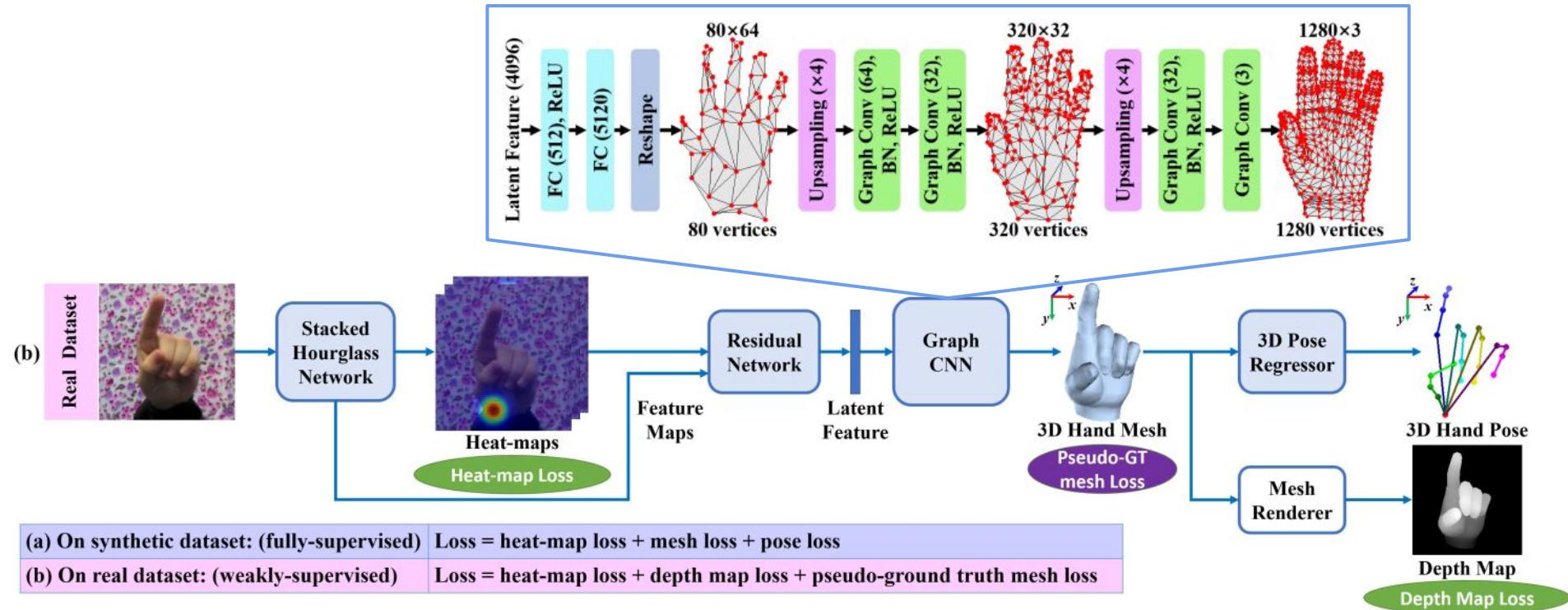


Shi, Weijing, and Raj Rajkumar. "Point-gnn: Graph neural network for 3d object detection in a point cloud." In Proceedings of the IEEE/CVF conference on computer vision and pattern recognition, pp. 1711-1719. 2020.

Image-text matching



3D hand mesh reconstruction



Ge, Liuhan, Zhou Ren, Yuncheng Li, Zehao Xue, Yingying Wang, Jianfei Cai, and Junsong Yuan. "3d hand shape and pose estimation from a single rgb image." In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp. 10833-10842. 2019.