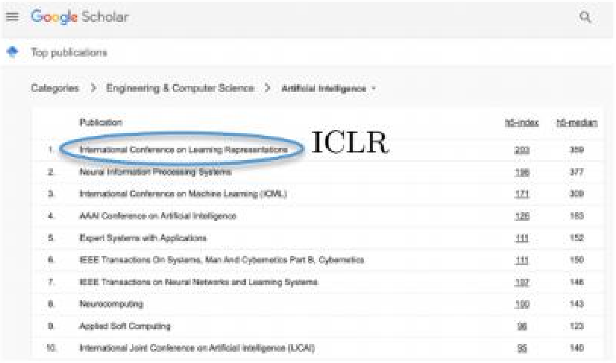
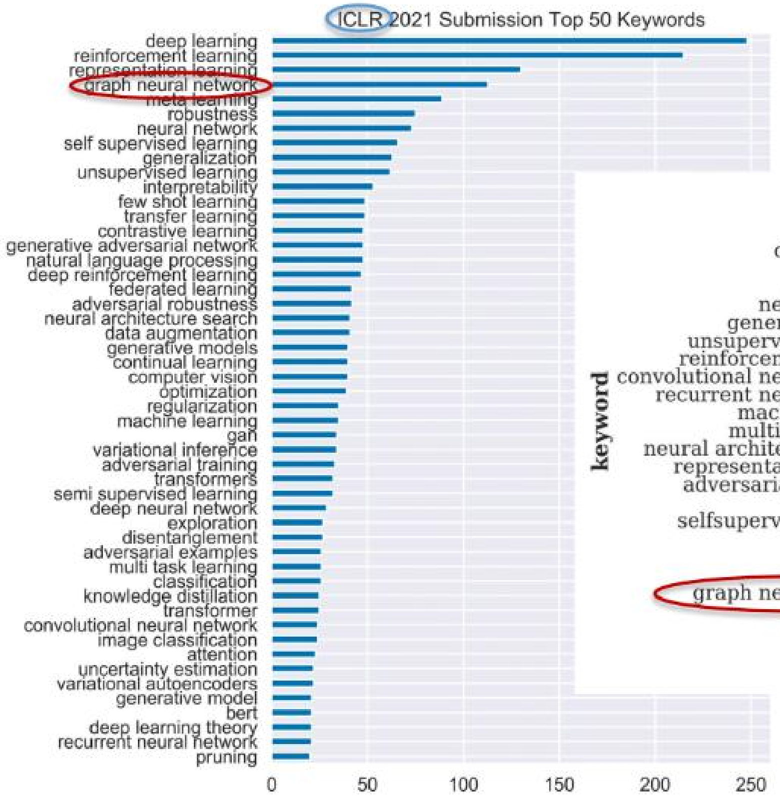
GNN

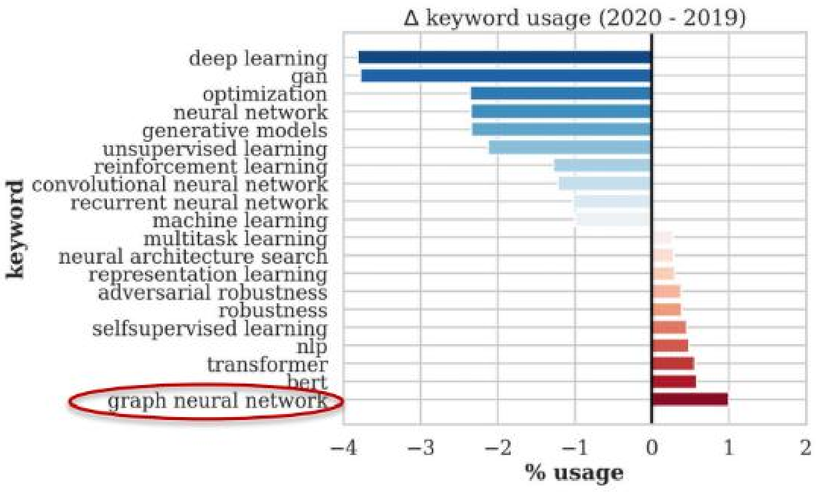
应用领域

学术圈子里那是越来越火，热度一个劲往上升



	Publication	h5-index	h5-median
1.	International Conference on Learning Representations	203	359
2.	Neural Information Processing Systems	198	377
3.	International Conference on Machine Learning (ICML)	171	309
4.	AAAI Conference on Artificial Intelligence	126	183
5.	Expert Systems with Applications	111	152
6.	IEEE Transactions On Systems, Man And Cybernetics Part B, Cybernetics	111	150
7.	IEEE Transactions on Neural Networks and Learning Systems	107	146
8.	Neurocomputing	100	143
9.	Applied Soft Computing	98	123
10.	International Joint Conference on Artificial Intelligence (IJCAI)	95	140

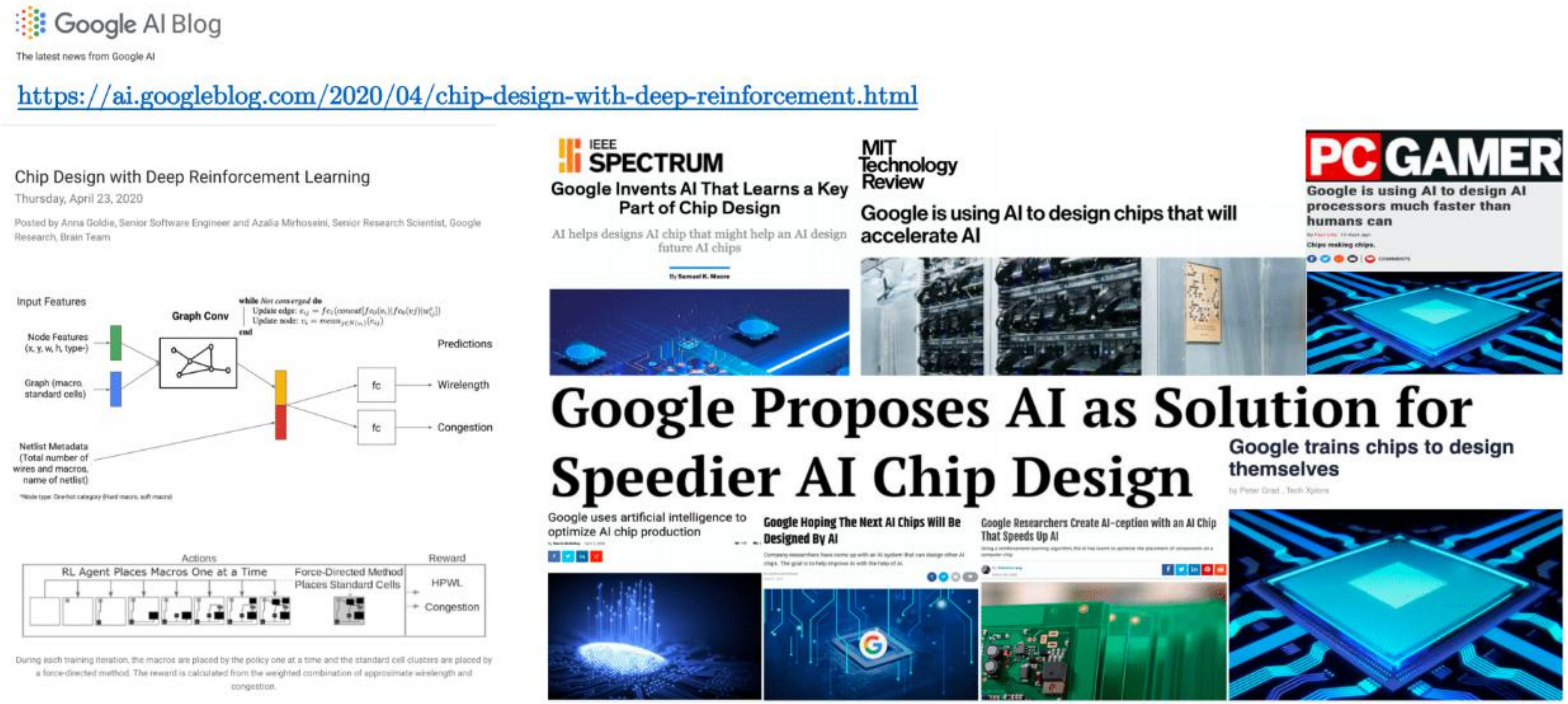




GNN

应用领域

先往大的层面整，芯片设计



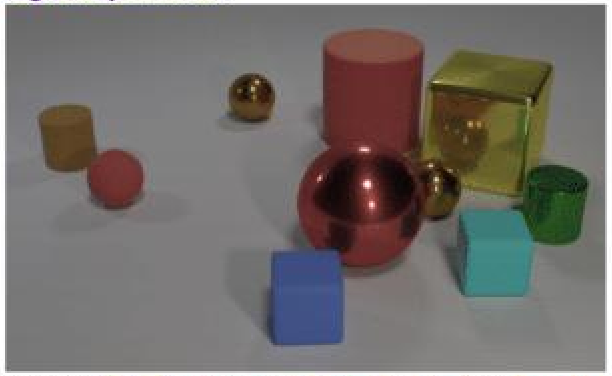
https://www.theverge.com/2021/6/10/22527476/google-machine-learning-chip-design-tpu-floorplanning

GNN

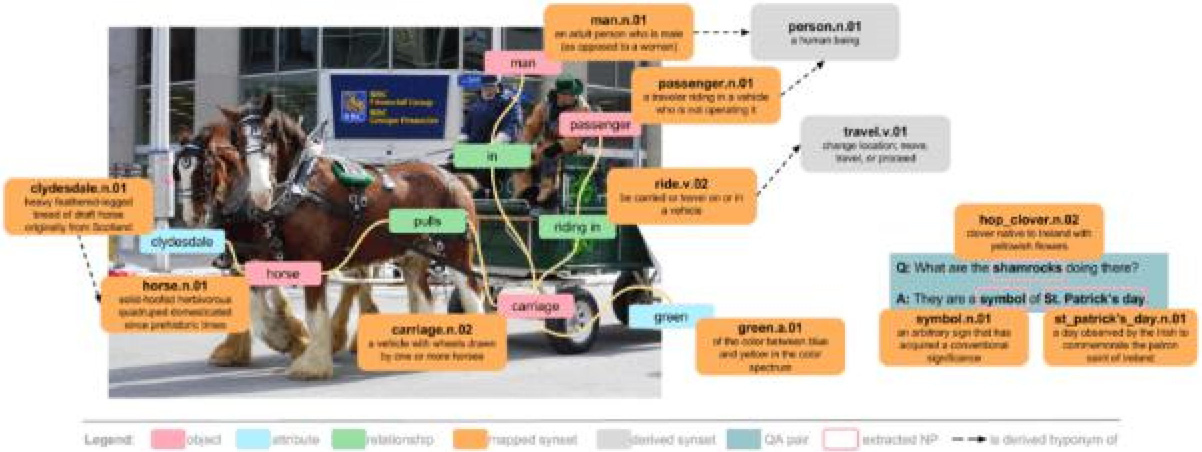
应用领域

场景分析与问题推理：

Questions in CLEVR test various aspects of visual reasoning including **attribute identification**, **counting**, **comparison**, **spatial relationships**, and **logical operations**.



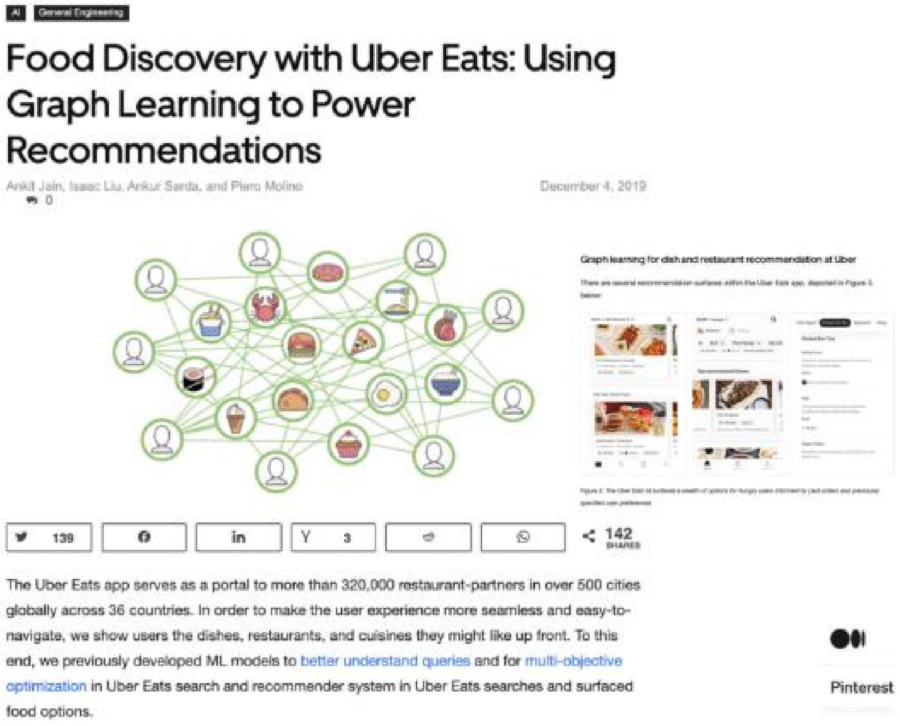
Q: Are there an **equal number** of **large things** and **metal spheres**?
Q: **What size** is the **cylinder that is left of** the **brown metal** thing **that is left of** the **big sphere**?
Q: There is a **sphere** with the **same size as** the **metal cube**; is it **made of the same material as** the **small red sphere**?
Q: **How many** objects are **either small cylinders** or **red** things?



GNN

应用领域

推荐系统相关，那肯定得图了：


AI General Engineering

Food Discovery with Uber Eats: Using Graph Learning to Power Recommendations

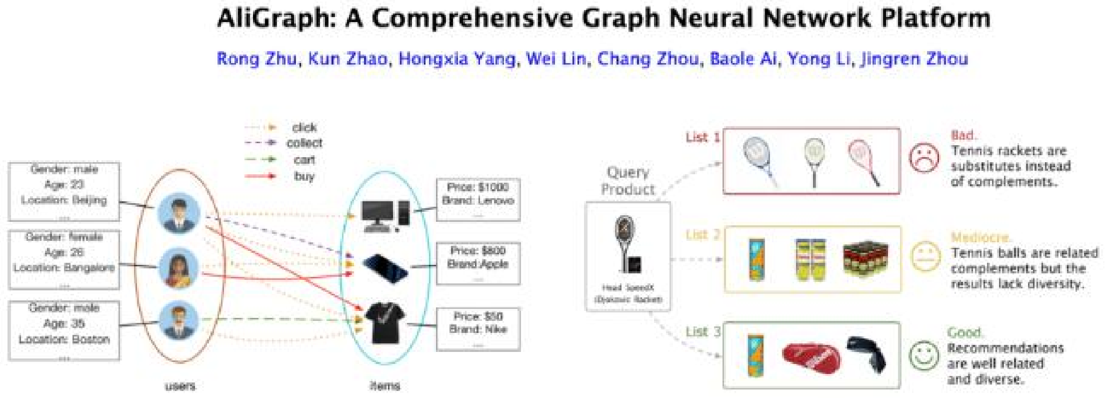
Ankit Jain, Isaac Liu, Ankur Sarda, and Piero Molino — December 4, 2019

Graph learning for dish and restaurant recommendation at Uber

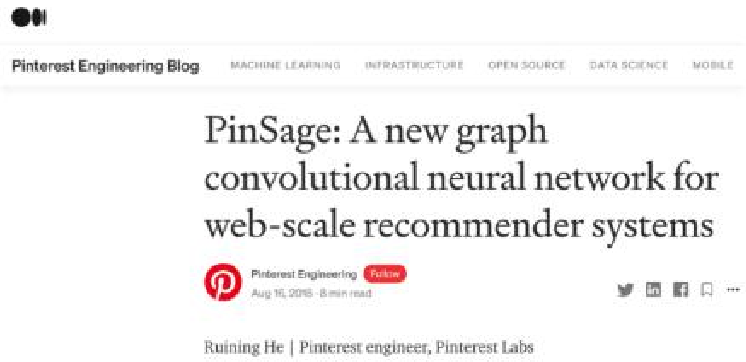
139 · 3 · 142 SHARES

The Uber Eats app serves as a portal to more than 320,000 restaurant-partners in over 500 cities globally across 36 countries. In order to make the user experience more seamless and easy-to-navigate, we show users the dishes, restaurants, and cuisines they might like up front. To this end, we previously developed ML models to better understand queries and for multi-objective optimization in Uber Eats search and recommender system in Uber Eats searches and surfaced food options.

Pinterest


AliGraph: A Comprehensive Graph Neural Network Platform

Rong Zhu, Kun Zhao, Hongxia Yang, Wei Lin, Chang Zhou, Baole Ai, Yong Li, Jingren Zhou


Pinterest Engineering Blog — MACHINE LEARNING · INFRASTRUCTURE · OPEN SOURCE · DATA SCIENCE · MOBILE

PinSage: A new graph convolutional neural network for web-scale recommender systems

Pinterest Engineering · Follow — Aug 16, 2018 · 8 min read

Ruining He | Pinterest engineer, Pinterest Labs

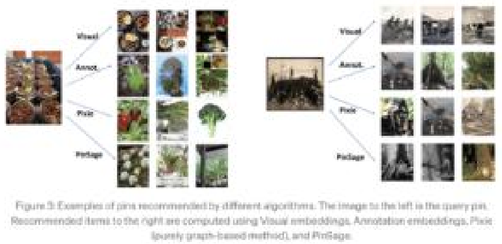
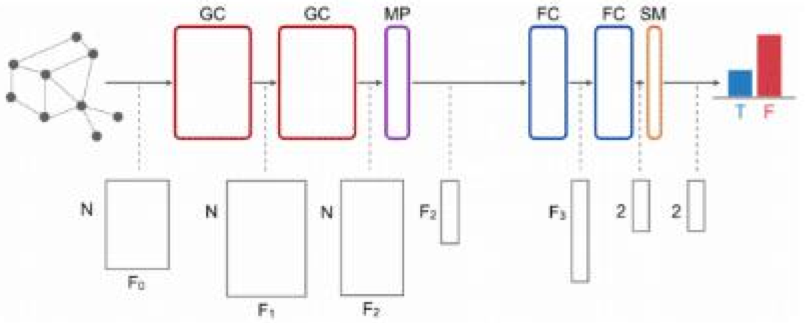


Figure 3: Examples of pins recommended by different algorithms. The image to the left is the query pin. Recommended items to the right are computed using Visual embeddings, Annotation embeddings, Pixie (purely graph-based method), and PinSage.

GNN

应用领域

欺诈检测，风控相关：



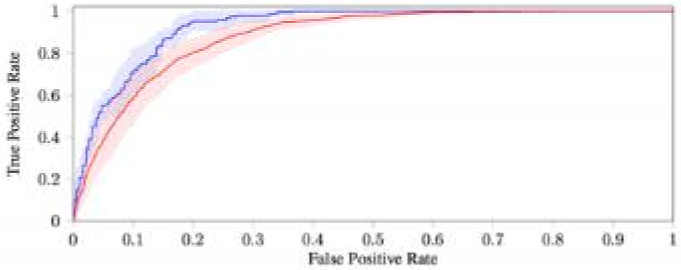
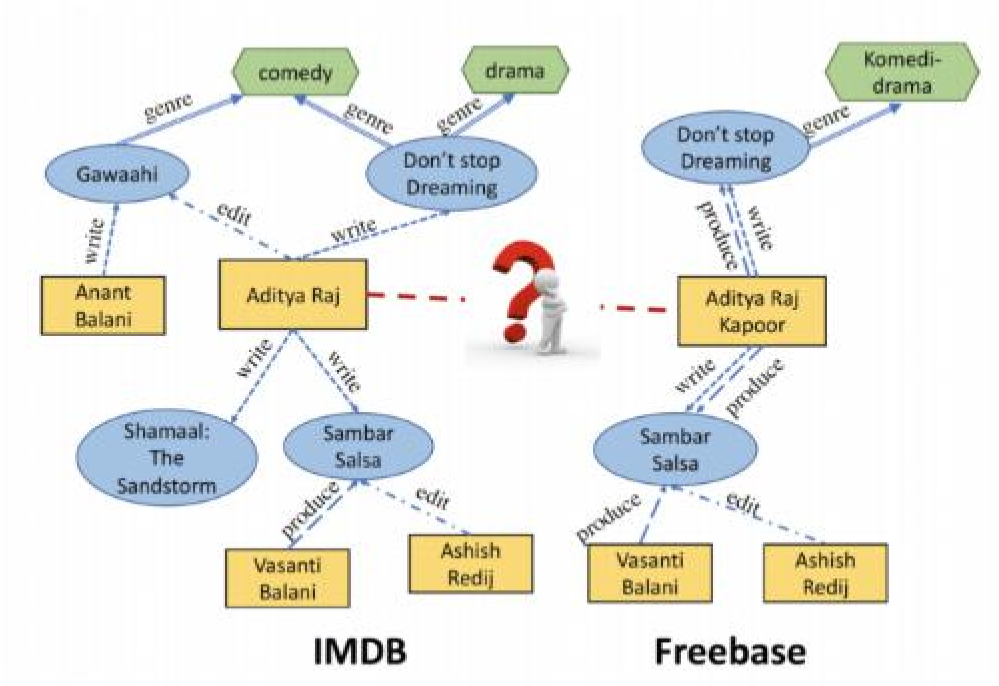


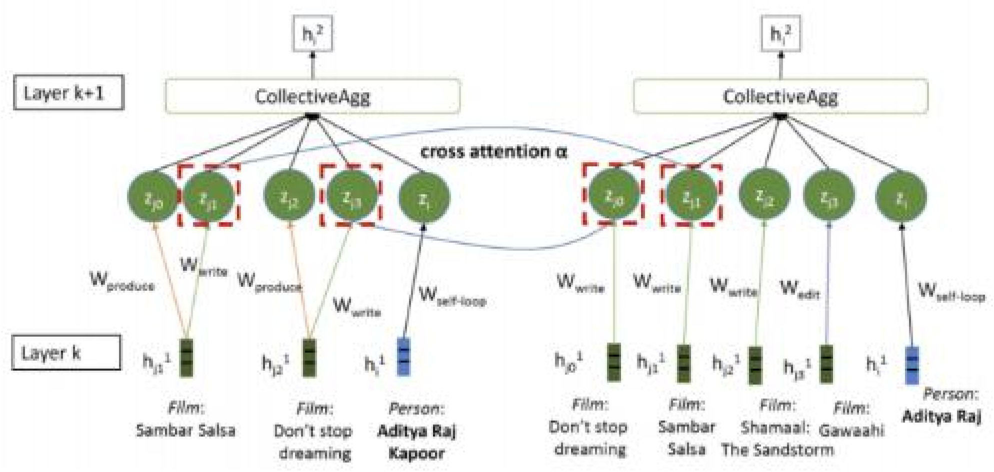
Figure 6: Performance of URL-wise (blue) and cascade-wise (red) fake news detection using 24hr-long diffusion time. Shown are ROC curves averaged on five folds (the shaded areas represent the standard deviations). ROC AUC is 92.70 ± 1.80% for URL-wise classification and 88.30 ± 2.74% for cascade-wise classification, respectively. Only cascades with at least 6 tweets were considered for cascade-wise classification.

GNN

应用领域

知识图谱本身也是个图模型

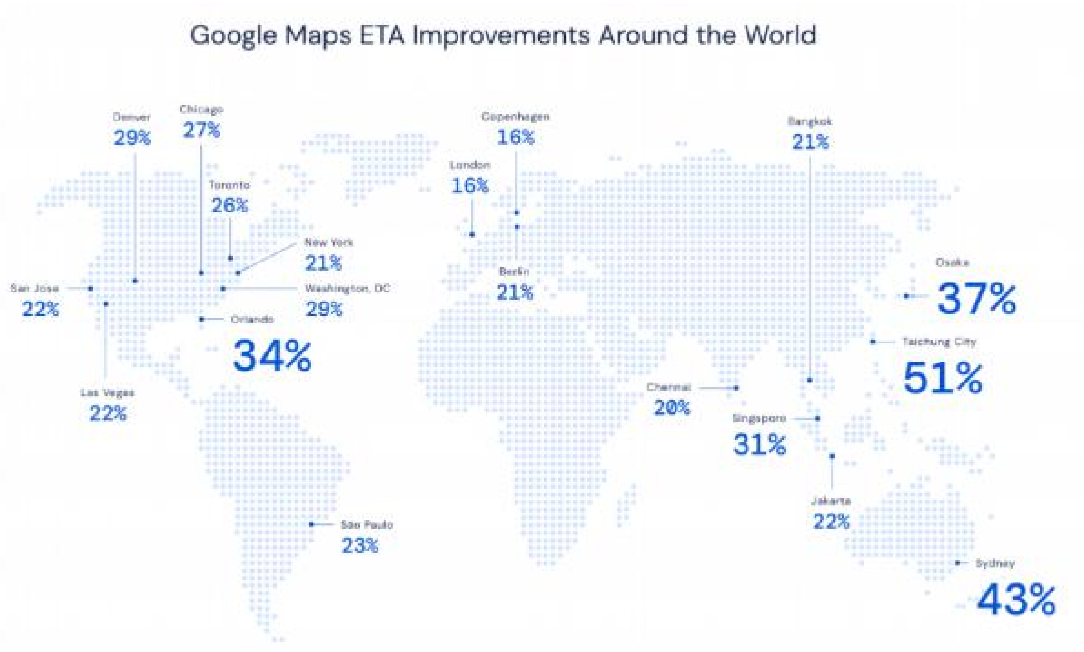




GNN

应用领域

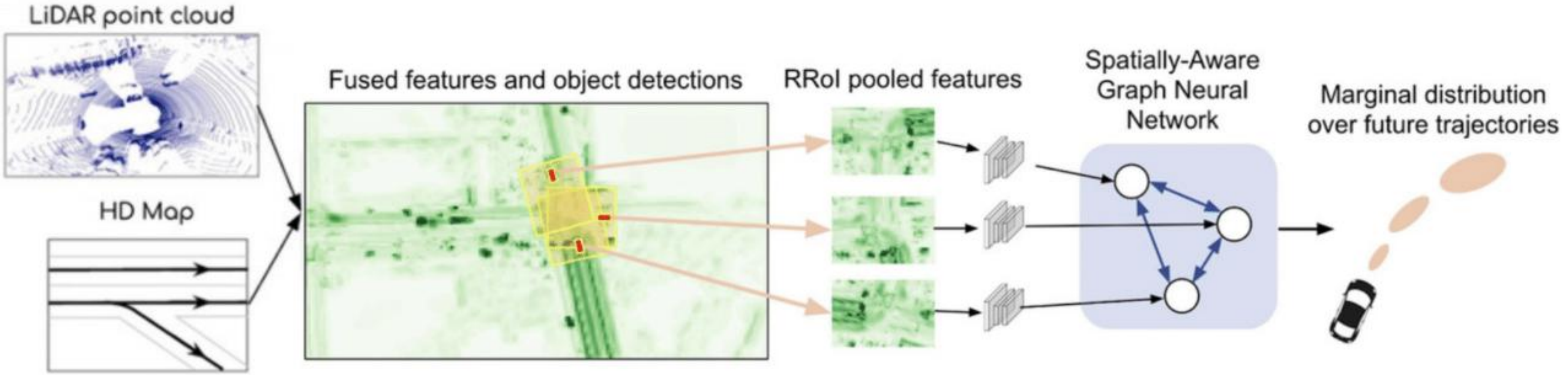
道路交通，动态流量预测

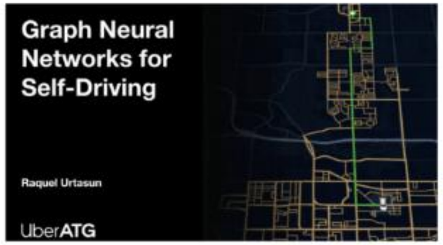


GNN

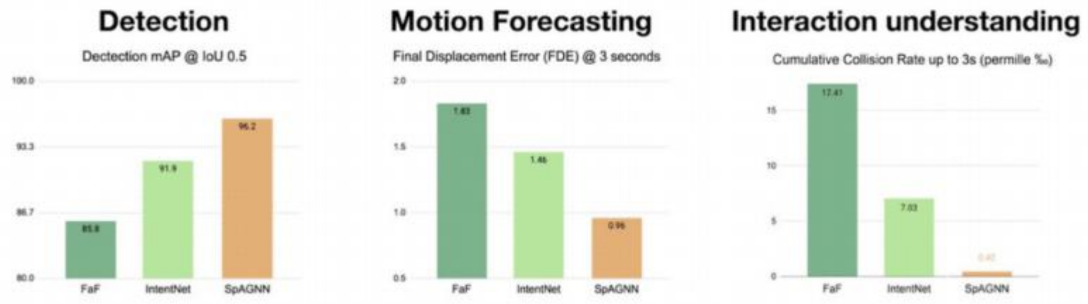
✓ 应用领域

自动驾驶，无人机等场景





https://slideslive.com/38930570/graph-neural-networks-for-selfdriving



GNN

应用领域

化学，医疗等场景

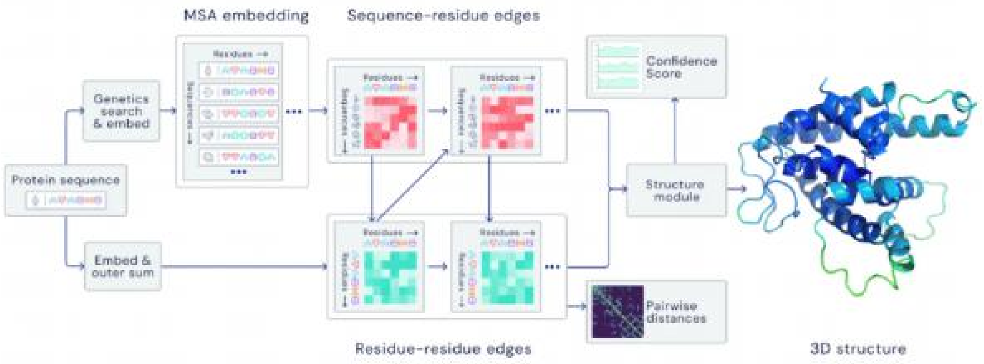

AlphaFold: a solution to a 50-year-old grand challenge in biology

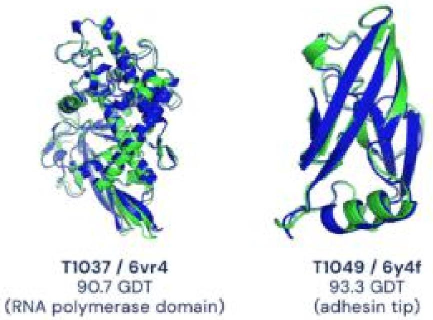
SHARE

AUTHORS

TAt The AlphaFold team

Proteins are essential to life, supporting practically all its functions. They are large complex molecules, made up of chains of amino acids, and what a protein does largely depends on its unique 3D structure. Figuring out what shapes proteins fold into is known as the "protein folding problem", and has stood as a grand challenge in biology for the past 50 years. In a major scientific advance, the latest version of our AI system AlphaFold has been recognised as a solution to this grand challenge by the organisers of the biennial Critical Assessment of protein Structure Prediction (CASP). This breakthrough demonstrates the impact AI can have on scientific discovery and its potential to dramatically accelerate progress in some of the most fundamental fields that explain and shape our world.

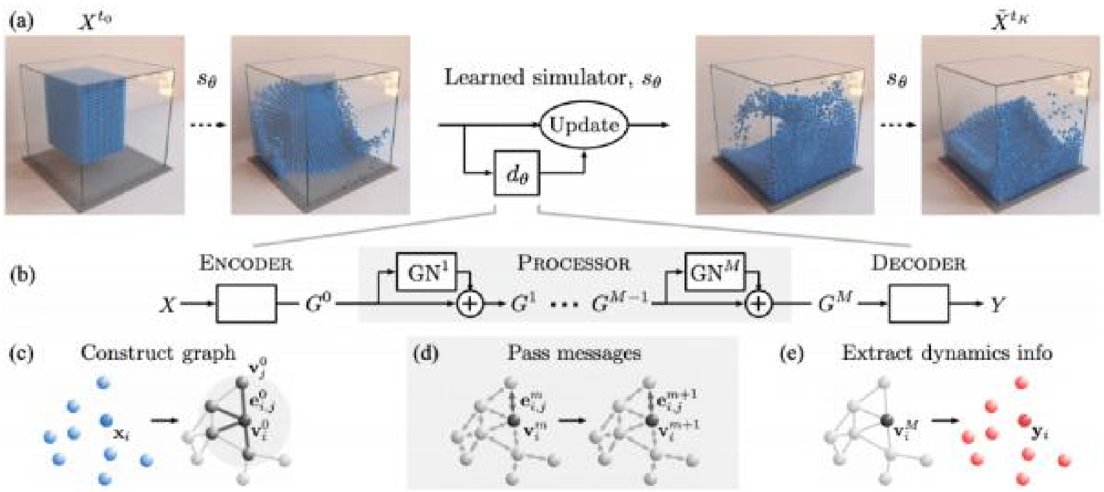


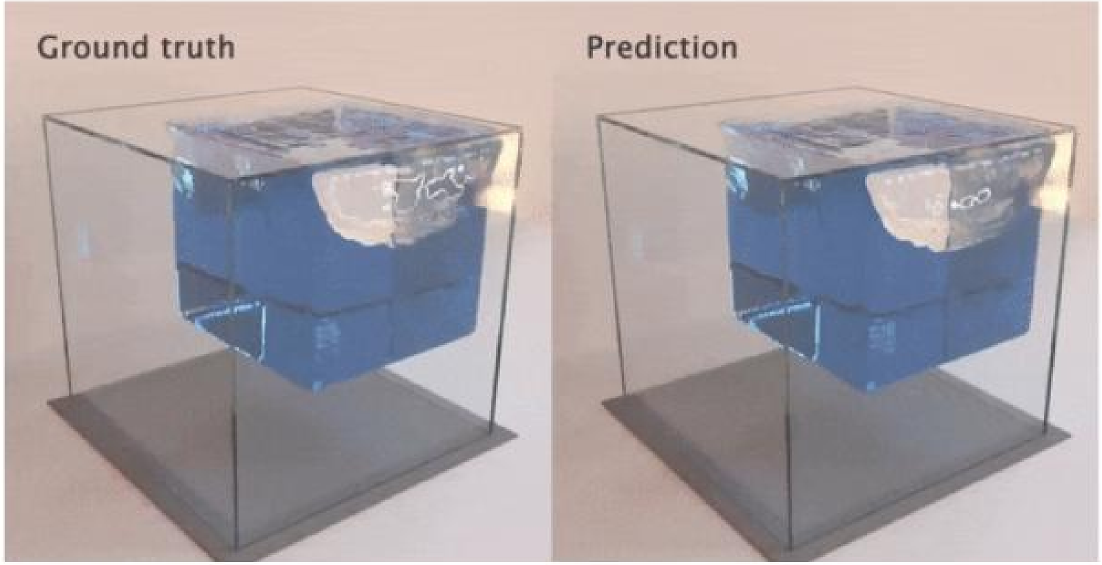


GNN

应用领域

物理模型相关

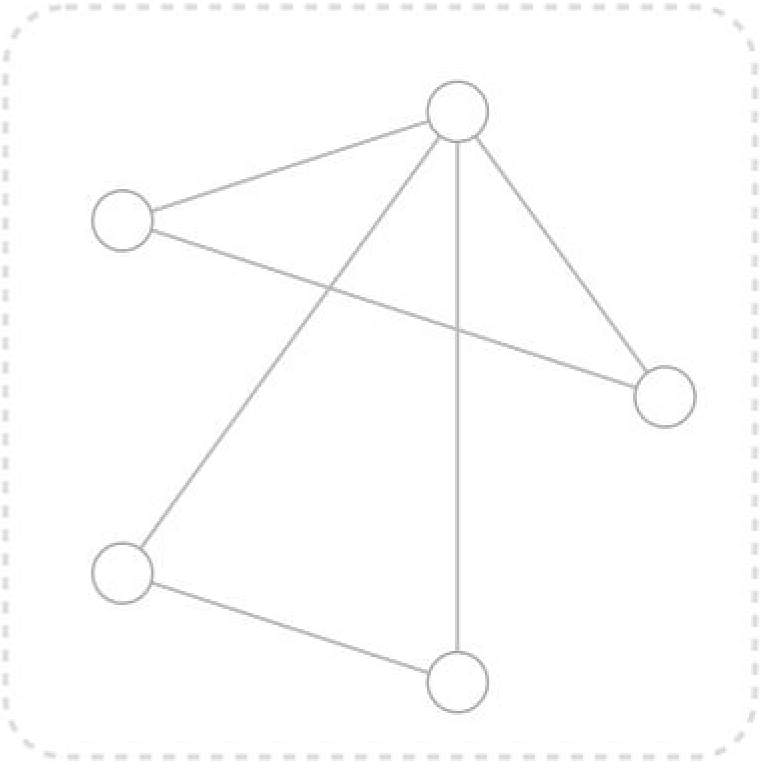




GNN

图的基本组成

跟大家想的一样，还是这点东西，我们要做的就是提取特征而已



V Vertex (or node) attributes

e.g., node identity, number of neighbors

E Edge (or link) attributes and directions

e.g., edge identity, edge weight

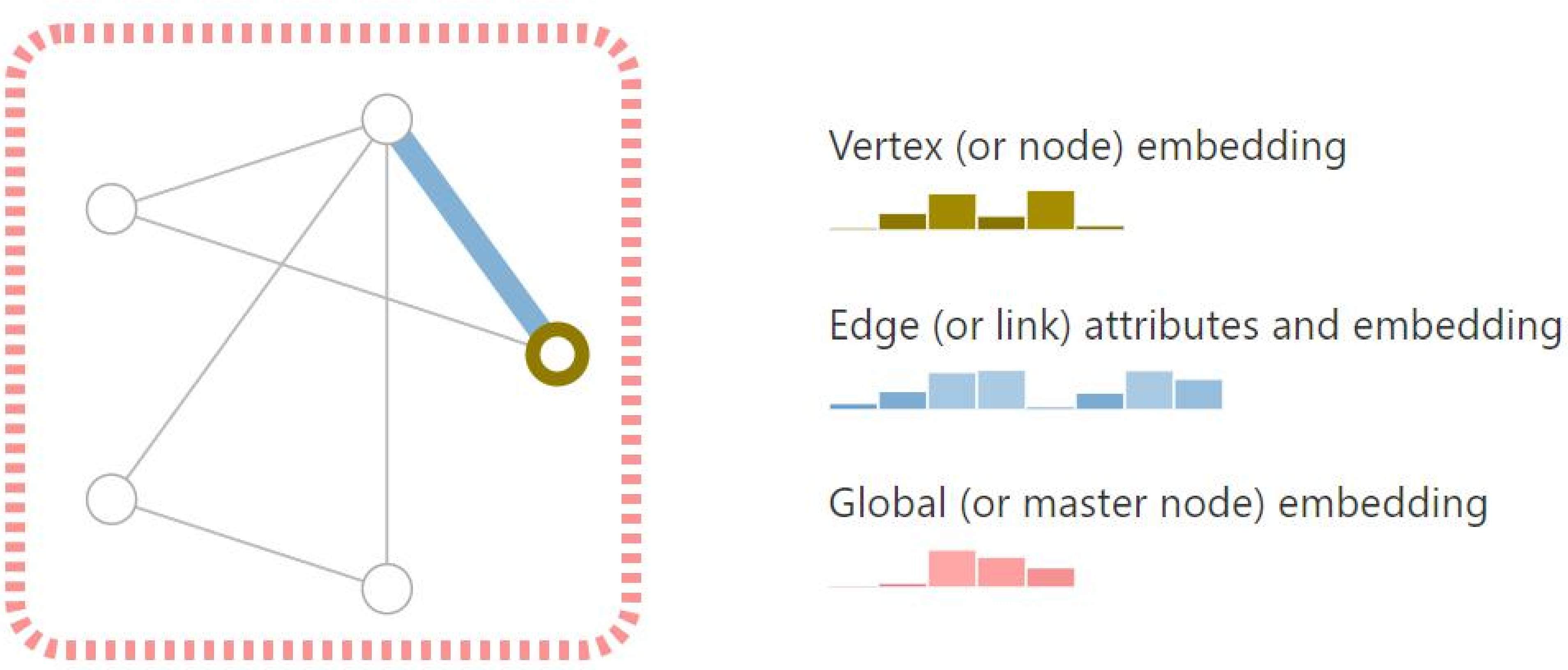
U Global (or master node) attributes

e.g., number of nodes, longest path

GNN

✓ 图神经网络要做啥

无论事整的多么复杂，我们利用图神经网络的目的就是整合特征



GNN

图的邻接矩阵

以图像为例子，每个像素点周围都有邻居，A就表示邻居之间的关系

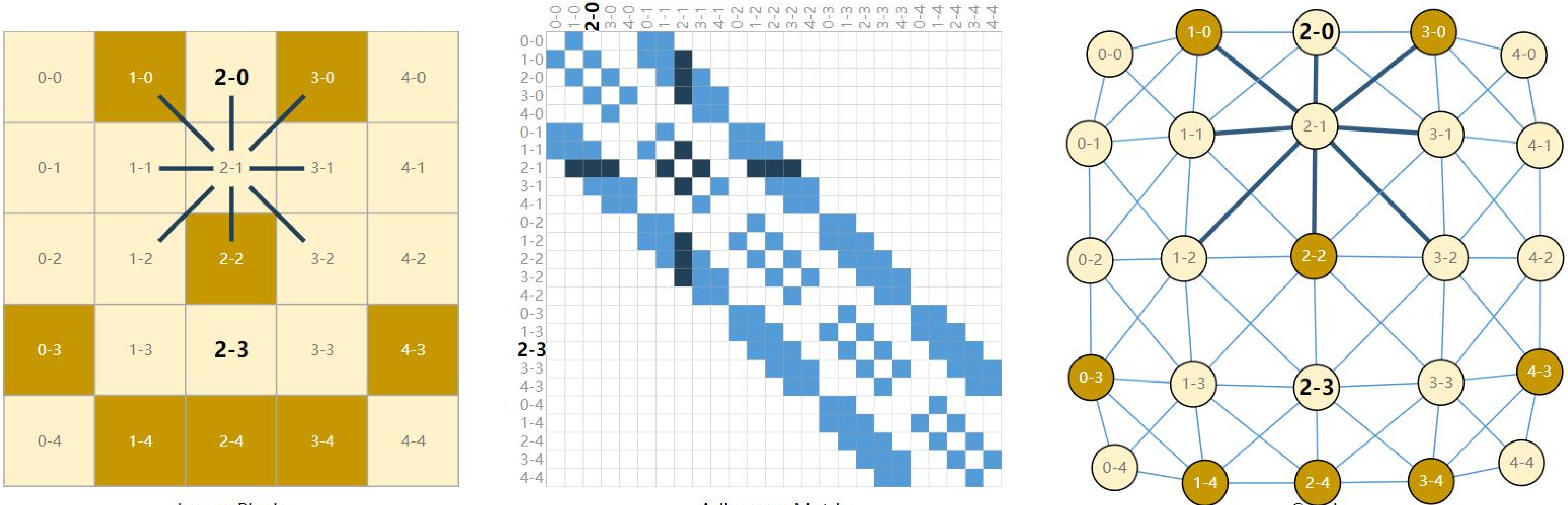
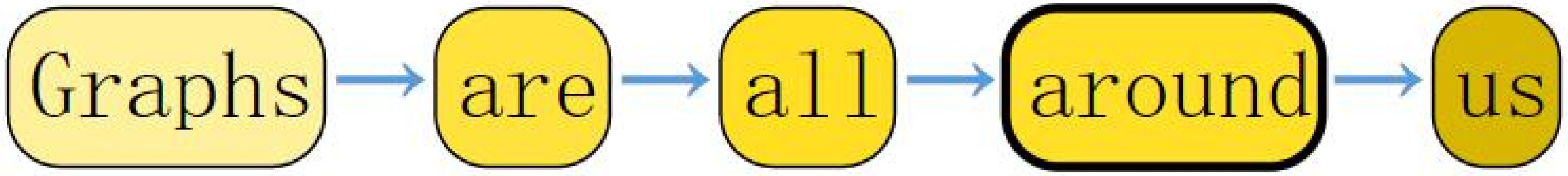


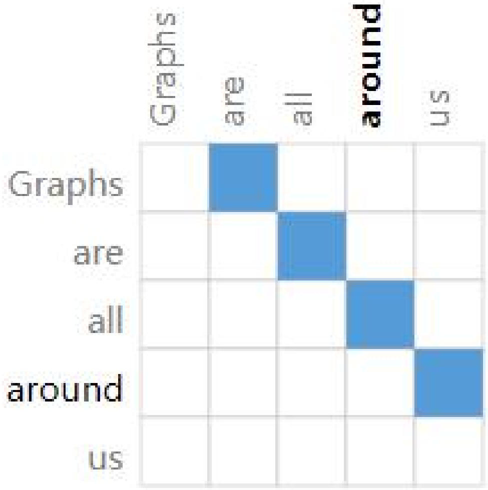
Image Pixels　　Adjacency Matrix　　Graph

GNN

图的邻接矩阵

文本数据也可以表示图的形式，邻接矩阵表示的连接关系





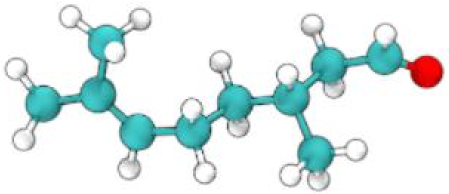
GNN

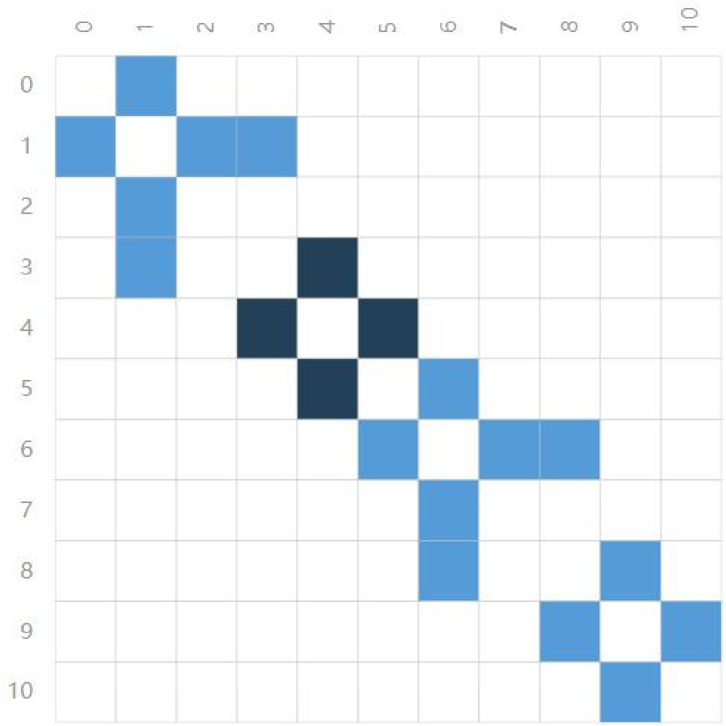
- 但是啊但是
  - 图像和文本任务中，你用过图相关的模型吗？好像木有吧
  - 为啥呢？因为图像和文本数据的格式都贼固定，想一想咱们的预处理
  - 所有图像resize成固定大小，然后进行卷积操作得到特征，格式很固定
  - 文本固定长度和词向量大小，然后也是这么个事，不需要特殊的邻接矩阵

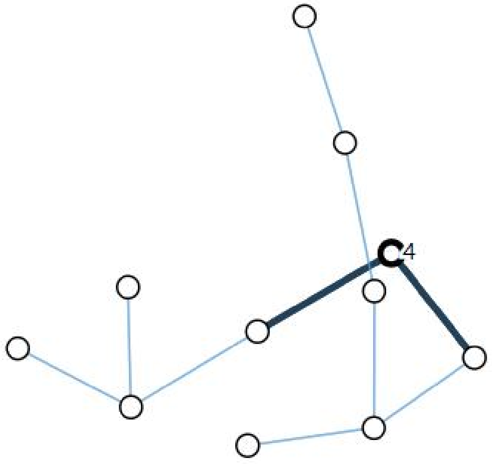
GNN

想想这些数据是固定格式吗?

分子相关的，还记得曾经的各种化学公式了嘛。。。



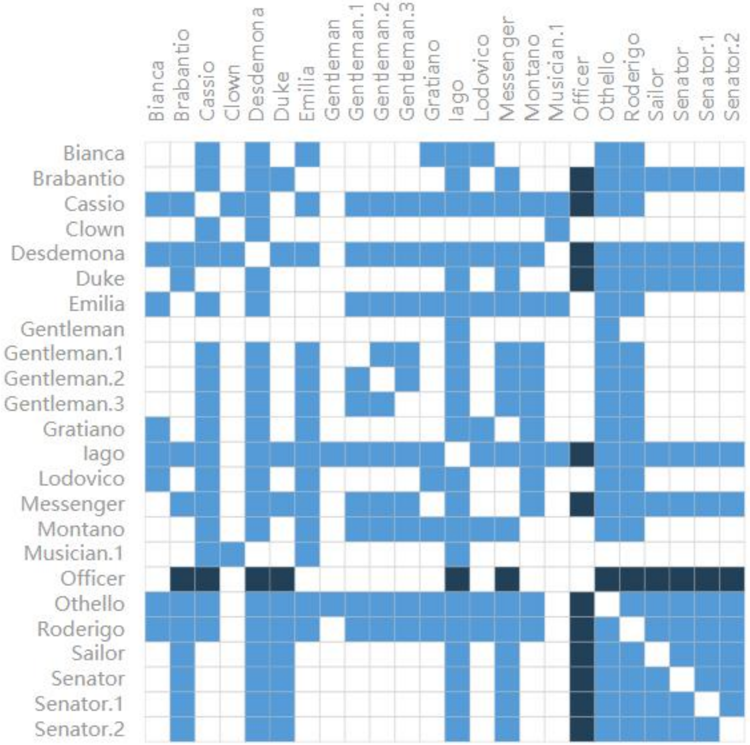


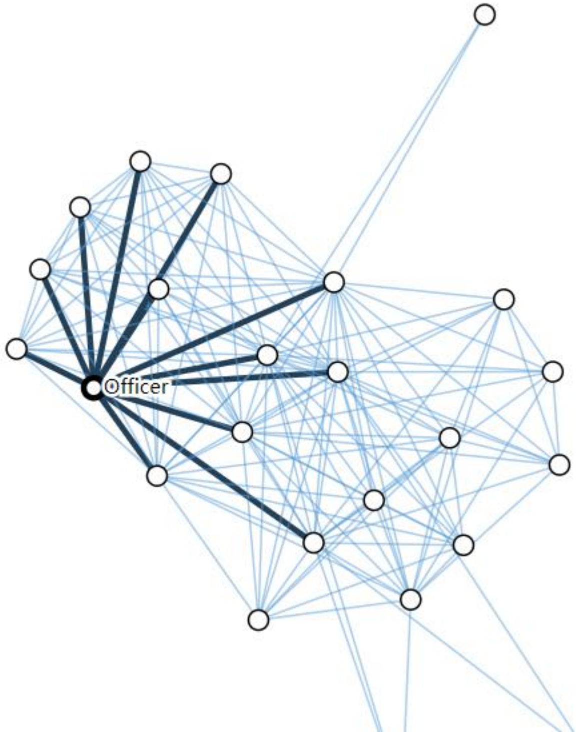


GNN

- 想想这些数据是固定格式吗？

- 社交网络中各个人物的关系，这种邻接矩阵会比较庞大

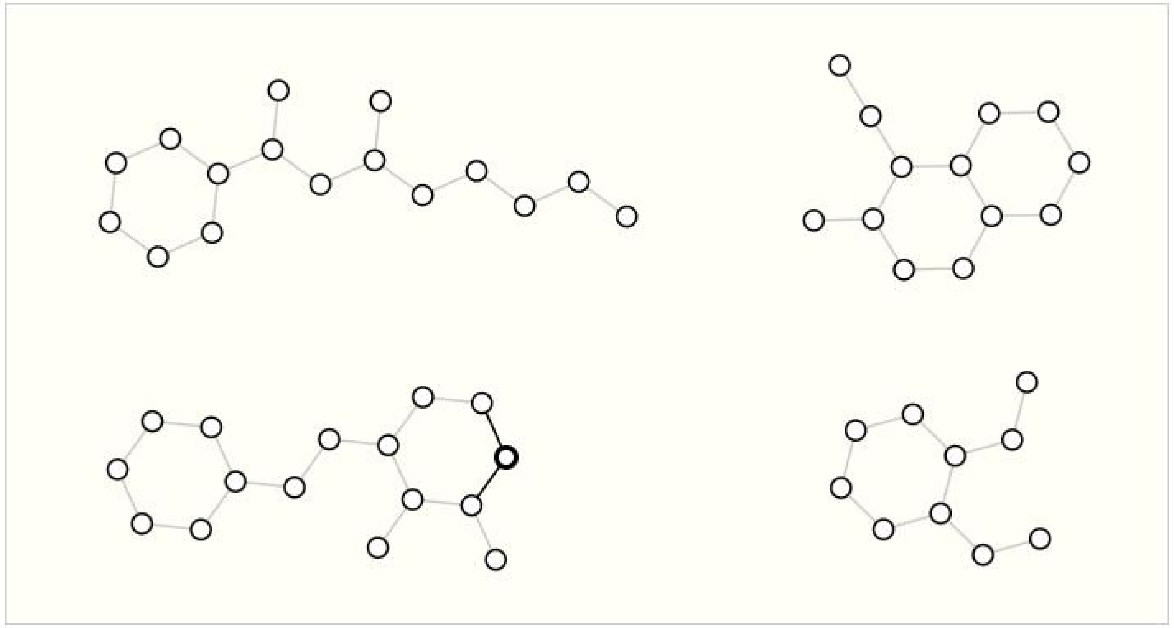


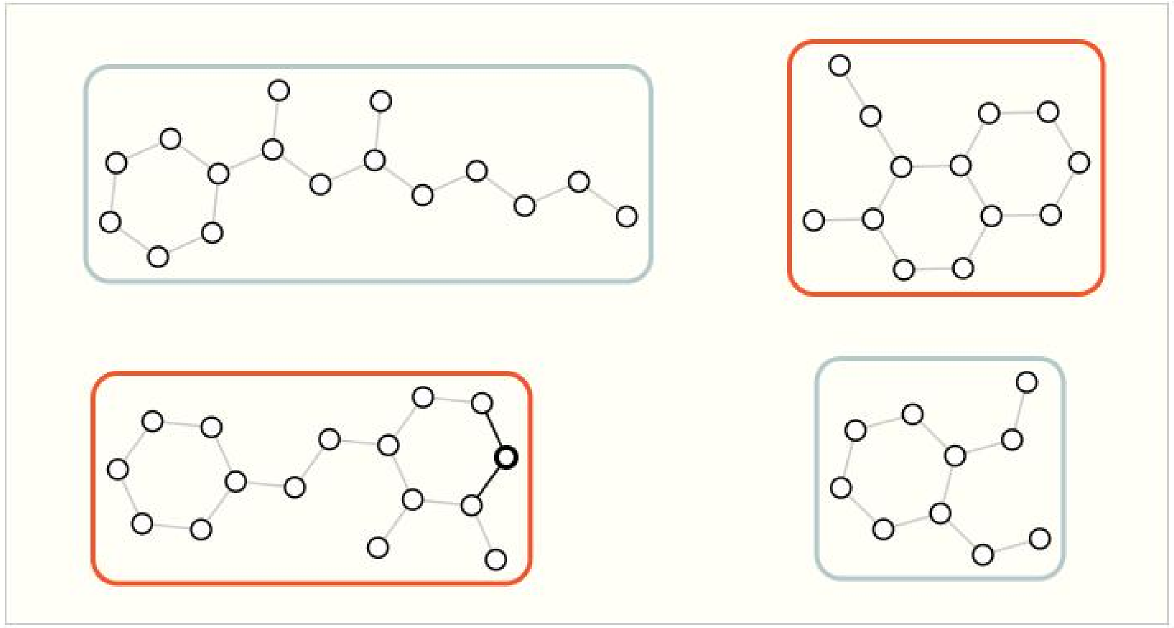


GNN

Graph级别任务

任务可以自己设计，例如这个分子有没有环路，这个分子是啥等

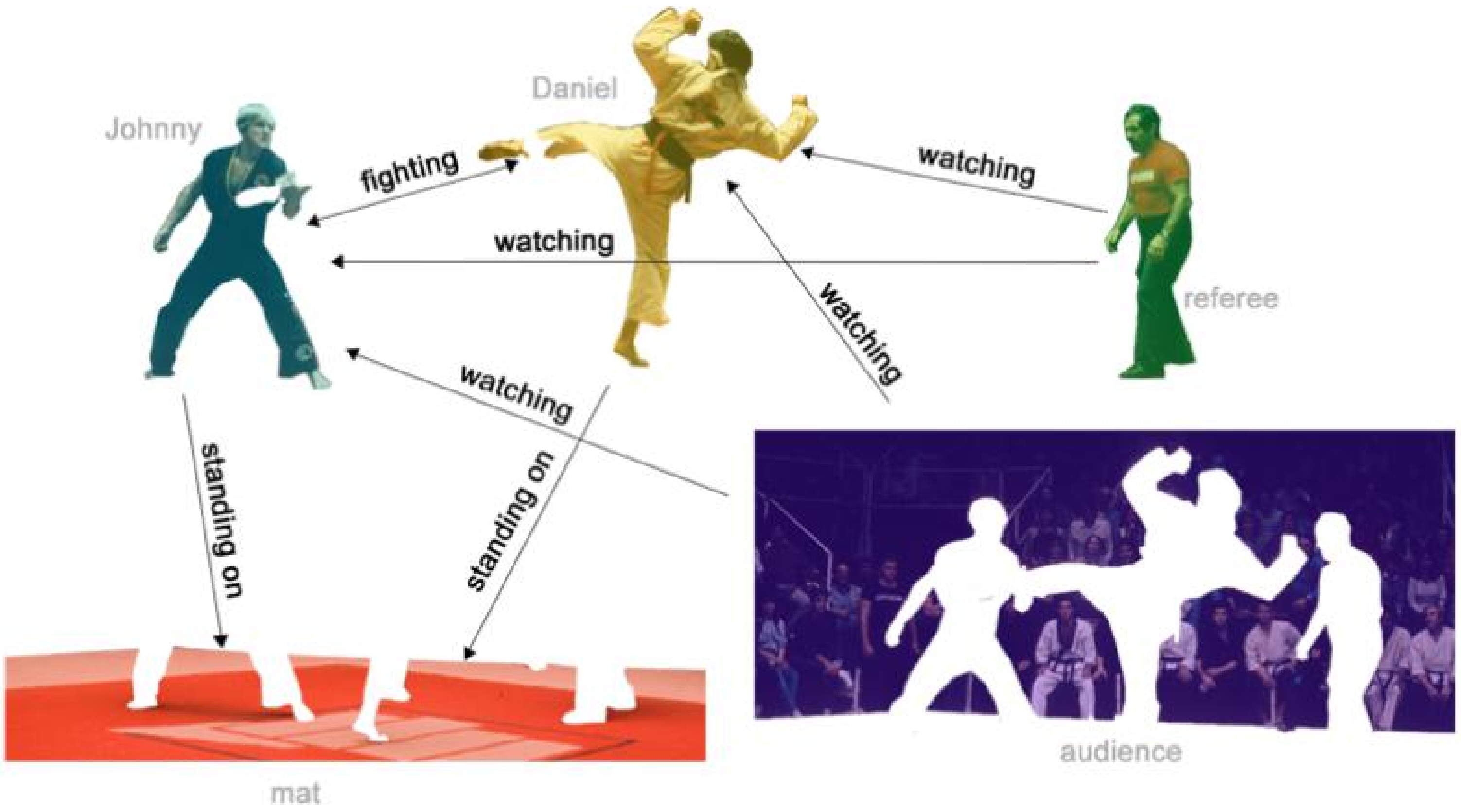




GNN

Node与Edge级别任务

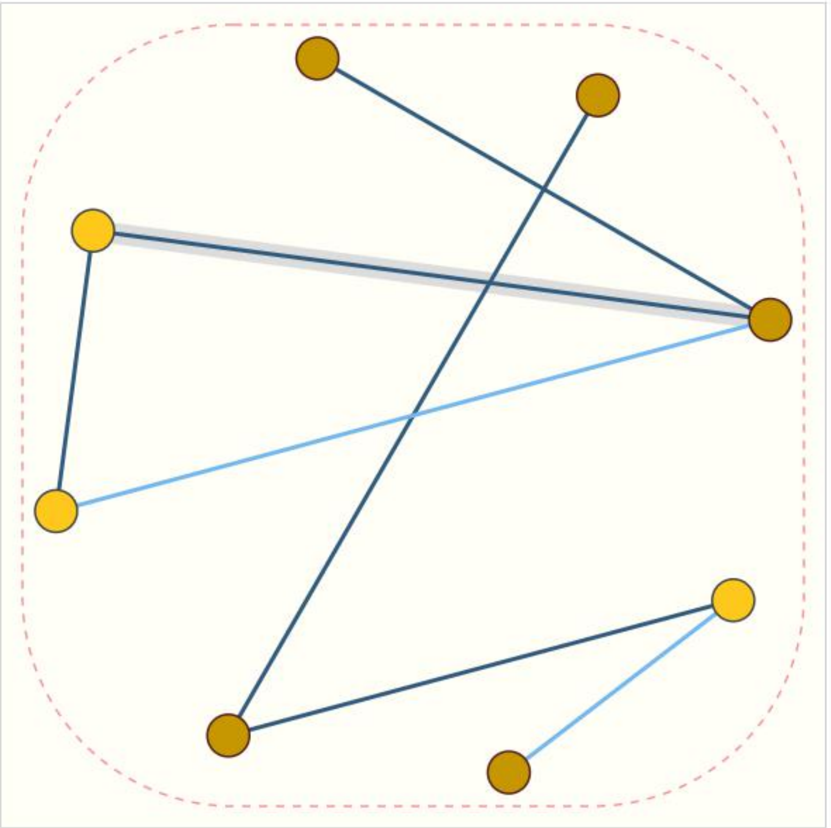
预测这个点是谁呢？这条边在做什么动作等



GNN

邻接矩阵

一般邻接矩阵表达形式如下，并不是一个N*N的矩阵，而是保存source,target



Nodes

[0, 1, 1, 0, 0, 1, 1, 1]

Edges

[2, 1, 1, 1, 2, 1, 1]

Adjacency List

[[1, 0], [2, 0], [4, 3], [6, 2],
[7, 3], [7, 4], [7, 5]]

Global

0

GNN

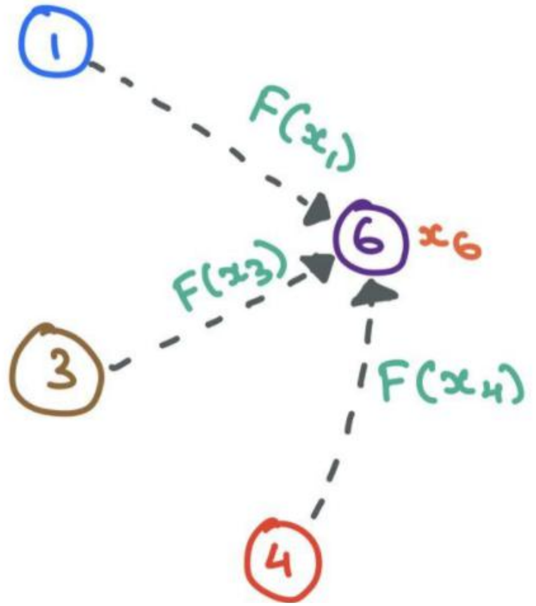
- message passing neural network

  - 每个点的特征该如何更新呢？肯定得考虑他们邻居的

GNN

- message passing neural network

  - 聚合操作可以当作全连接层
  - 但是更新的方法有很多，可以自己设置
  - 结合邻居与自身信息：$\bar{m}_i = G(\{\mathbf{W}_j \cdot x_j : j \in \mathcal{N}_i\})$
  - 汇总：$h_i = \sigma(W_1 \cdot h_i + \sum_{j \in \mathcal{N}_i} \mathbf{W}_2 \cdot h_j)$



$$\text{Sum} = \sum_{j \in \mathcal{N}_i} \mathbf{W}_j \cdot x_j$$

$$\text{Mean} = \frac{\sum_{j \in \mathcal{N}_i} \mathbf{W}_j \cdot x_j}{|\mathcal{N}_i|}$$

$$\text{Max} = \max_{j \in \mathcal{N}_i}(\{\mathbf{W}_j \cdot x_j\})$$

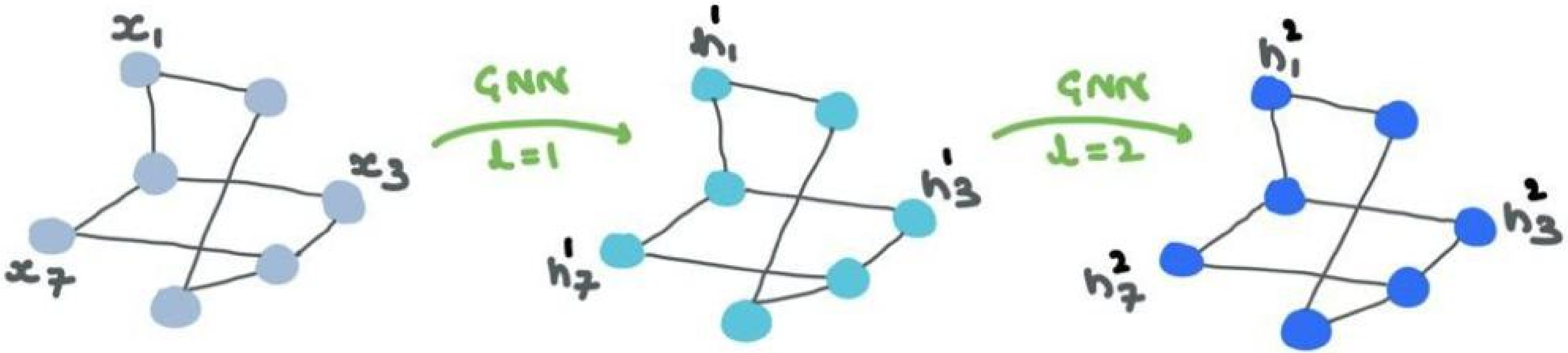
$$\text{Min} = \min_{j \in \mathcal{N}_i}(\{\mathbf{W}_j \cdot x_j\})$$

GNN

- GNN也可以有多层

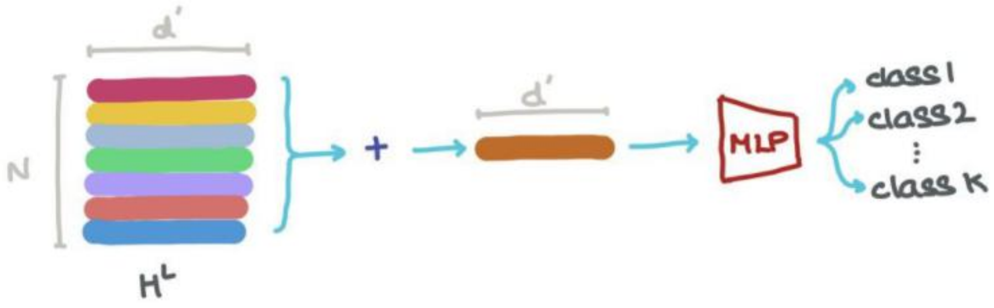
  - GNN的本质就是更新各部分特征

  - 其中输入是特征，输出也是特征，邻接矩阵也不会变的

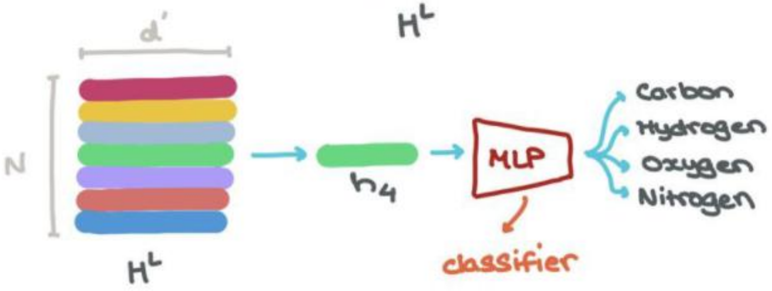


GNN

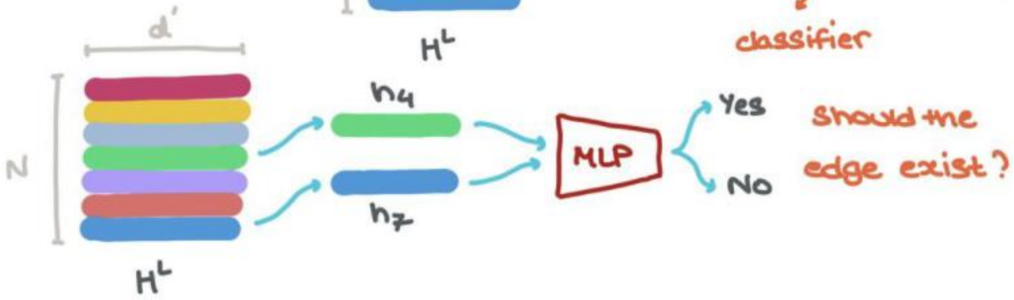
- 输出特征能干啥呢?
  - 各个点特征组合，可以图分类:



  - 各个节点也可以分类:



  - 边也是如此:



  - 其实只是利用图结构得到特征，最终要做什么还是我们自己定