Graph neural networks
lecture

TIF 360

25/3'22

Graph neural networks =

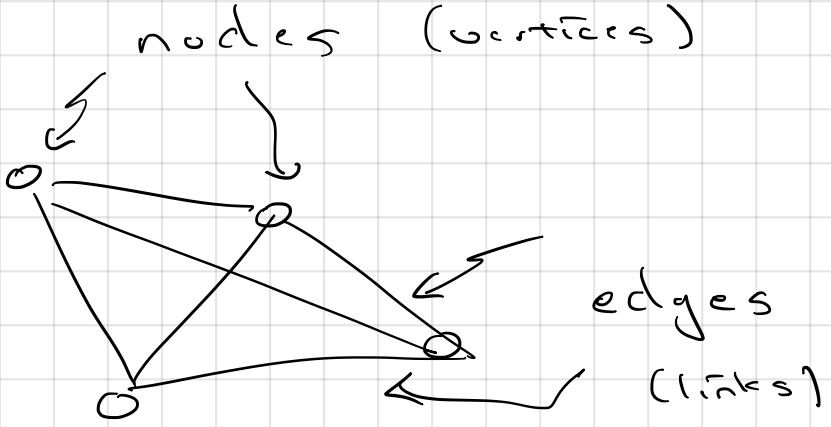
= neural networks acting on graphs

Outline

- Why interesting to apply NN to graph objects?
- How is a graph defined?
- What type of machine learning task may we want to do?
- Basic GNN layer:

  Graph convolution
- Other layers + Graph Pooling
- Homework A

Graph

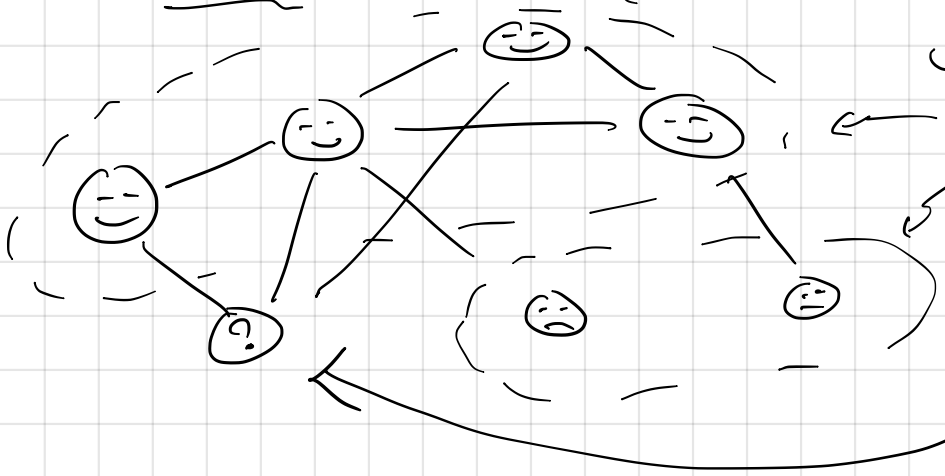


More specific shortly

Why NN on graphs / what tasks?

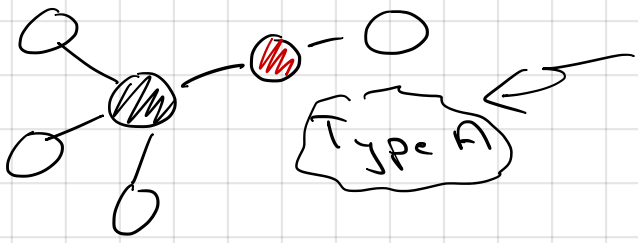
Many interesting forms of data that can be nicely represented as graphs:

Social networks:



We may want to do clustering. Or node prediction.

Molecules



We may want to do classification or regression

e.g. how chemically active (in some sense) is the molecule

Different methodology for different tasks

[4] Graph classification / regression

⇕

Supervised learning

⇕

Data: large number of labeled graphs

⇕

The network needs to handle different size graphs with varying connectivity (node degree)

[4] Node-prediction

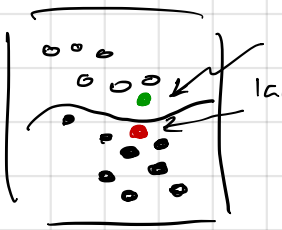
⇕

Semi-supervised learning:

⇕

typically single graph, node degree may very

Ex



some labeled nodes, also edge info taken into account e.g. neighboring nodes may be more likely to be similar

[3] Clustering: can be unsupervised

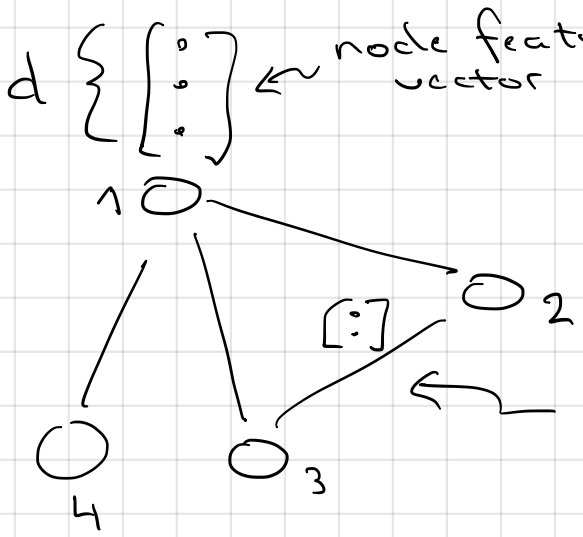
The GNN may do some automatic clustering

graph → new graph where info from neighboring nodes is absorbed

also, lower dim. embedding

Graphs: not only nodes and edges (in this context)

Information on nodes and edges



$\Rightarrow \vec{x}_i \quad i = 1, \dots n$

$\vec{x}_i$: dimension d; n: nr of nodes

$\vec{e}_{23}$, e_{23}: node feature vector, or scalar

$\vec{e}_{ij}, e_{ij}$

The structure is given by an

Adjacency matrix A_{ij}

$A_{ij} = 1$ if edge $i \to j$

$A_{ij} = 0$ if no edge

Undirected graph $A_{ij} = A_{ji}$

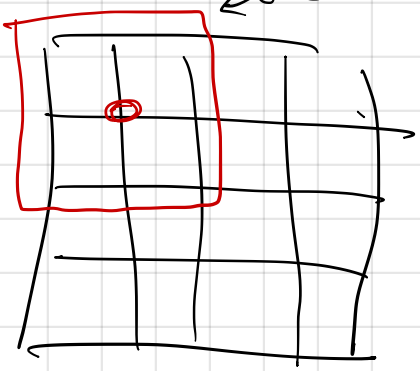
Ex above

$$A = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Convolutions on graphs

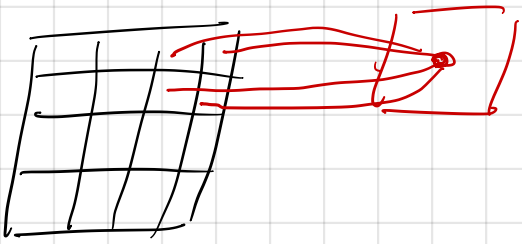
Collect information from neighboring nodes seems like a natural construction.

Similar to CNN:



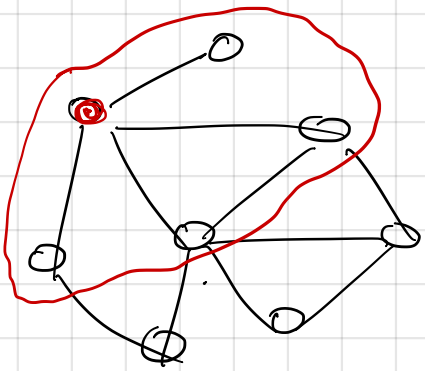
← CNN filter

regular set of neighbors on a grid (matrix)



2×2 filter (on one channel) has 4 weights + bias

On a graph?

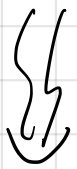


Discuss ingredients

$\vec{x}_i$ feature vector on node i

A_{ij} adjacency matrix

σ: non-linear fcn (i.e ReLU or other)



new graph with new node features

NB! Since the number of neighbors vary, not simple to have different weights to diff nodes

- Basic construction GCN Conv (Kipf & Welling)

- Isomorphic mapping: $A'_{ij} = A_{ij}$

same number of nodes, same connectivity

- Include self-loops in A:

$$\tilde{A} = A + \mathbb{1} \qquad (\tilde{A}_{ij} = A_{ij} + \delta_{ij})$$

- Degree matrix $\tilde{D}_{ii} = \sum_{j=1}^{n} \tilde{A}_{ij} = \deg_i$ = number of neighbors incl self

$$\tilde{D}_{ij} = 0$$

- Map node feature to new node feature

$\vec{x}_i \rightarrow \vec{x}'_i$

$\dim d \qquad \dim d'$

$$\begin{bmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vec{x}_3 \\ \vdots \end{bmatrix}$$

Write $\vec{x}_i$ as matrix $X \leftarrow n \times d$

act. fcn, incl. bias

$$X' = \sigma\left(\underbrace{\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2}}_{\text{adds up all neighbor vectors normalized by degree}} \underbrace{X W}_{\text{transforms each node vector } d \to d'} \right)$$

W: weight matrix $d \times d'$

$$\vec{x}'_i = \sigma\left(\sum_j \frac{\tilde{A}_{ij}}{\sqrt{\deg_i}\sqrt{\deg_j}} W^T \vec{x}_j \right)$$

"just like a non-activated dense layer on each node"

Collects information "one-hop" per layer. Isotropically, i.e. all neighbors have equal influence.

- Simple variation GraphConv

$$\vec{x}_i' = \sigma\left(\omega_1 \vec{x}_i + \omega_2 \sum_j e_{ij} \vec{x}_j\right)$$

e_{ij}: edge weight
$e_{ij} = 0$ if $A_{ij} = 0$

takes edge weights into account

fixed

- We can also make the absorption of information from neighboring nodes adaptive (trainable).

Graph attention layer GATConv

$$\vec{x}_i' = \sigma\left(\sum_j \alpha_{ij} \omega \vec{x}_j\right)$$

ω: d'xd weight matrix

- $\alpha_{ij} = \text{softmax}(e_{ij}) = \dfrac{e^{e_{ij}}}{\sum_k e^{e_{ik}}}$

$$\sum_j \alpha_{ij} = 1$$

$$\Sigma_{ij} = \sigma'\left(\vec{a} \cdot \underbrace{[\omega\vec{x}_i \| \omega\vec{x}_j]}_{\text{concatenation}}\right) \tilde{A}_{ij}$$

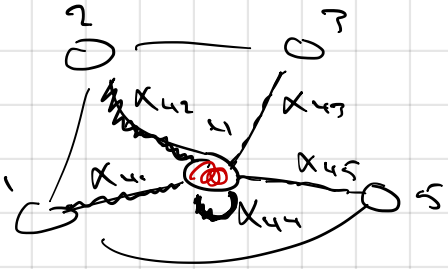
possibly other activation

$2d'$ attention vector

$$\begin{bmatrix} \omega\vec{x}_i \\ \vdots \\ \omega\vec{x}_j \end{bmatrix} \quad d' \quad d'$$

to make sure $\alpha_{ij} = 0$ if nodes are not adjacent

Attention coefficients, trainable edge weights



more input from some neighboring nodes

- One can also have several attention heads with attention coeffs a^k & weights ω^k

$$\vec{x}_i' = \Big\|_k \vec{x}_i^{\,k} = \begin{bmatrix} \vdots \\ \vec{x}_i^{\,1} \\ \vdots \\ \vec{x}_i^{\,2} \\ \vdots \\ \vec{x}_i^{\,3} \\ \vdots \end{bmatrix} \begin{matrix} \\ \text{head1} \\ \\ \text{head2} \\ \\ \text{head3} \\ \end{matrix}$$

These types of structures have had great success for Natural Language Processing

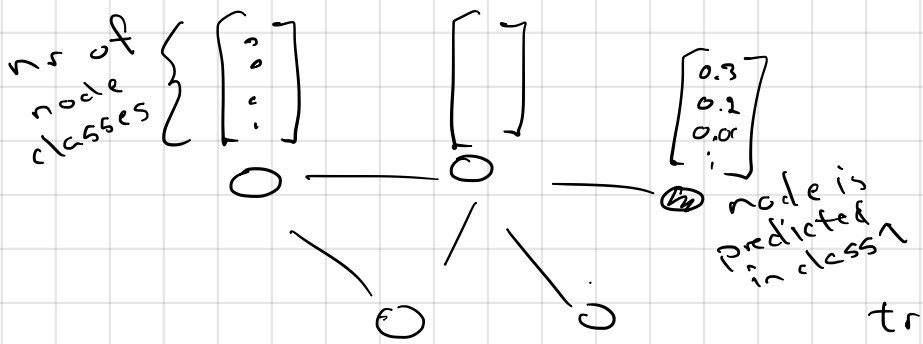
- NB! Convolutional graph layers collect information similarly to each node $\Rightarrow$ after each layer info tends to get smeared out. Don't want too many layers.

Now we have learned how to collect information in the graph.

New graph with node features $\vec{x}'_i$ that reflect surrounding of node i.

What's next? Depends on task — Discuss

- To do node classification: end with a softmax activated convolut. layer with d' = number of classes



train over loss w.r.t. labeled nodes.

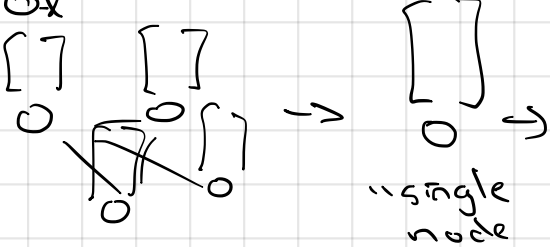
- To do graph classification we need to reduce info to one vector, a.k.a. graph embedding.

For this use Pooling layer

- Simplest Global pooling

E.g. global mean pool

$$\vec{x}'_1 = \frac{1}{n}\sum_{i=1}^{n} \vec{x}_i$$



dense → softmax [class predic.]

- More sophisticated: max-k pooling

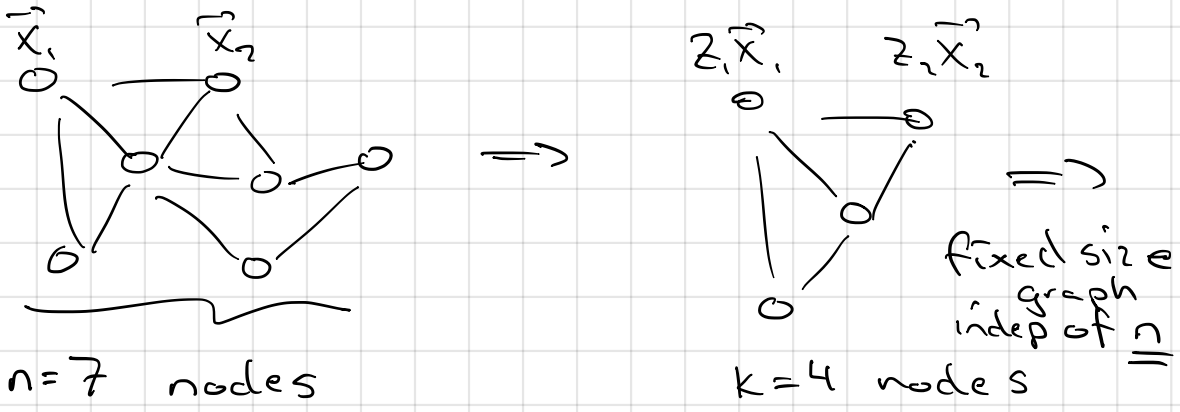
  select k most important nodes

  using "self-attention"

$$Z_i = \sigma(\vec{q} \cdot \vec{x}_i)$$

$\vec{q}$: attention vector

pick k-nodes with highest value Z



Homework A

- Prob. 1 (5p) Do semisupervised node-classification (most code available)

- Prob 2 Do graph-classification data from a problem related to quantum computing