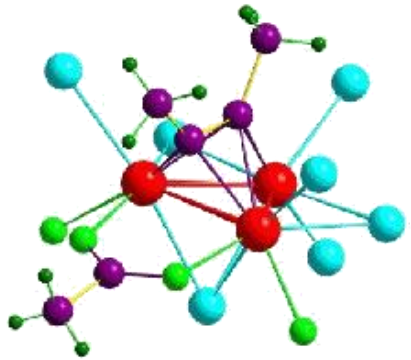
Modelling Structure with Graph Neural Networks

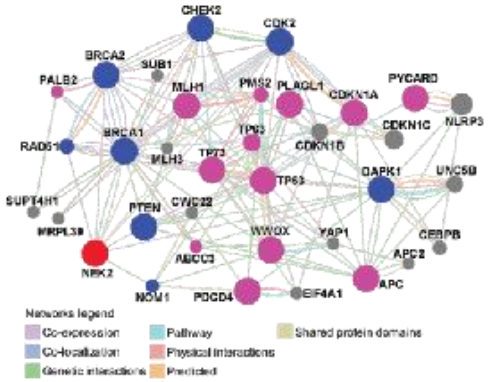
Lei Li

Language Technologies Institute | Carnegie Mellon University School of Computer Science

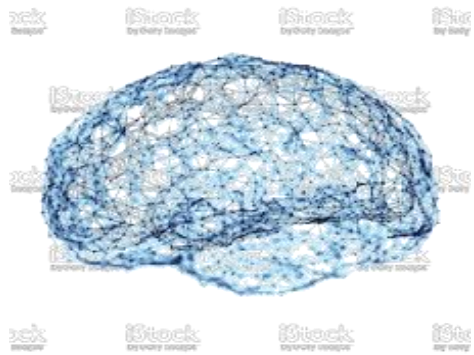
Graph Data is everywhere



Molecular Graphs

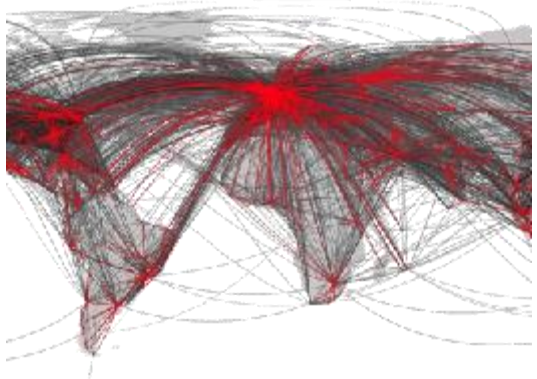


Gene Graphs



Brain Graphs

Web Graphs



Transportation Graphs

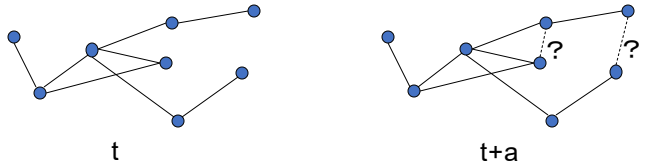
Social Graphs

Tasks on Graph Data

Node-level

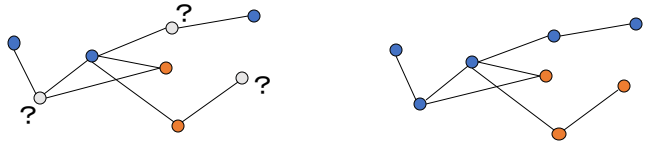
Link Prediction

is there a bond between two atoms?



Node Classification

is this atom C or N?

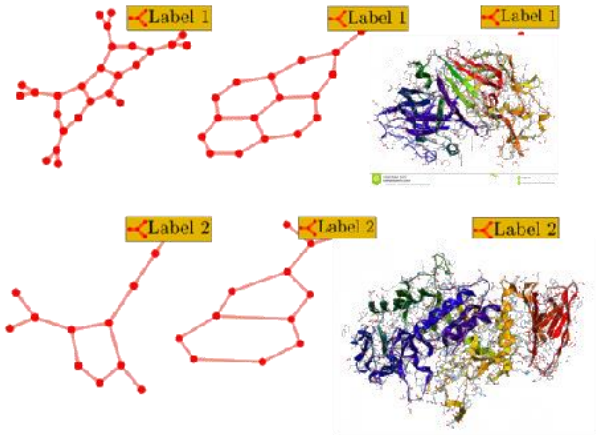


Structure prediction

what are 3D coordinates of atoms/residues?

Graph-level

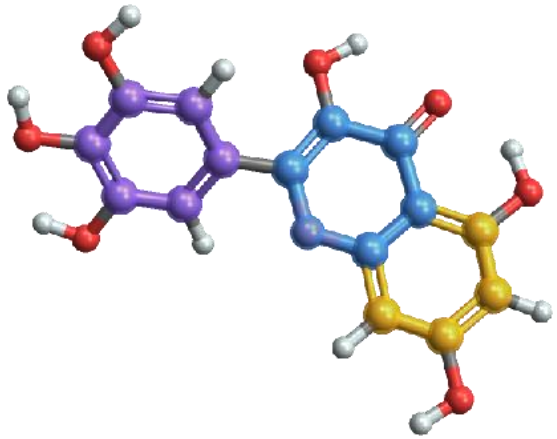
Predicting properties of a graph

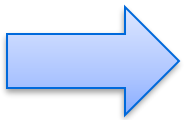


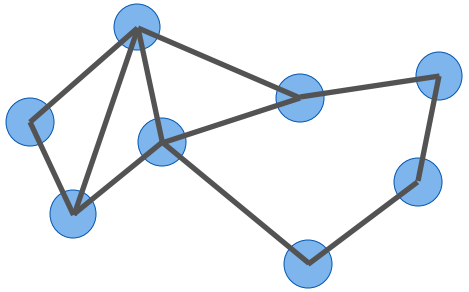
Is a molecule toxic to animals?

Example: predict toxicity of a drug

Toxic?



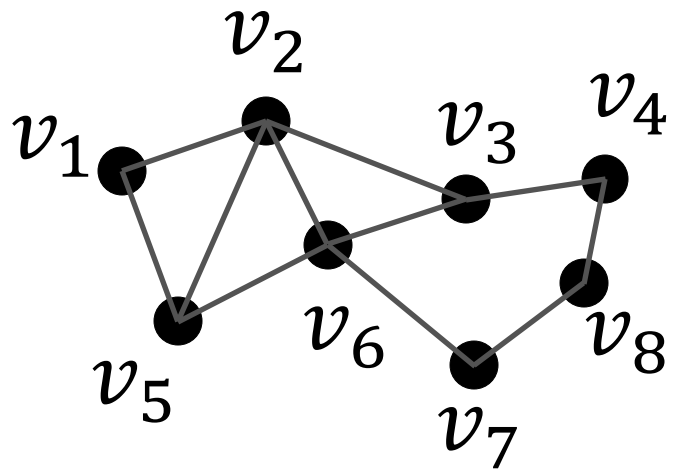




Outline

- Message Passing Neural Network
- Equivariant Graph Neural Network
- Code Example

Graph Representation



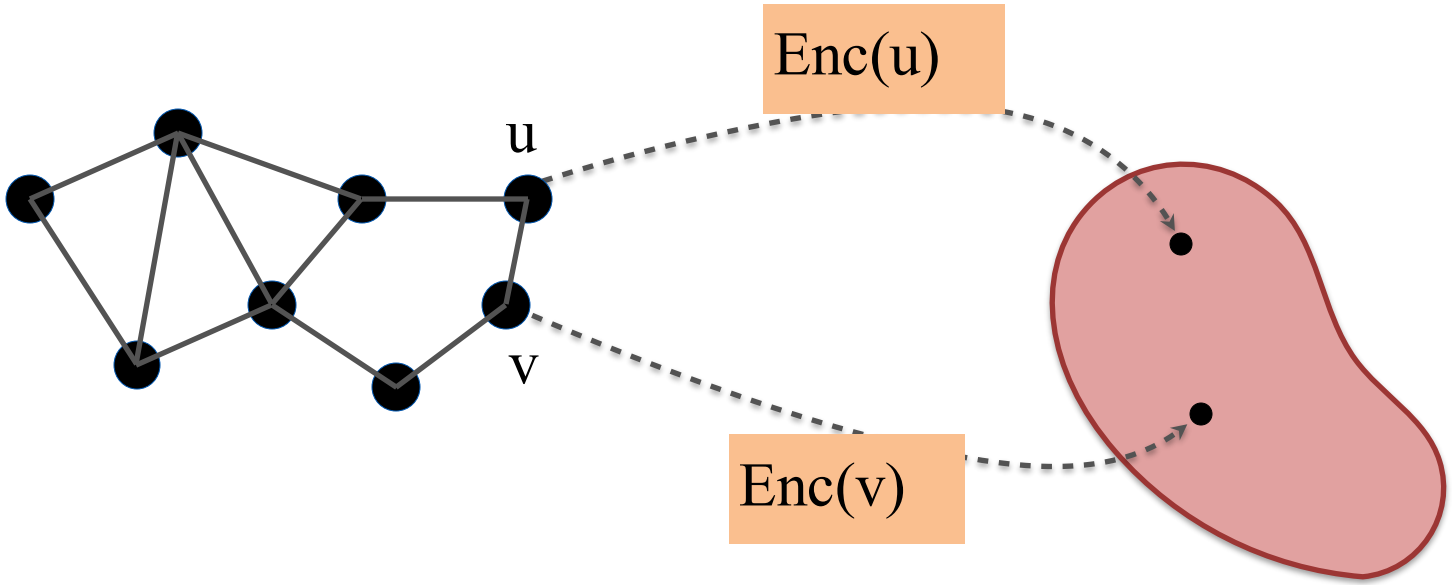
Graph: $G = \{V, E\}$

Nodes: $V = \{v_1, v_2, \ldots, v_N\}$

Edges: $E = \{e_1, e_2, \ldots, e_M\} \subset V \times V$

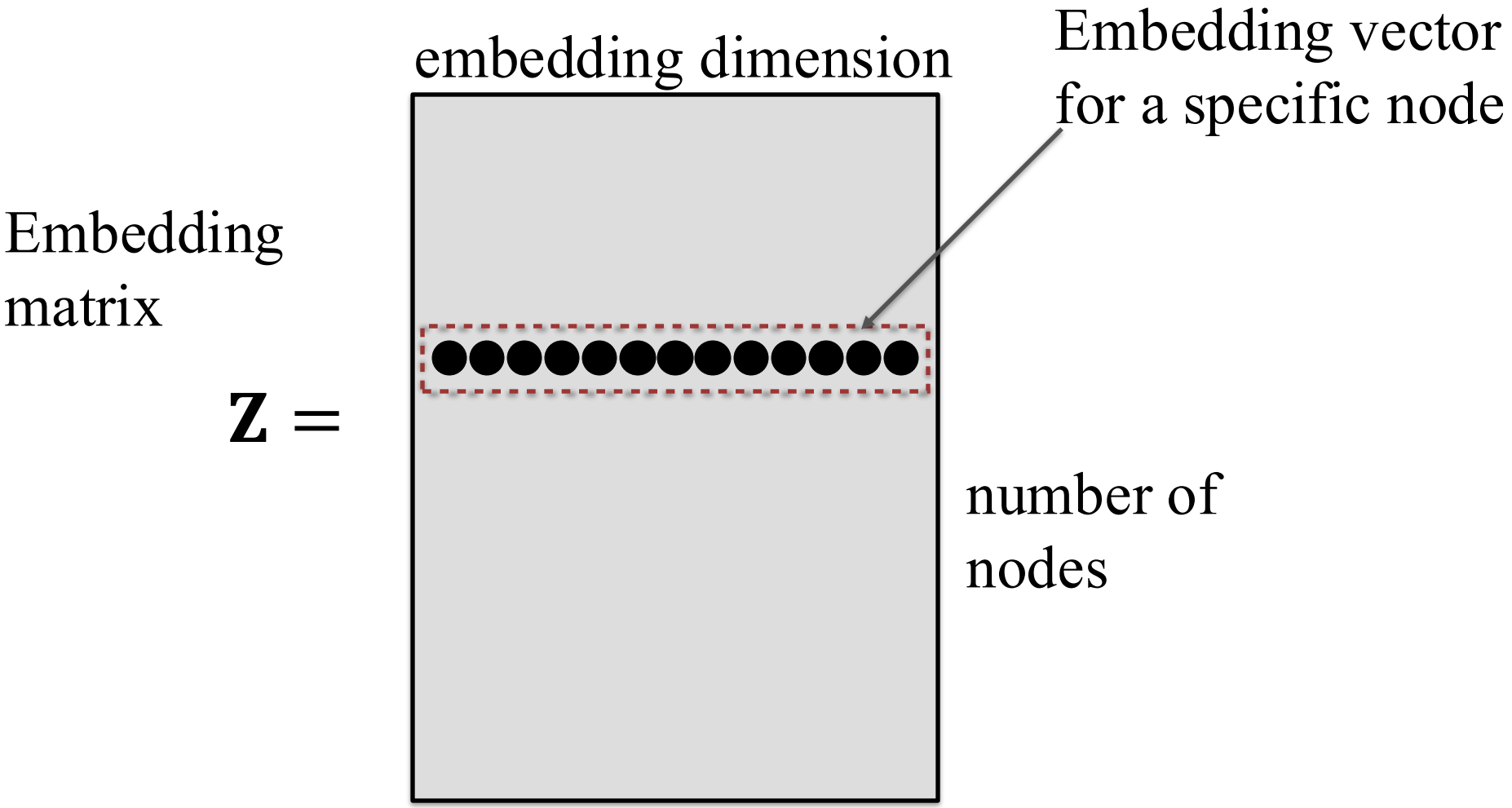
Node Embedding

$$Enc(\cdot): V \rightarrow \mathbb{R}^d$$

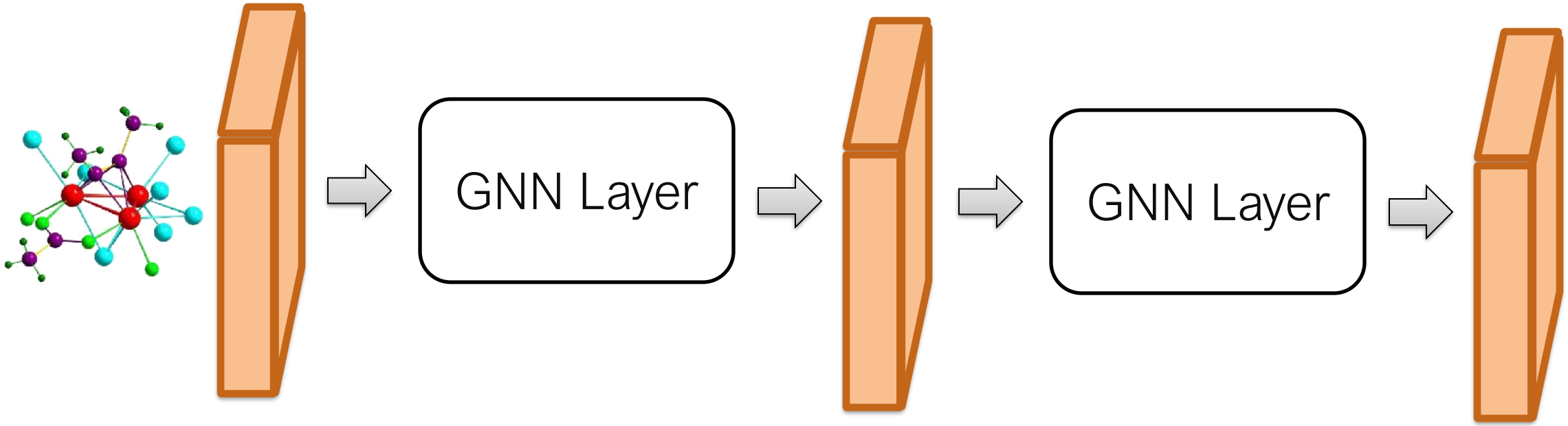


“Shallow” Node Embedding

- is just a lookup-table



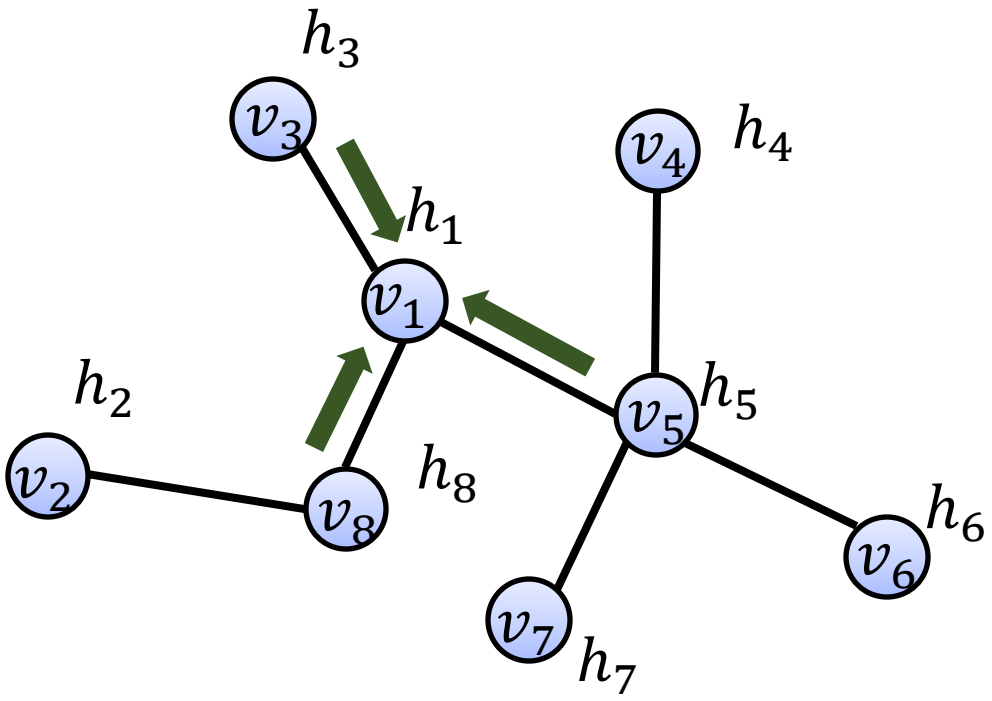
Graph Neural Network



Output is an embedding matrix for nodes
for further downstream tasks: e.g. node property prediction

Message Passing Neural Network

Every node receives message from its neighbors, aggregate and update



$\mathbf{h_i}$: node embedding vector

aggregate information from its neighbors

$$h_i^{k+1} = U^k\left(\text{Aggregate}_{v_j \in N(v_i)} m_{j\to i}^k\right), \forall v_i \in V$$

$\mathbf{N(v_i)}$: Neighbors of the node $\mathbf{v_i}$

$\mathbf{m_{j\to i}^k}$: message from node j to i at k-th layer

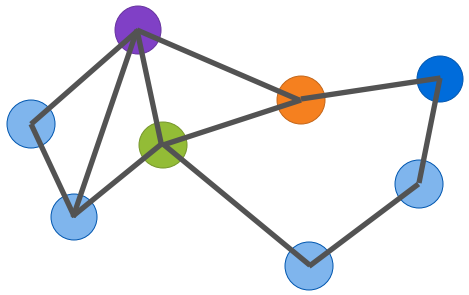
Aggregate can be avg, sum, max/min etc.

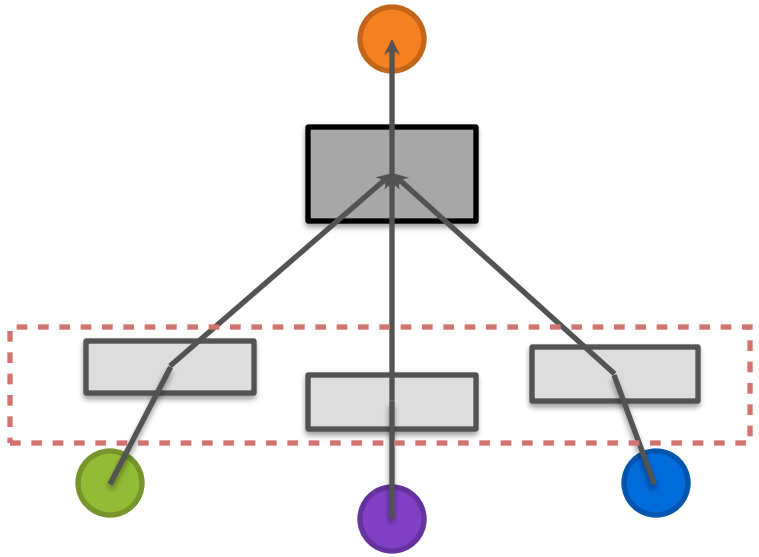
MPNN Message Computation

- Each node will create a message $m_{j \to i} = M^k(h_i^k, h_j^k, e_{ij})$
  - Dependent on incoming node (h_j^k), target node (h_i^k), edge feature

- e.g. Linear projection or FFN

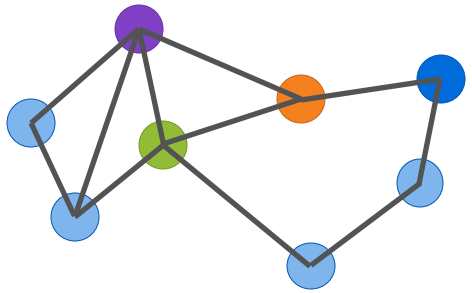
$\sigma(W_k \cdot [h_i^k, h_j^k, e_{ij}])$

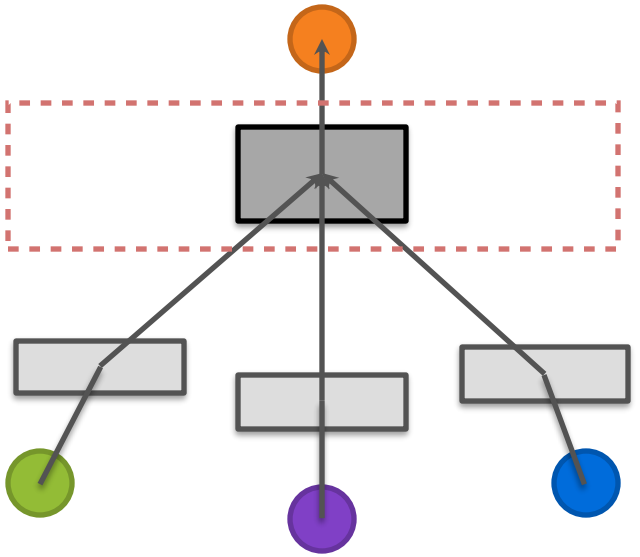




Message Aggregation/Pooling

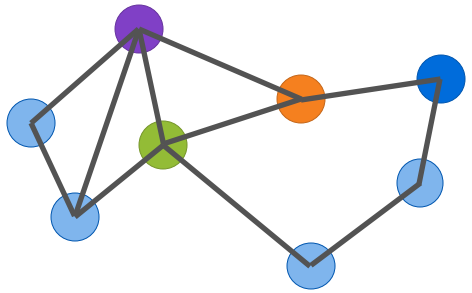
- Each node will aggregate messages from its neighbors
- Aggregate function can be
  - Sum, Mean, Max operator
  - $m_i^{k+1} = \sum_{v_j \in N(v_i)} M^k(h_i^k, h_j^k, e_{ij})$

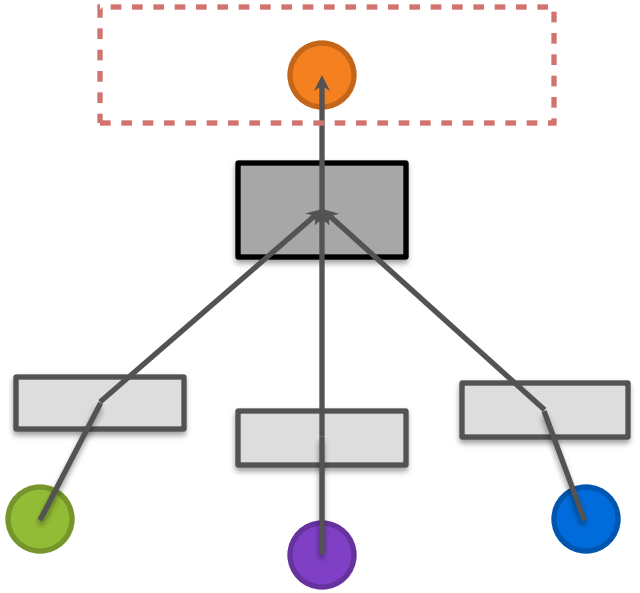




Message Update

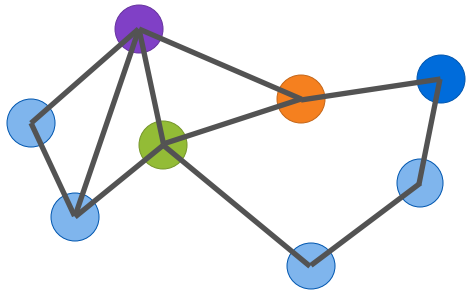
- Combine message and current node embbeding
- Apply FFN
  - $h_i^{k+1} = U^k(h_i^k, m_i^{k+1})$

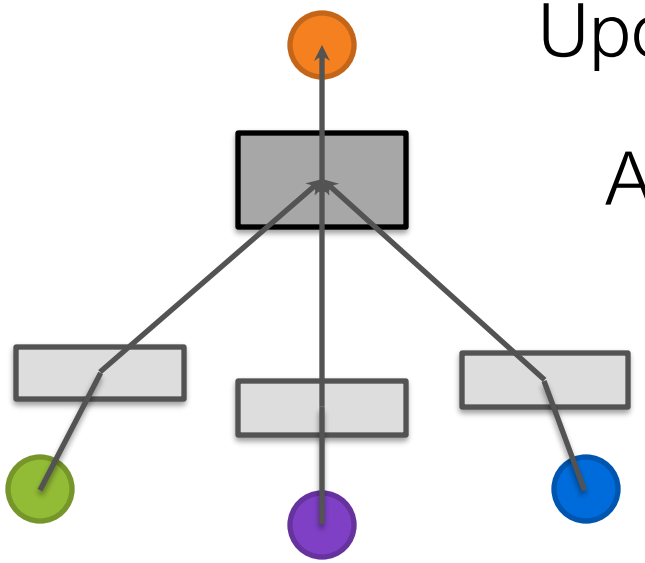




Generic framework: Message Passing NN

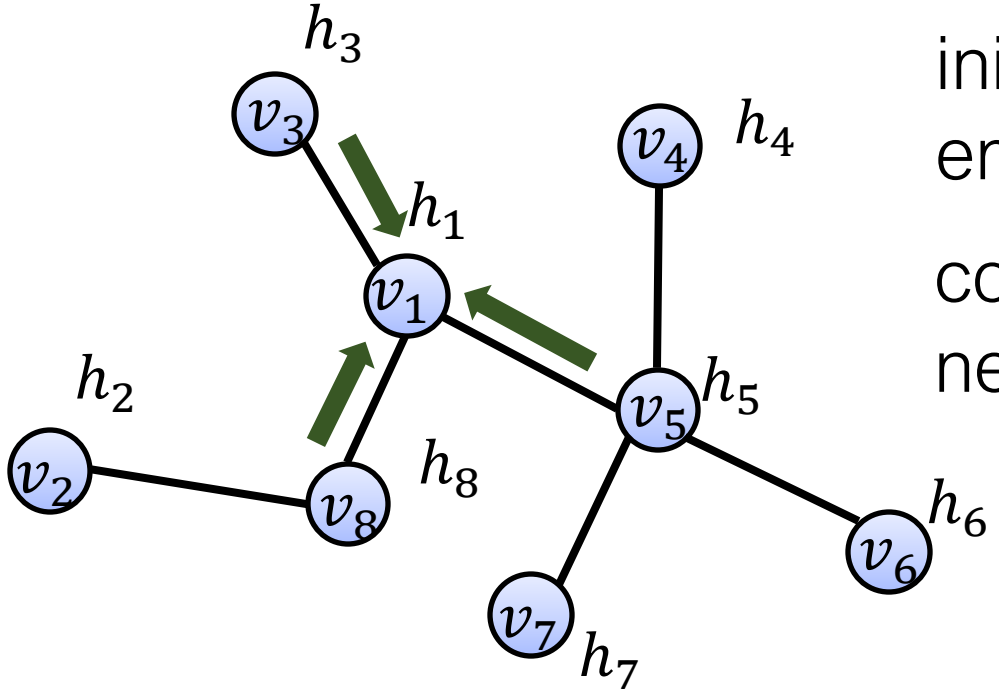
- MPNN = Message passing + Aggregation + Update
  - propagate nonlinear messages along graph topology
  - flexible and generic design choices under this framework
  - Graph convolutional network (GCN)
  - GraphSAGE
  - Graph Attention Network (GAT)





A Simple Graph Convolution Network

- averaging neighbor's message and apply nonlinear transformation



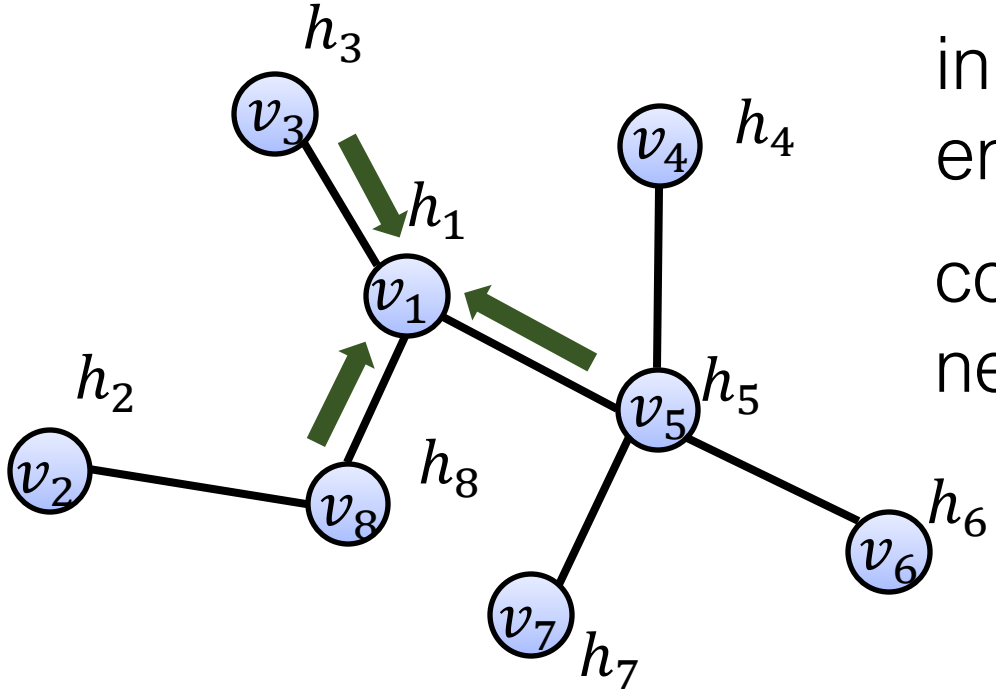
initial embedding: $\mathrm{h_i^0 = x_i}$

computing next layer: $h_i^{k+1} = \sigma\left(W_k \frac{1}{|N(v_i)|} \sum_{v_j \in N(v_i)} h_j^k + B_k h_i^k\right)$

example: $h_1^2 = tanh\left(W_1 \cdot \frac{1}{3}(h_3^1 + h_5^1 + h_8^1) + B_1 h_1^1\right)$

A Simple Graph Convolution Layer

- averaging neighbor's message and apply nonlinear transformation

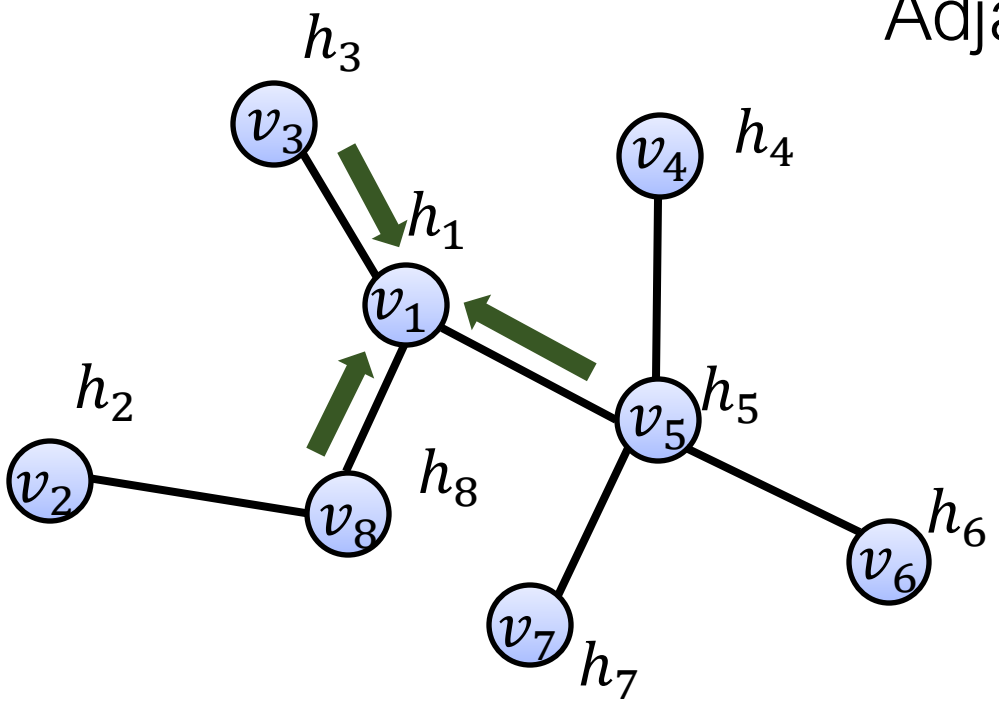


initial embedding: $\mathrm{h_i^0 = x_i}$

computing next layer: $\mathrm{h_i^{k+1} = \sigma\left(W_k \frac{1}{|N(v_i)|} \sum_{v_j \in N(v_i)} h_j^k + B_k h_i^k \right)}$

next layer: $h_1^{(3)} = tanh\left(W_2 \cdot \frac{1}{3}(h_3^{(2)} + h_5^{(2)} + h_8^{(2)}) + B_2 h_1^{(2)} \right)$

Matrix Representations of Graphs



Adjacency Matrix: $\mathrm{A[i,j]} = 1$ if $\mathrm{v_i}$ is adjacent to $\mathrm{v_j}$

$\mathrm{A[i,j]} = 0$, otherwise

Adjacency Matrix $\boldsymbol{A}$

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Matrix Representation of GCN

- Neighbor Aggregation can be performed efficiently using matrix operations

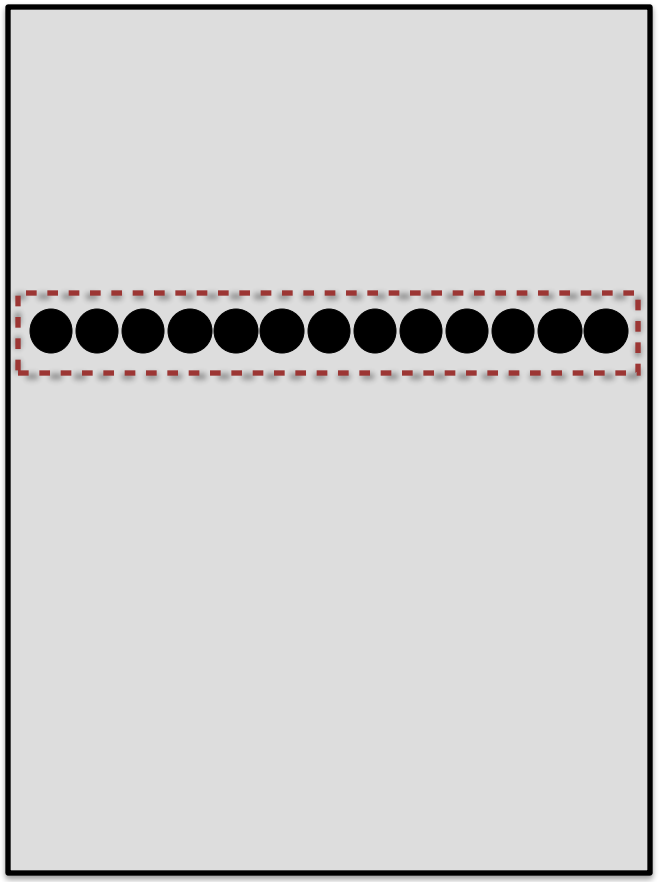
$H^k = [h_1^k, \ldots, h_{|V|}^k]^T$

Then $\sum_{v_j \in N(v_i)} h_j^k = A_{i,:} H^k$

Let D be diagonal matrix (0 elsewhere)

$D_{i,i} = \text{Degree}(v_i) = \sum_j A_{i,j}$

Then $\frac{1}{|N(v_i)|} \sum_{v_j \in N(v_i)} h_j^k = D^{-1} A H^k$



Aggregation Neighbor's Information in Matrix form

$$\frac{1}{|N(v_i)|}\sum_{v_j \in N(v_i)} h_j^k = D^{-1}AH^k$$

D^{-1}

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}^{-1}$$

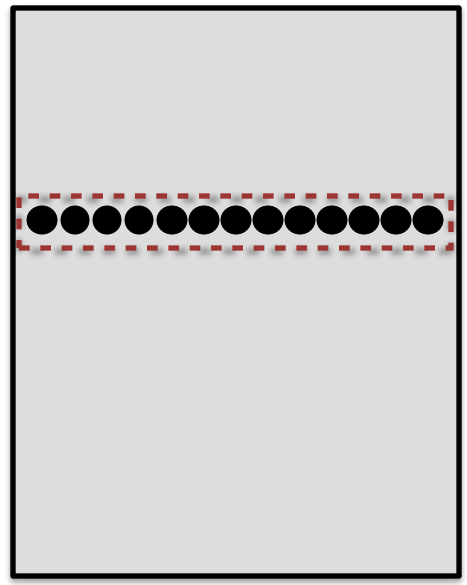
$\cdot$

A

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

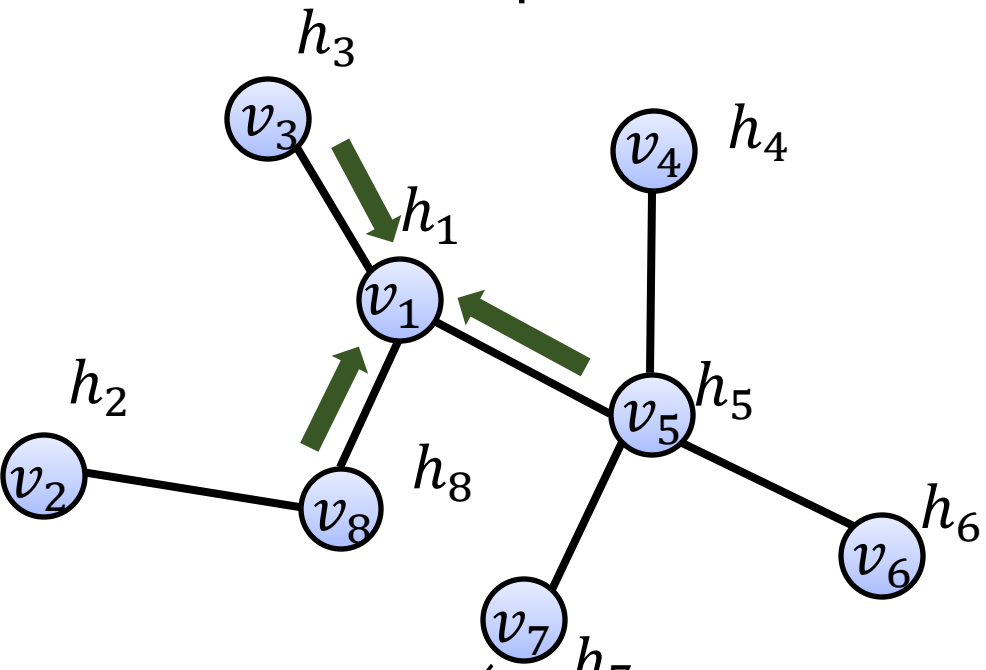
$\cdot$

H^k



Graph Convolution in Matrix Form

- Neighbor Aggregation can be performed efficiently using matrix operations



$$h_i^{k+1} = \sigma\left(W_k \frac{1}{|N(v_i)|} \sum_{v_j \in N(v_i)} h_j^k + B_k h_i^k \right)$$

$$H^k = [h_1^k, \ldots, h_{|V|}^k]^T$$

$$\tilde{A} = D^{-1}A$$

$$H^{k+1} = \sigma\left(\tilde{A} H^k \cdot W_k^T + H^k B_k^T \right)$$

(Better) Graph Convolution Network

- Neighbor Aggregation can be performed efficiently using matrix operations

- To make $\tilde{A}$ symmetric

$$H^k = [h_1^k, \ldots, h_{|V|}^k]^T$$

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

$$H^{k+1} = \sigma(\tilde{A} H^k \cdot W_k^T + H^k B_k^T)$$

Prediction Layer

$$H^k = [h_1^k, \ldots, h_{|V|}^k]^T$$
$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$
$$H^{k+1} = \sigma(\tilde{A} H^k \cdot W_k^T + H^k B_k^T)$$

- For node classification (e.g. predicting atom type):

$$o_i = \mathrm{Softmax}(h_i^{(m)})$$

- For graph classification (e.g. predicting toxicity):

$$o = \mathrm{Softmax}(\frac{1}{N} \sum_i h_i^{(m)})$$

Property of GCN: Equivariant

- the embeddings computed from graph convolution layers is invariant to node permutation

$$h_i^0 = x_i$$

$$h_i^{k+1} = \sigma(W_k \frac{1}{|N(v_i)|} \sum_{v_j \in N(v_i)} h_j^k + B_k h_i^k)$$

$$H^k = [h_1^k, \dots, h_{|V|}^k]^T$$

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

$$H^{k+1} = \sigma(\tilde{A} H^k \cdot W_k^T + H^k B_k^T)$$

Training GCN

- Parameters: weight matrix for each layer

$$H^k = [h_1^k, \dots, h_{|V|}^k]^T$$

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

$$H^{k+1} = \sigma(\tilde{A} H^k \cdot W_k^T + H^k B_k^T)$$

- Supervised training: e.g. Node classification
  - Cross entropy loss

$$L = -\sum y_i \cdot \log f(h_i^K) \qquad f_i = \mathrm{Softmax}(h_i^{(K)})$$

  - y_i is node label (in one-hot vector or smoothed version)

Training GCN

- Parameters: weight matrix for each layer

$$H^k = [h_1^k, \dots, h_{|V|}^k]^T$$

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

$$H^{k+1} = \sigma(\tilde{A} H^k \cdot W_k^T + H^k B_k^T)$$

- Unsupervised training:
  - Linked nodes have similar embedding

$$L = \sum_{i,j} CE(y_{i,j}, Sim(h_i^K, h_j^K))$$

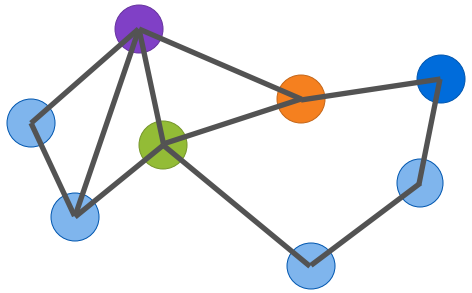
  - $y_{i,j} = 1$ if there is edge from v_i to v_j
  - Similarity can be defined in many ways: e.g. inner product $h_i \cdot h_j$

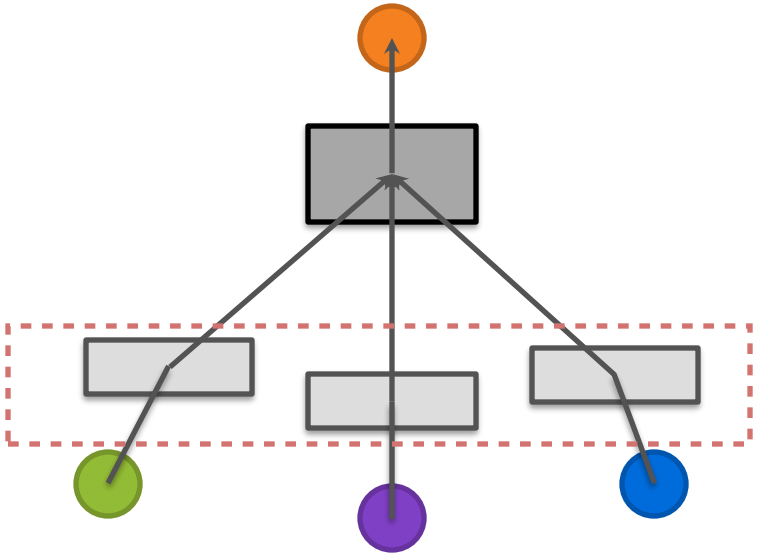
GraphSAGE

Also a special case of MPNN

$$h_i^{k+1} = \sigma\left(W_k \cdot \text{CONCAT}\left(h_i^k, \text{AGG}(\{h_j^k, \forall v_j \in N(v_i)\})\right)\right)$$

AGG can be designed in multiple ways, like pooling (sum, avg, max)





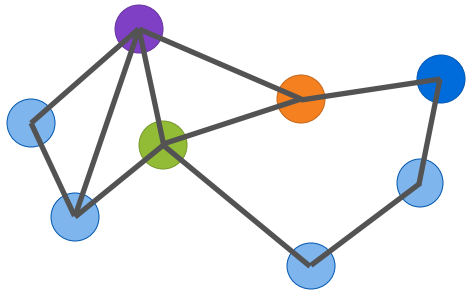
Graph Attention Network (GAT)

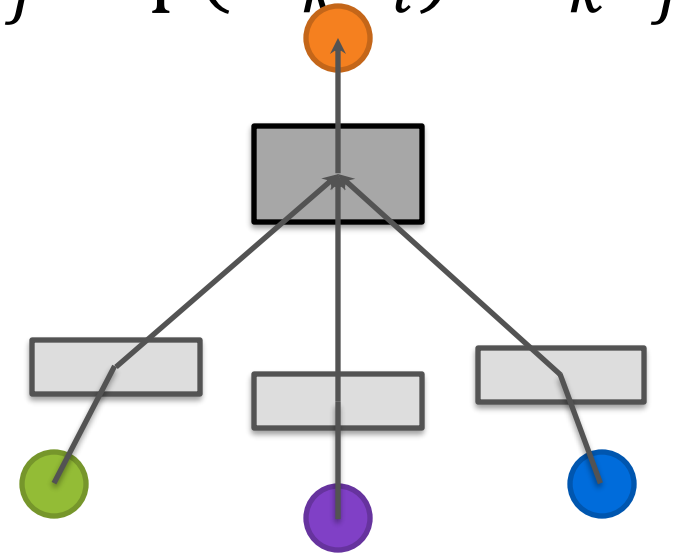
not strictly MPNN, but a generalized one

$$h_i^{k+1} = \sigma\Big(\sum_{v_j \in N(v_i)} \alpha_{ij} W_k h_{v_j}^k \Big)$$

attention weight

$$\alpha_{ij} = \text{Attention}(W_k h_i, W_k h_j) = \frac{\exp(W_k h_i)^T W_k h_j}{\sum_{j'} \exp(W_k h_i)^T W_k h_{j'}}$$

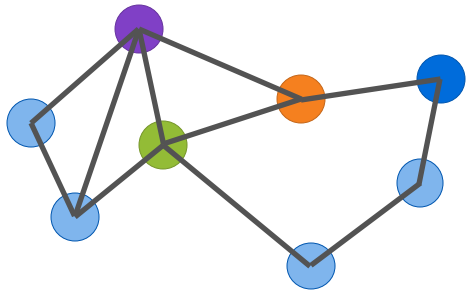


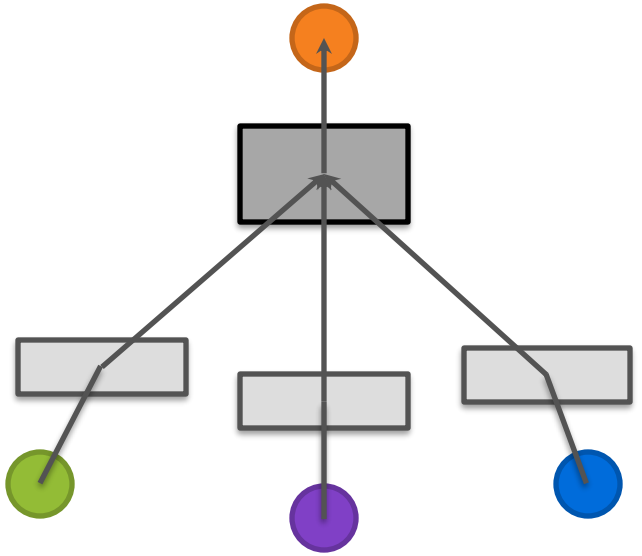


Multi-head Attention for GAT? Yes

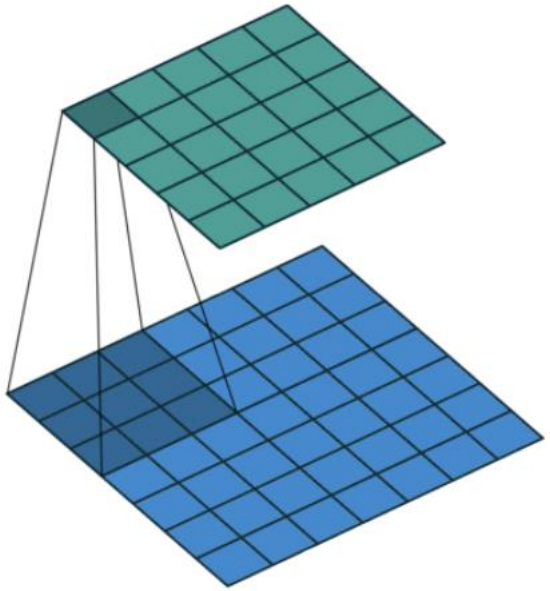
$$h_i^{k+1} = \sigma\Big(\sum_{v_j \in N(v_i)} \alpha_{ij} W_k h_{v_j}^k \Big)$$

$$\alpha_{ij} = \text{Attention}(W_k h_i, W_k h_j) = \frac{\exp(W_k h_i)^T W_k h_j}{\sum_{j'} \exp(W_k h_i)^T W_k h_{j'}}$$

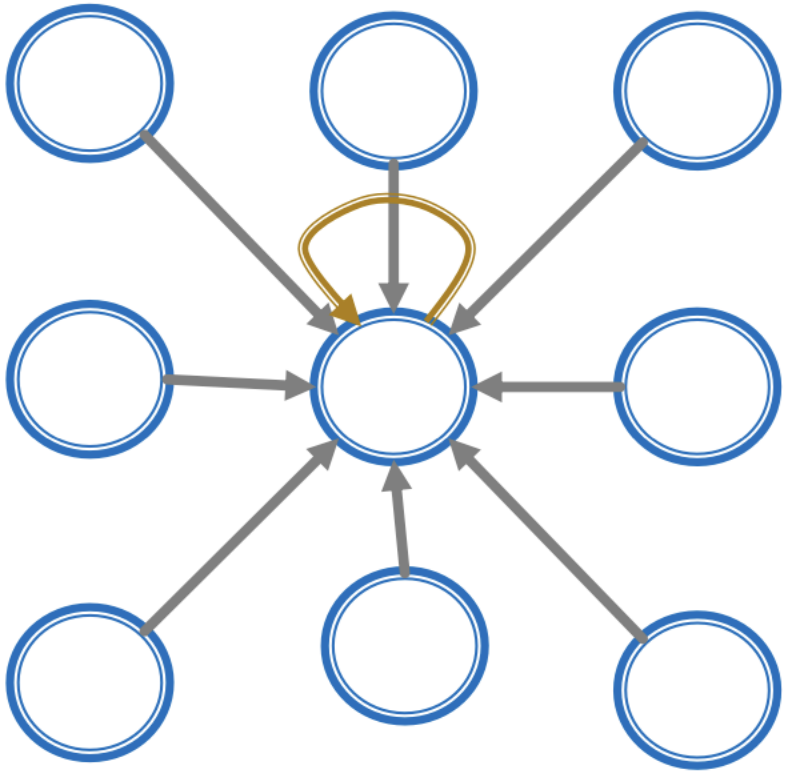




Relation between GNN and CNN



Image



Graph

CNN can be viewed as a special GNN on grid graph

GNN vs. Transformer

- Transformer is special GNN on a full-connected graph

Outline

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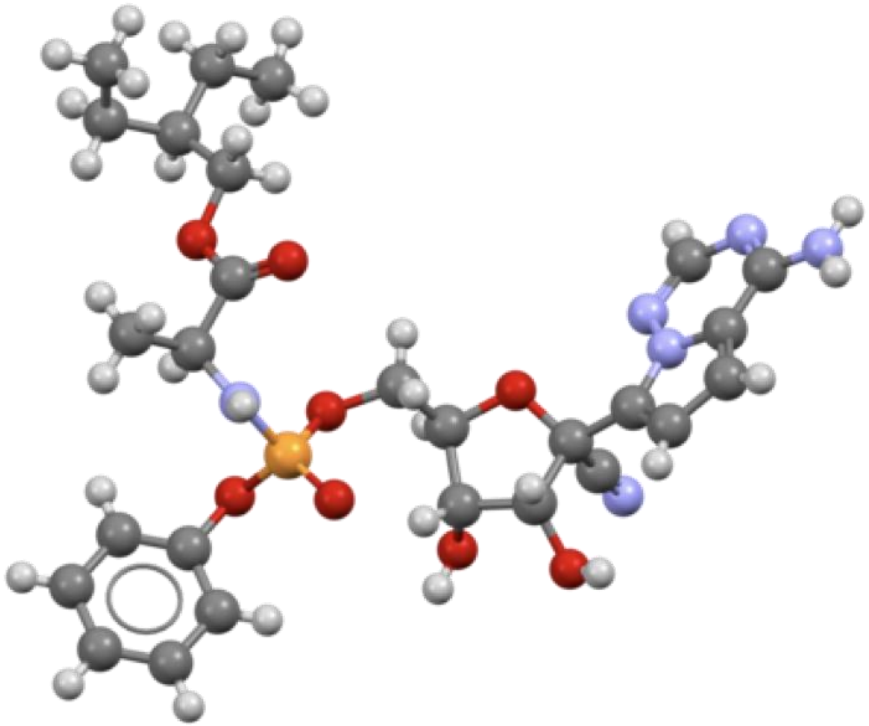
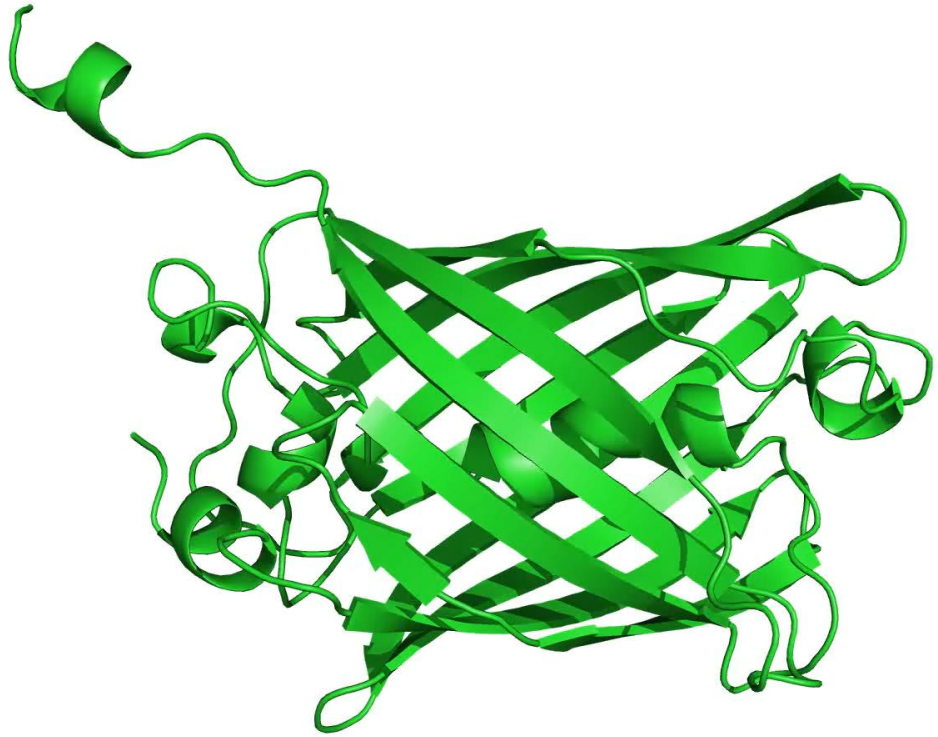
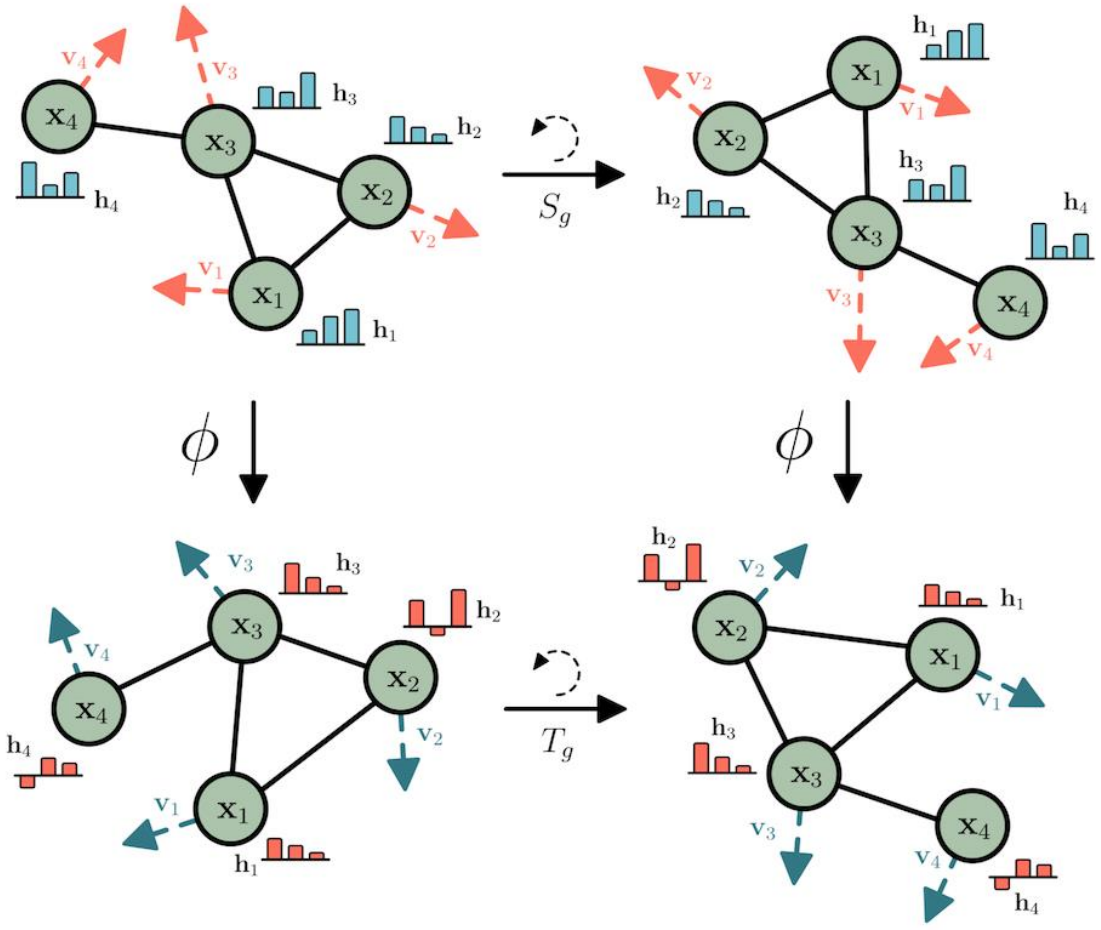
Structure and Geometry of Molecules

- Matrix of 3D coordinates, in addition to node features
- Equivariance: translation, rotation invariant





Equivariance in Embedding Transformation



f is Equivariant (SE3 invariant):

$$f(R(x) + z) = f(x)$$

No matter how we rotate and move the molecule, the NN will compute the same embeddings

X are coordinates

H are features

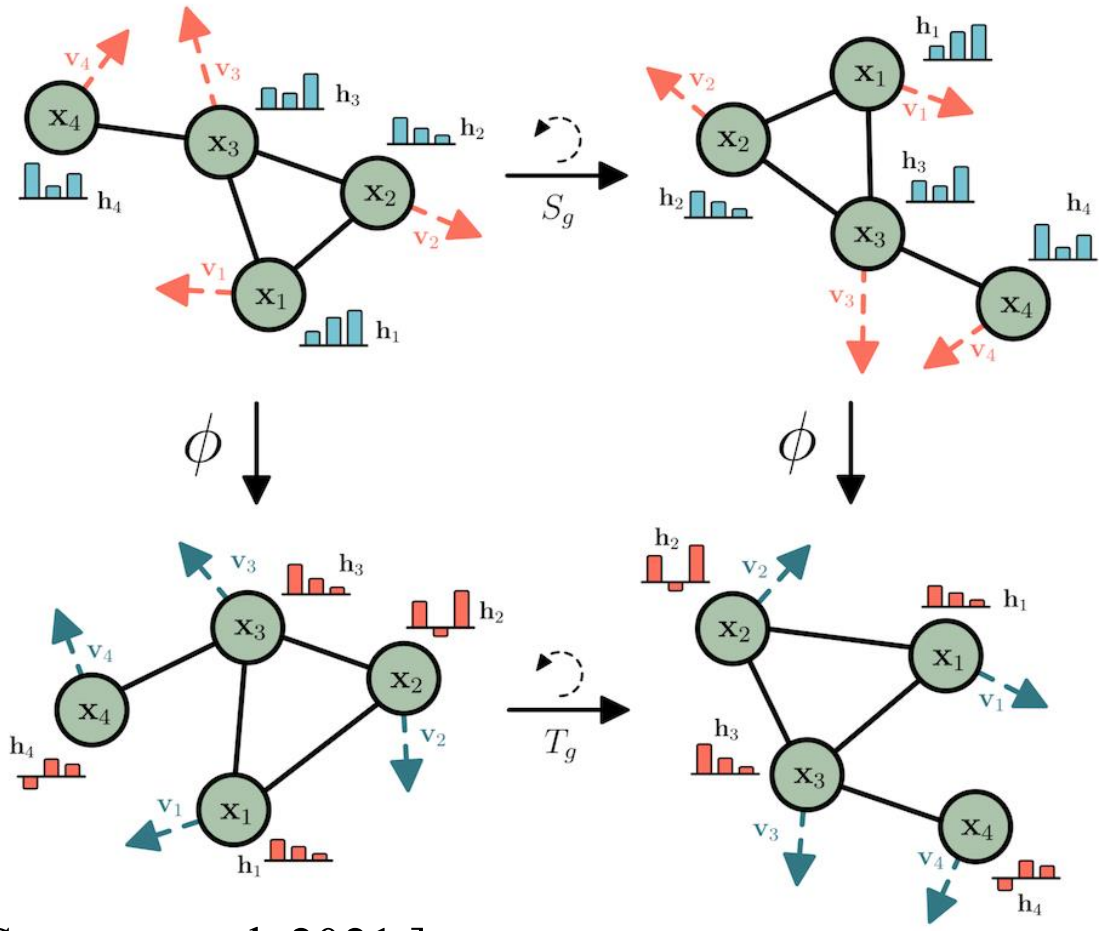
g is the rotation/translation

$$F\big(H, g(X)\big) = F(H, X)$$

[Satorres et al, 2021.]

Equivariant Graph Neural Network (EGNN)

- EGNN is an equivariant MPNN



[Satorres et al, 2021.]

$$d_{ij} = \left|x_i - x_j\right|_2$$

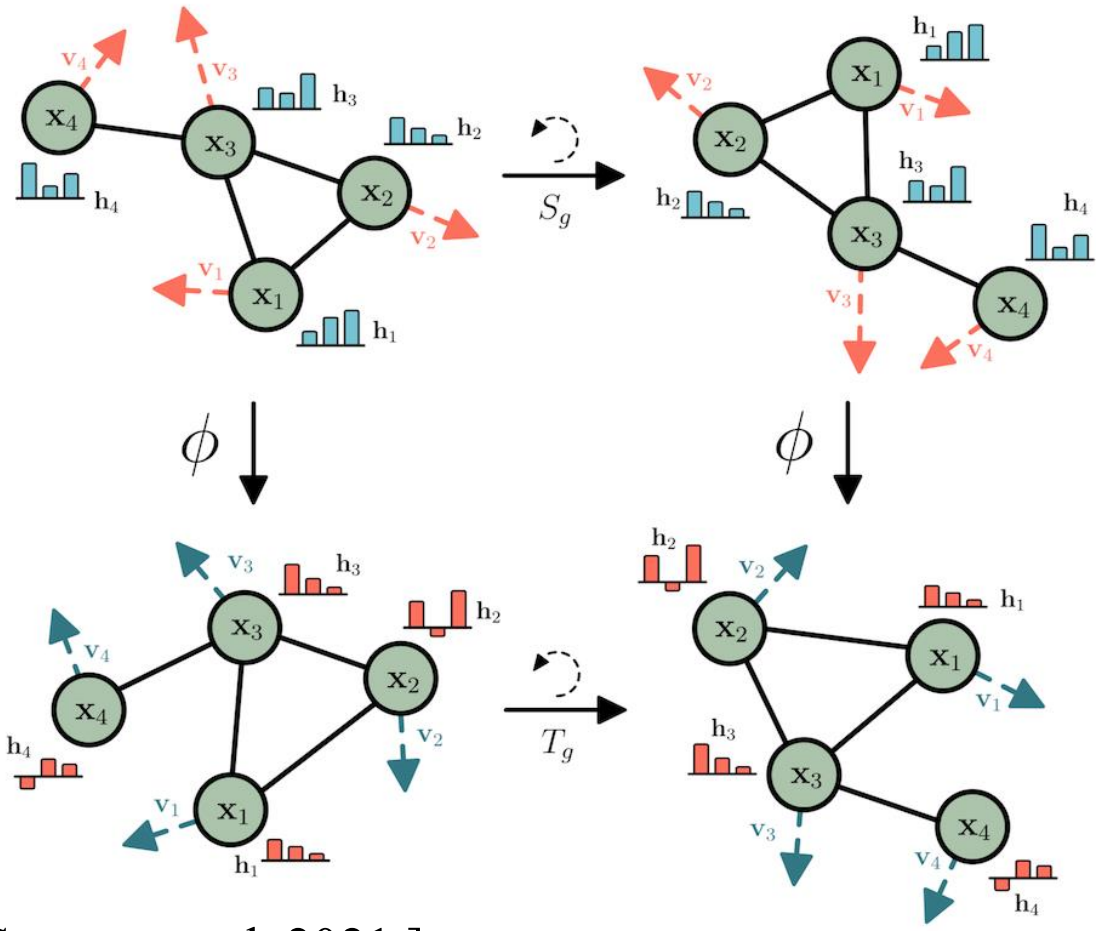
$$m_{j\to i} = M^k\left(h_i^k, h_j^k, d_{ij}\right)$$

$$m_i^{k+1} = \sum_{v_j \in N(v_i)} m_{j\to i}$$

$$h_i^{k+1} = U^k\left(h_i^k, m_i^{k+1}\right)$$

Equivariant Graph Neural Network (EGNN)

- EGNN is an equivariant MPNN, optionally updating coordinates



$$d_{ij}^k = \left|x_i^k - x_j^k\right|_2$$

$$m_{j\to i} = M^k\left(h_i^k, h_j^k, d_{ij}^k\right)$$

$$m_i^{k+1} = \sum_{v_j \in N(v_i)} m_{j\to i}$$

$$h_i^{k+1} = U^k\left(h_i^k, m_i^{k+1}\right)$$

$$x_i^{k+1} = x_i^k + \sum_{v_j \in N(v_i)} \left(x_i^k - x_j^k\right) F^k\left(m_{j\to i}\right)$$

[Satorres et al, 2021.]

Using MPNN and EGNN

- Code example at

https://projects.volkamerlab.org/teachopencadd/talktorials/T036_e3_equivariant_gnn.html

Summary

- Message Passing Neural Network
  - Nodes carry embeddings
  - message (embeddings) passed along graph edges
  - message + aggregation + update
  - many variants: GCN, GAT
- Equivariant Graph Neural Network
  - A special case of MPNN
  - modelling the embedding of nodes, along with 3D structures
  - rotation/translation invariant