Geometric deep learning with graph neural networks
Deep Learning ❤️ Euclidean data
Deep Learning 💗 Non-Euclidean data
Graphs to the rescue
Basic concepts

Undirected

Directed

Node

Edge

Adjacency matrix

\[ A = \begin{bmatrix}
1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 & 1 \\
0 & 0 & 1 & 1 & 1
\end{bmatrix} \]
Convolutional Neural Network (CNN)

Vincent Dumoulin, Francesco Visin - A guide to convolution arithmetic for deep learning
Image = Graph
Image = Graph
Convolutions
Curved surfaces
Objects with relations
Convolution = Message passing

Node feature vector
Message passing layer

https://www.outsystems.com/blog/posts/graph-neural-networks/
Message passing

**Message** from node $j \rightarrow i$:

$$m_j = m(x_i, x_j, e_{ij})$$

**Aggregate** messages from all neighbors:

$$a = a(m_j \mid j \text{ neighborhood of } i)$$

**Update** node $i$:

$$x'_i = u(x_i, a)$$
Message passing

Message

\[ m_1 = m(x_3, x_1, e_{31}) \]
\[ m_2 = m(x_3, x_2, e_{32}) \]
\[ m_3 = m(x_3, x_4, e_{34}) \]
\[ m_4 = m(x_3, x_5, e_{35}) \]

Aggregate (mean)

\[ a = \frac{m_1 + m_2 + m_4 + m_5}{4} \]

Update

\[ u(x_3, a) \]
\[ x_3' \]
Two layer GNN
Graph Convolutional Network
Thomas N Kipf and Max Welling 2017

Message from node $j \rightarrow i$:
$$m_j^k = \frac{e_{ij}}{\sqrt{d_i d_j}} x_j^k, \quad d_i = 1 + \sum_{j \in N(i)} e_{ij}$$

Aggregate messages from all neighbors:
$$a^k = \sum_j m_j^k$$

Update node $i$:
$$x_i^{k+1} = Aa^k$$
Supervised learning

Node classification:

Graph classification:

Link prediction:
Graph Auto Encoders

Traditional Auto Encoder:

\[ X \rightarrow \text{Encoder} \rightarrow Z \rightarrow \text{Decoder} \rightarrow \hat{X} \]

Input Encoder Compressed Latent Space Decoder Output
Graph Auto Encoders

Traditional Auto Encoder:

- Input: $X$
- Encoder: $Z$
- Compressed Latent Space: $\hat{X}$

Graph Auto Encoder:

- Node features: $X \in \mathbb{R}^{N \times D}$
- Adjacency matrix: $A \in \{0, 1\}^{N \times N}$
- Encoder GNN
- Graph embedding $Z \in \mathbb{R}^{N \times F}$
- Decoder
- Reconstructed adjacency matrix $\hat{A} \in \{0, 1\}^{N \times N}$

Variational Graph Auto-Encoders by Thomas N Kipf and Max Welling
Attention in GNN

Graph Attention Network (Vaswani et al NIPS 2017)

Message

\[ m_j = m(x_i, x_j) \]

Attention score

\[ \alpha_{ij} = f(x_i, x_j) \]

Aggregation function

\[ a = \sum_{j \in N(i)} \alpha_{ij} m_j \]

neighborhood of i
GNN vs Transformers

\[ x_1' \]

Layer Norm

Feed Forward

Layer Norm

Self attention

\[ z_1 = \sum_{i=1}^{4} \alpha_{1,k}(Vx_k) \]

For all k:

\[ \alpha_{1,k} = f(x_1, x_k) \]
Graph neural network vs Transformers
Graph neural network vs Transformers

Message Passing

Message

\[ m_j = V x_j, \quad j \in N(i) \]
\[ \alpha_{ij} = f(x_i, x_j) \]

Aggregate

\[ \sum_j \alpha_{ij} (m_j) \]

Update

Layer Norm
Feed forward
Layer Norm

\[ x'_i \]
My research with GNN

Predict molecular toxicity

Geometry of molecule
Mesh-based simulation

Learning mesh-based simulation with Graph Networks (Deepmind),
Deep mind and google maps use Graph Neural networks to improve traffic predictions
Antibiotic Discovery


They have, for the first time, identified completely new kinds of antibiotic from scratch, without using any previous human assumptions. Published in *Cell*.
Libraries

Pytorch
• [Pytorch geometric](#)
• [Deep graph library](#)

Tensorflow
• [Deep graph library](#)
• [Graph Nets library](#)
• [Spektral](#)

Jax
• [Jraph](#)
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References:

• About Non-Euclidean Spaces

