飞桨

图神经网络七日打卡营

小斯妹　百度PGL团队成员

2020.11.25

昨晚课程内容的问题

陈轻歌 1小时前

deepwalk相关问题

deepwalk论文中用的加速方法是层次的softmax，而不是用的负采样吧。。。
这两种加速方法，会影响最终模型的性能吗?
毕竟是讲论文，还是尊重一下作者在论文中的表述吧。。。

赞 回复

Desmon 老师 1小时前

因为实际情况中，我们会选择用负采样的方式优化（可以看到后续的论文基本都是采用负采样的方法）。所以我们选择讲解负采样这种方式，对于大家来说比较好理解，同时实现起来也方便一些。另外，我们在讲述游走模型时，其实关注点是放在如何游走上面哈~ 晚上我会跟大家说一下，我们是有选择的对论文内容进行筛选讲解。

赞 回复 删除

昨晚的作业

AIStudio 红白黑： https://aistudio.baidu.com/aistudio/projectdetail/1265981?shared=1

红白黑

1小时前

图网络基本概念复习总结与思考，以及相关作业代码的详细注解（逐行解释，上下文联系，容易理解），算注册

路理解

或者博

图网络

今晚是

1

Notebook　文件(5)　«

一、图基础及分类

1.1 什么是图?

1.2 图具有的信息/属性

1.3 图节点的概念补充--度、出度与入度

1.4 概念理解

1.5 图的基本分类

二、同构图与异构图

2.1 同构图基本定义

*2.2 异构图的定义

*2.3 异构图的补充概念(图元（子图))

2.4 同构图与异构图的数学表示

/1260103

1　回复

3.1 Node2Vec采样算法转换代码注解

1. 这部分代码，用于随机游走后得到的路径，然后对这些路径进行吸收学习，训练图结构

In [16]

```
%%writefile userdef_sample.py
import numpy as np

# 随机节点的获取
def node2vec_sample(succ, prev_succ, prev_node, p, q):

    """
    输入：succ – 当前节点的下一个相邻节点id列表 list (num_neighbors,)
        prev_succ – 前一个节点的下一个相邻节点id列表 list (num_neighbors,)
        prev_node – 前一个节点id int
        p – 控制回到上一节点的概率 float
        q – 控制偏向DFS还是BFS float
    输出：下一个节点id int
    """
```

多看看课程讨论区

课程大纲

第一课：图学习初印象

- 图学习概述、入门路线
- 实践：环境搭建

第二课：游走类算法

- DeepWalk, node2vec, metapath2vec
- 实践：DeepWalk

第三课：图神经网络算法(一)

- GCN, GAT
- 实践：GCN, GAT

第四课：图神经网络算法(二)

- 图采样、邻居聚合
- 实践：GraphSage

第五课：GNN 进阶

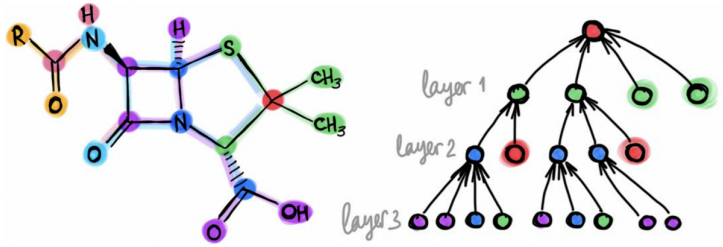
- ERNIESage, UniMP
- 实践：有趣的应用

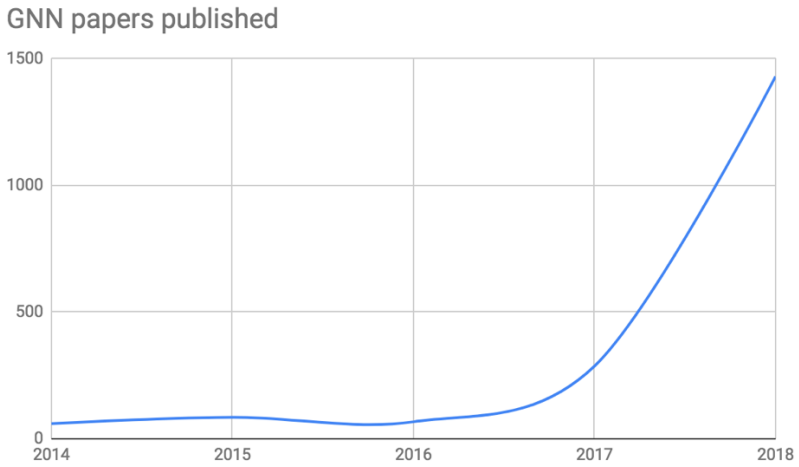
后续：新冠项目实战，带你助力疫情防控

参考材料：

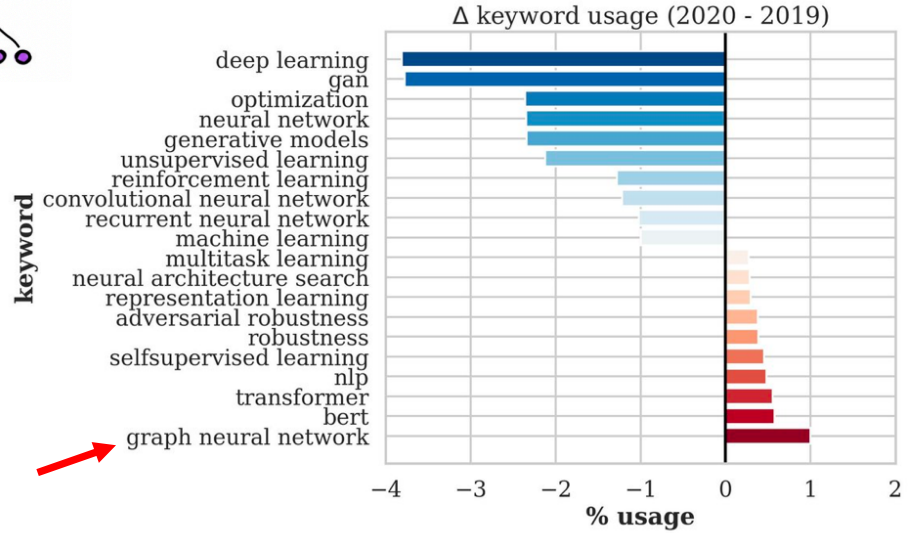
- 斯坦福CS224W课程： http://cs224w.stanford.edu
- 图学习库 PGL：https://github.com/PaddlePaddle/PGL

图神经网络的兴起：业界论文发表

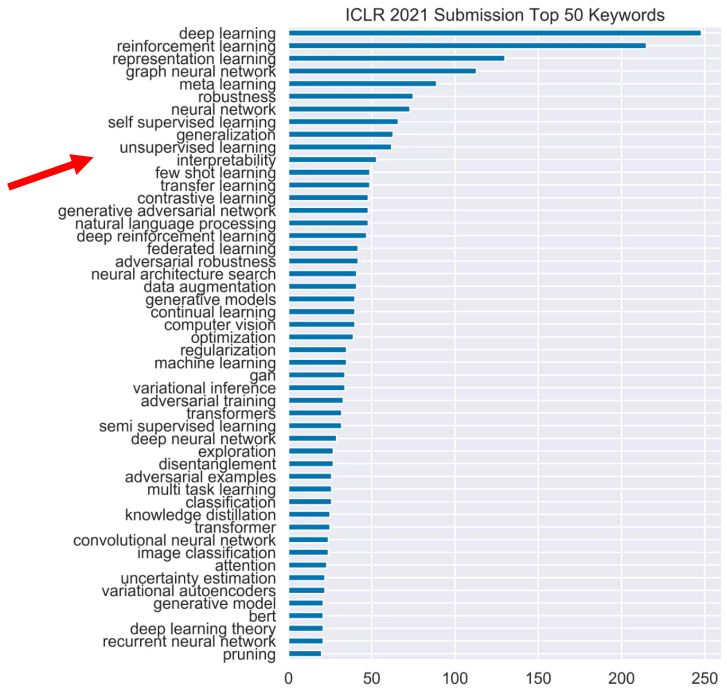




图神经网络发表论文数（2014-2018）

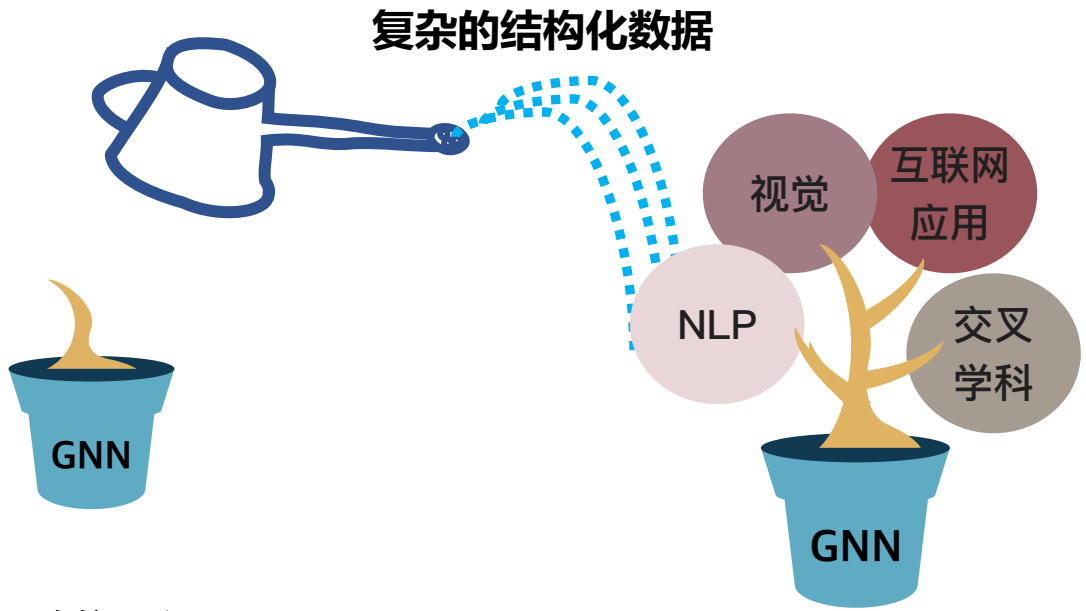


ICLR 2020 提交论文情况



ICLR 2021 提交Top50关键词

图神经网络的兴起：各领域的渗透

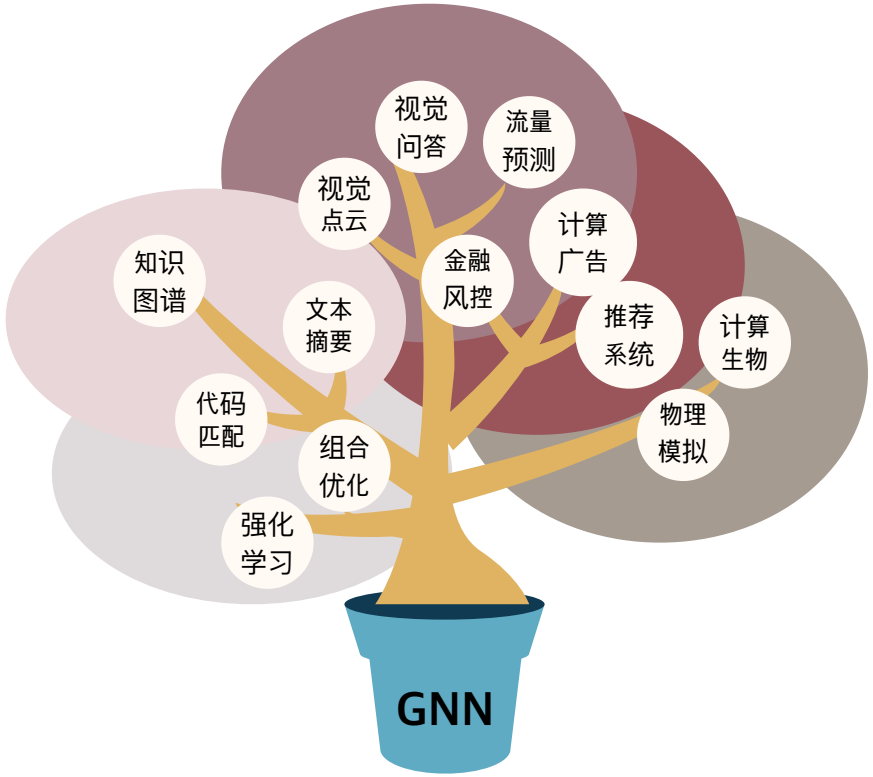


图网络结构雏形

- 涌现不同的图网络如GCN、GAT
- 提供了建模复杂结构的工具

图网络领域初探

- 在不同的领域引入复杂结构化信息，而信息增益带来收益
- 可迁移性，图网络可以统一不同领域的模型。



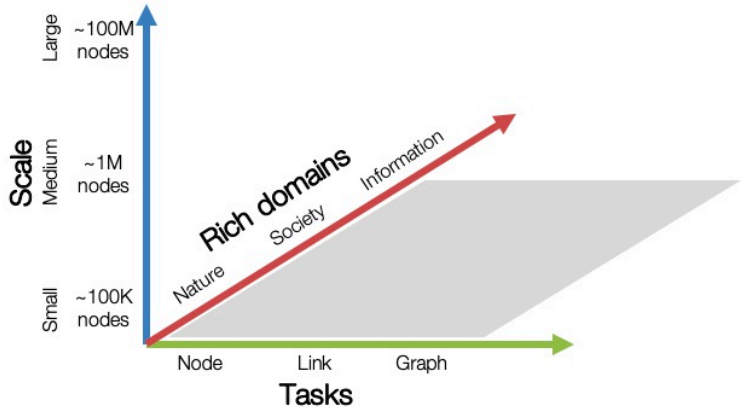
图网络应用爆炸

- 全新的解决方案：解决交叉学科的问题，生物计算、药物发现、粒子运动模拟
- 大量落地推荐系统、搜索广告、金融风控

图神经网络的兴起：权威榜单出现

OPEN GRAPH BENCHMARK

- Jure Leskovec、Yoshua Bengio、Will Hamilton、Max Welling等学者提出



图神经网络领域目前最**权威**的评测榜单：

① 规模大：最大为10亿级

② 领域多：Nature/Society/Information

③ 任务多：Node/Link/Graph

https://ogb.stanford.edu/

https://github.com/graphdeeplearning/benchmarking-gnns

Benchmarking Graph Neural Networks

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[2] Department of Mathematics, Loyola Marymount University
[3] Mila, University of Montréal [4] CIFAR

http://keg.cs.tsinghua.edu.cn/cogdl/leaderboard.html

Leaderboard

CogDL provides several downstream tasks including node classification (with or without node attributes), link prediction (with or without attributes, heterogeneous or not). These leaderboards maintain state-of-the-art results and benchmarks on these tasks.

NODE CLASSIFICATION

LINK PREDICTION

GRAPH CLASSIFICATION

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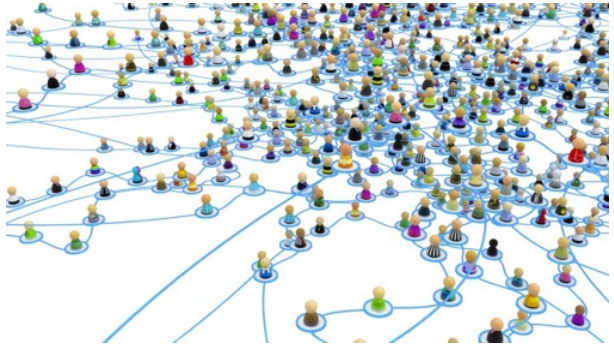
第三课 图神经网络算法(一)

小斯妹 百度PGL团队成员

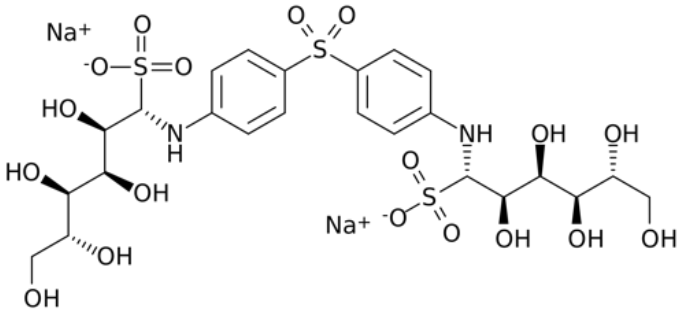
2020.11.25

简单回顾

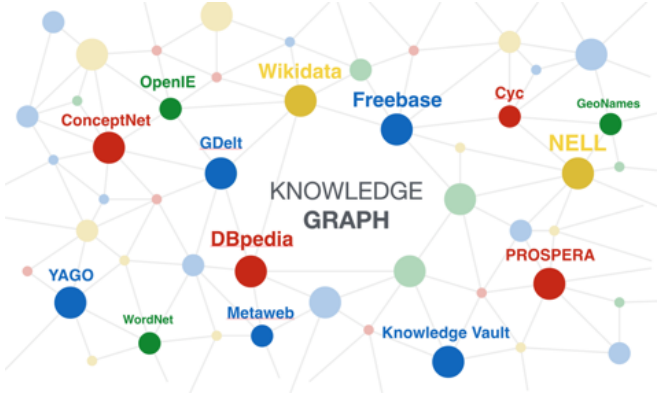
社交关系



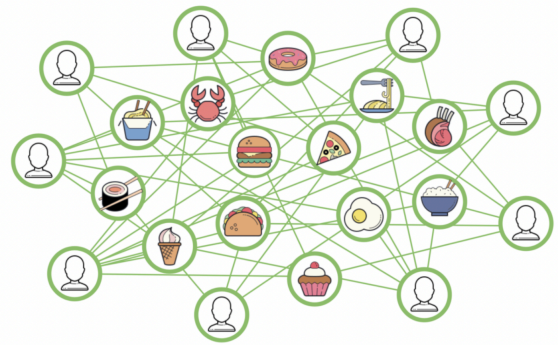
化学分子



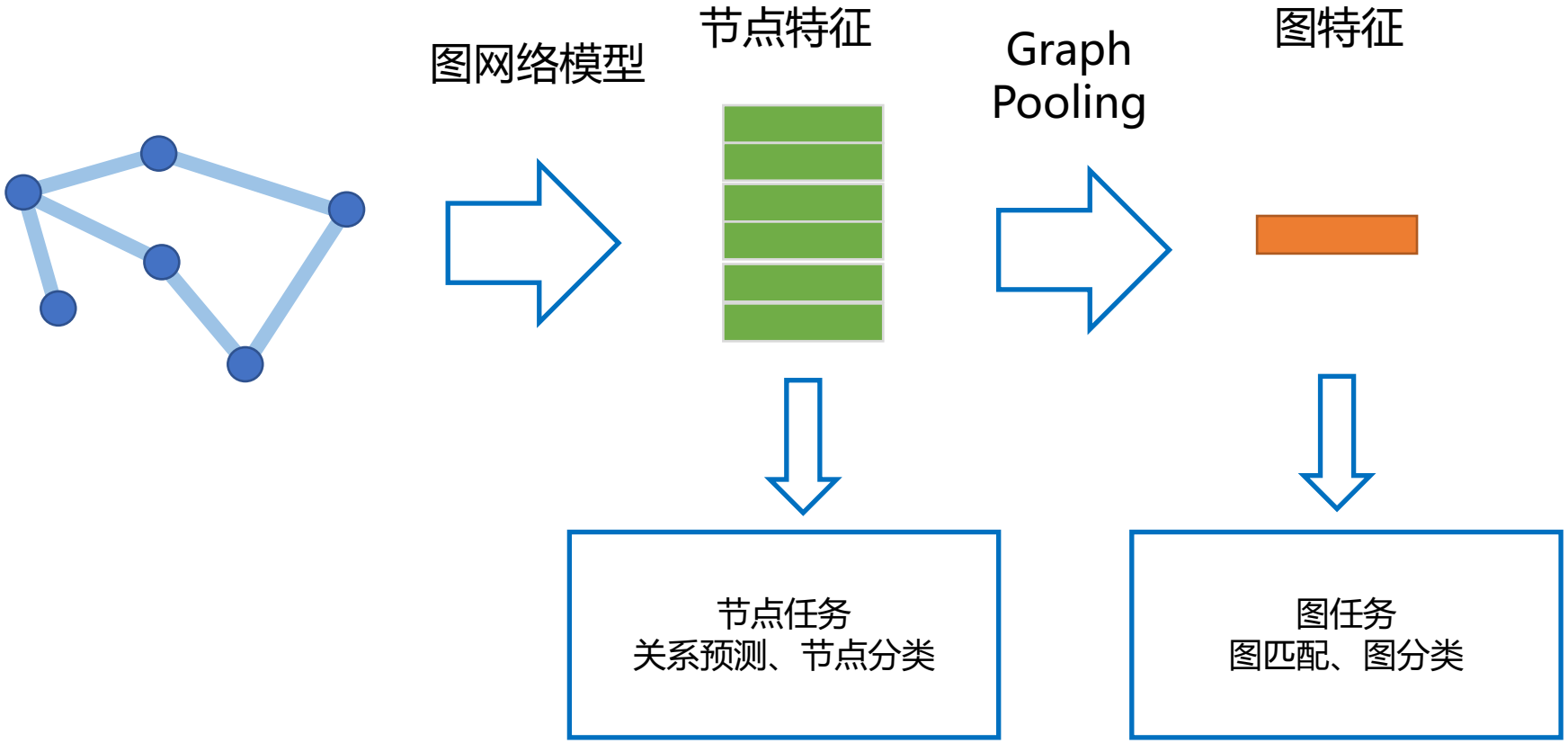
知识图谱



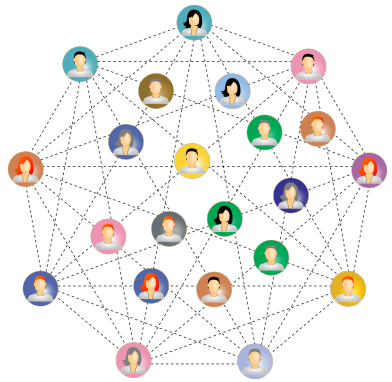
推荐系统



图网络的目的

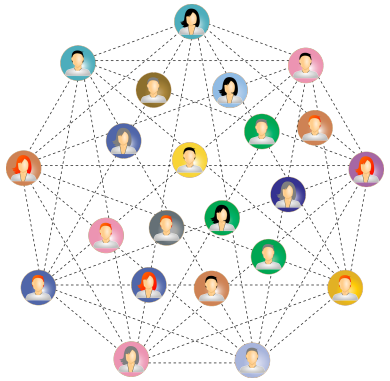


训练方式



图游走类模型

下游任务，如分类

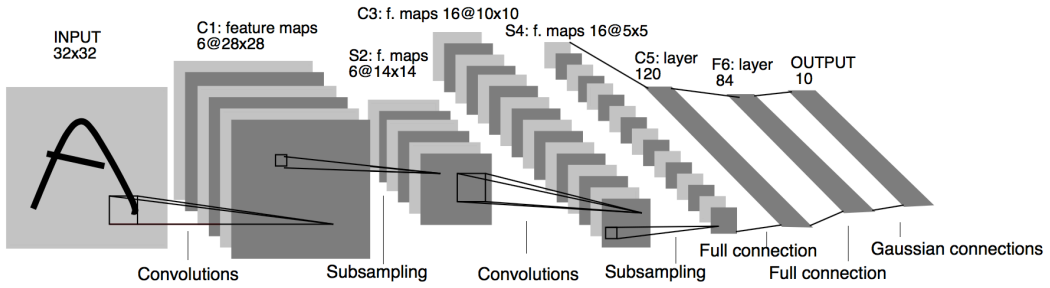


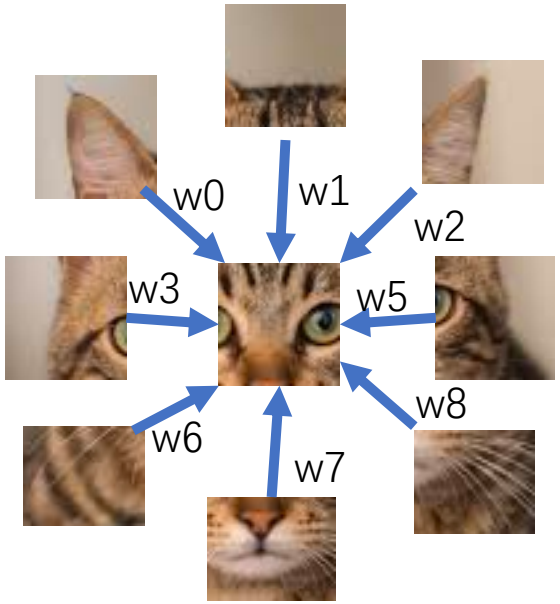
具体任务，如分类

端到端训练

回顾DNN在文本以及图像的发展

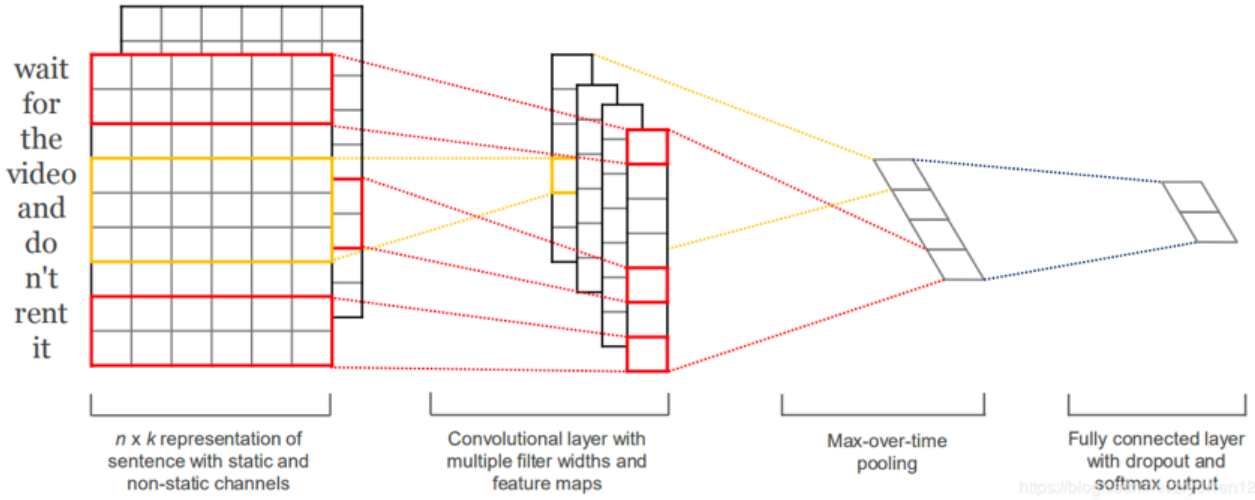
图像上的卷积网络
2D-Convolution





回顾DNN在文本以及图像的发展

文本上的卷积网络 1D-Convolution

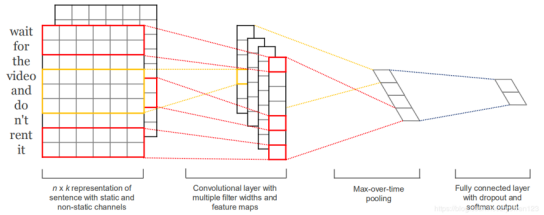


TextCNN: Convolutional Neural Networks for Sentence Classification

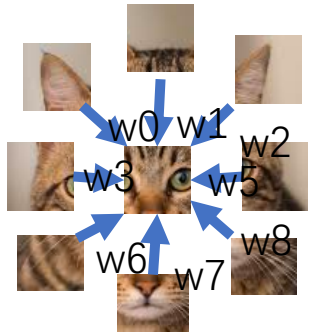
规则性数据

排列整齐的数据
Grid-Like Data

文本

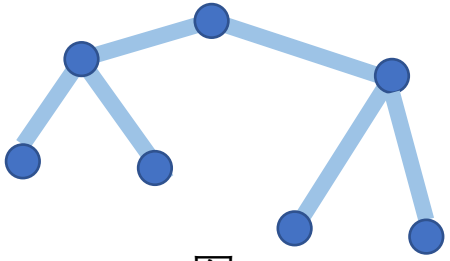


图像

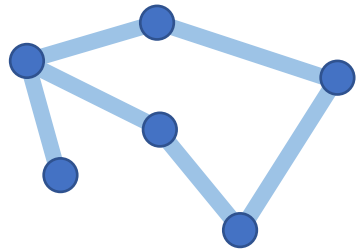


不规则数据

树

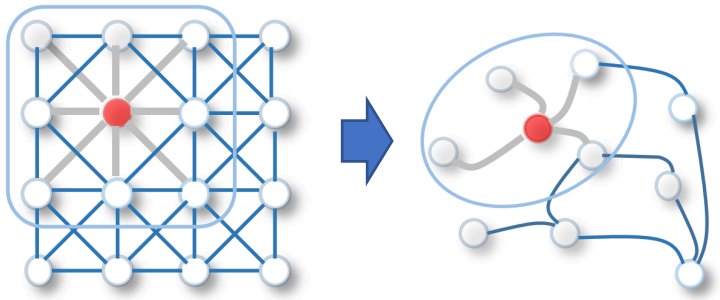


图

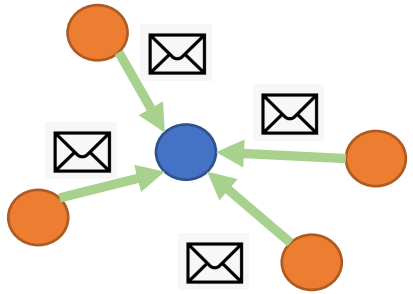


图卷积网络

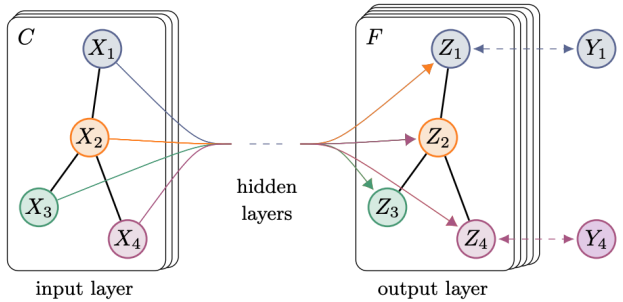
Graph Convolutional Network



如何从**图像卷积**，类比到**图结构卷积**



怎么用**消息传递**方式实现图卷积网络

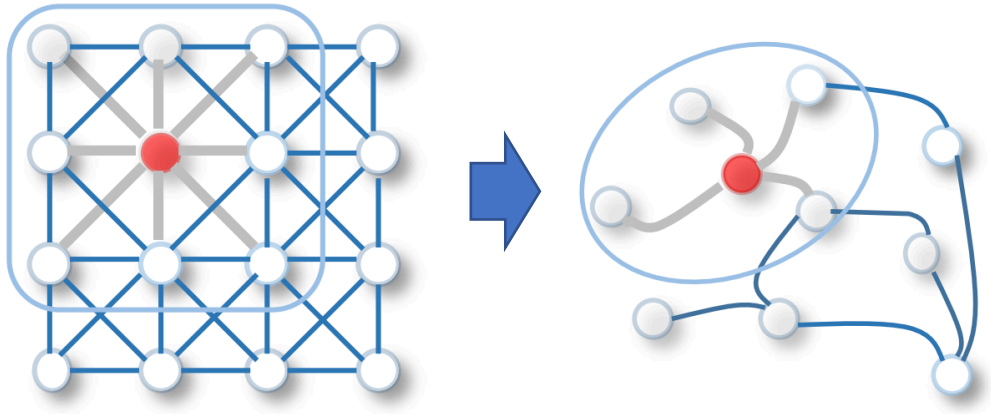


怎么用多层图网络完成**节点分类任务**

参考文献: SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS (ICLR 2017)

图卷积网络

Graph Convolutional Network

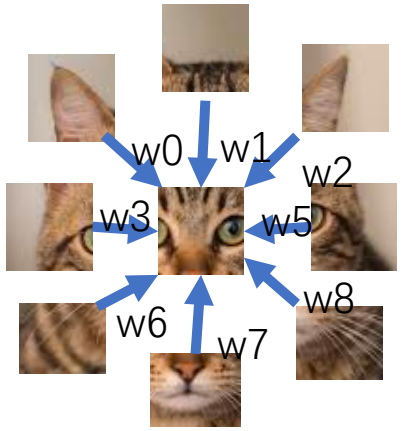


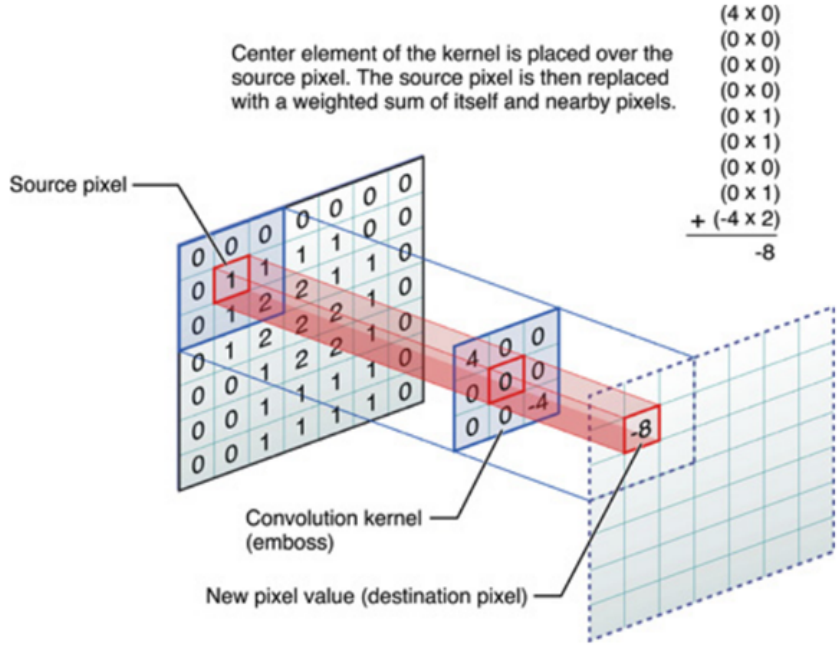
如何从**图像卷积**，类比到**图结构卷积**

图卷积网络

Graph Convolutional Network

图像上的卷积操作





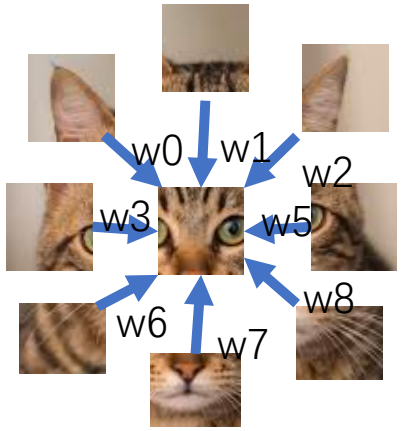
图像卷积

将一个**像素点**周围的**像素**按照不同的**权重叠加**起来。

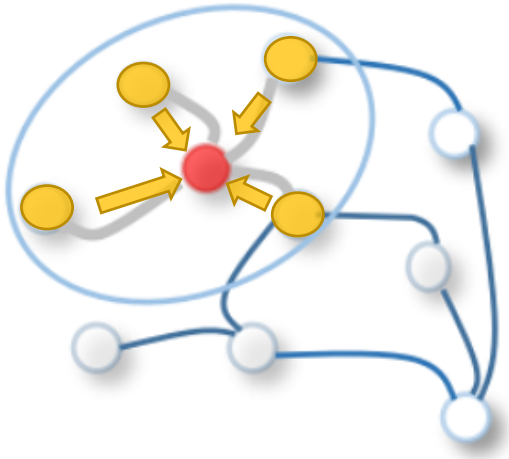
图卷积网络

Graph Convolutional Network

图像上的卷积操作



图结构上的卷积



图像卷积

将一个**像素点**周围的**像素**按照不同的**权重叠加**起来。

图结构卷积

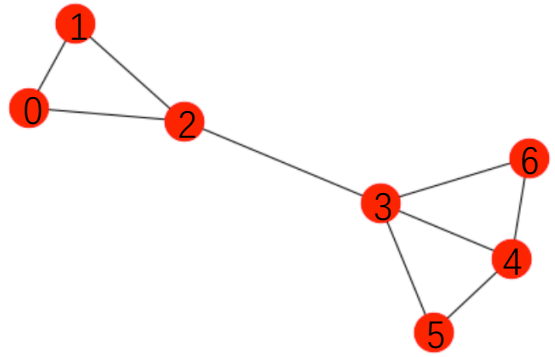
将一个**节点**周围的**邻居**按照不同的**权重叠加**起来。

图卷积网络

Graph Convolutional Network

图卷积网络的计算公式

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$



红框 是图卷积网络的**核心公式**

$\hat{A}$ 邻接矩阵

$\hat{D}^{-\frac{1}{2}}$ 与度矩阵相关

$H^{(l)}$ 每一层的节点表示

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

邻接矩阵

图卷积网络

Graph Convolutional Network

图卷积网络的计算公式

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

红框 是图卷积网络的**核心公式**

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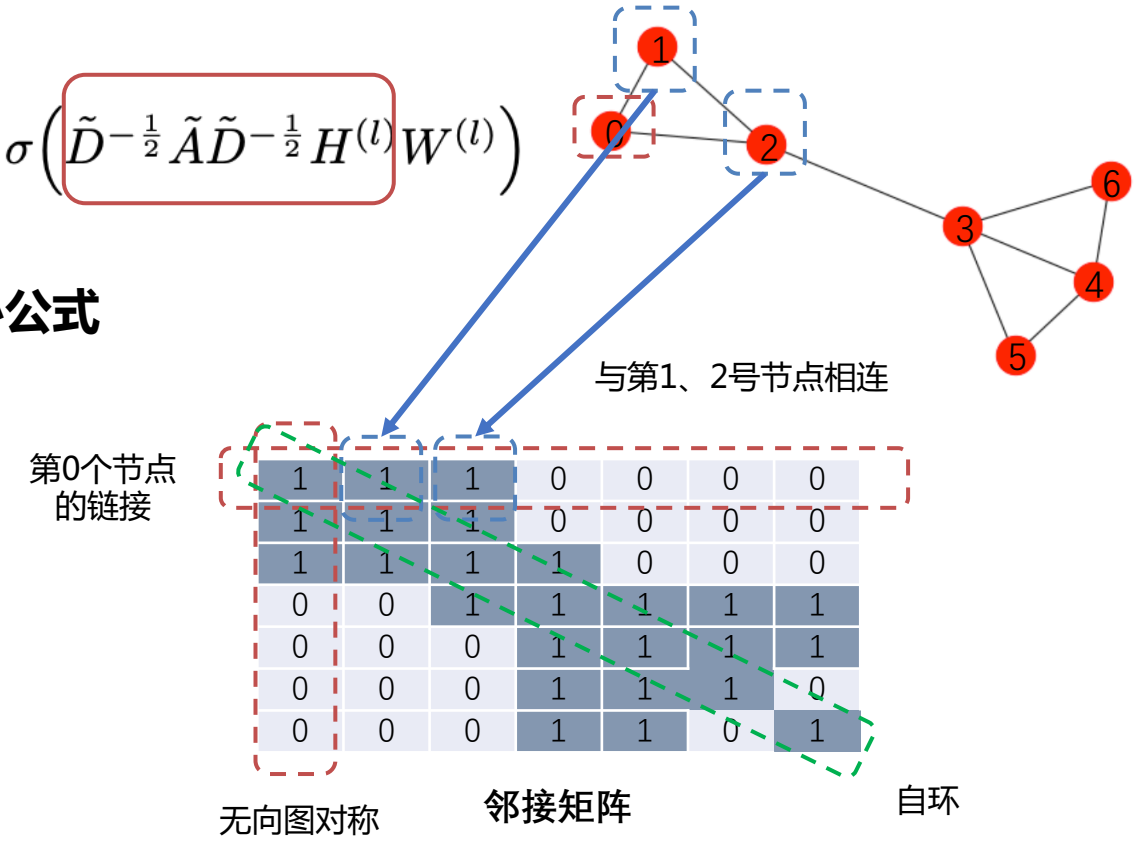
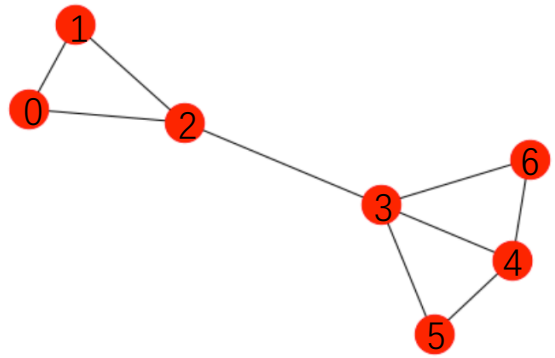


图卷积网络

Graph Convolutional Network



图卷积网络的计算公式

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

$\hat{A}$ 是邻接矩阵

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

求和

$\hat{D}$ 是度矩阵

3	0	0	0	0	0	0
0	3	0	0	0	0	0
0	0	4	0	0	0	0
0	0	0	5	0	0	0
0	0	0	0	4	0	0
0	0	0	0	0	3	0
0	0	0	0	0	0	3

$\hat{D}^{-\frac{1}{2}}$

$1/\sqrt{3}$	0	0	0	0	0	0
0	$1/\sqrt{3}$	0	0	0	0	0
0	0	$1/\sqrt{4}$	0	0	0	0
0	0	0	$1/\sqrt{5}$	0	0	0
0	0	0	0	$1/\sqrt{4}$	0	0
0	0	0	0	0	$1/\sqrt{3}$	0
0	0	0	0	0	0	$1/\sqrt{3}$

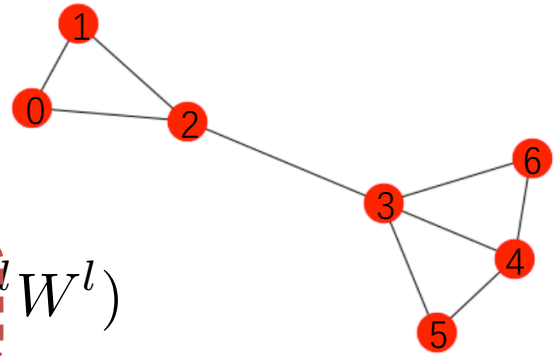
图卷积网络

Graph Convolutional Network

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

简化

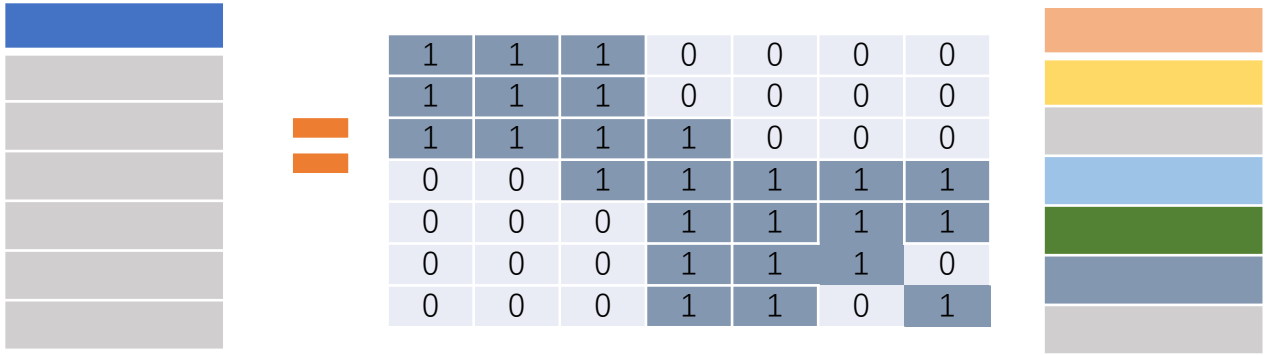
$$H^{(l+1)} = \sigma(\hat{A}H^{l}W^{l})$$



$AH^{(l)}$ 公式的物理含义是什么

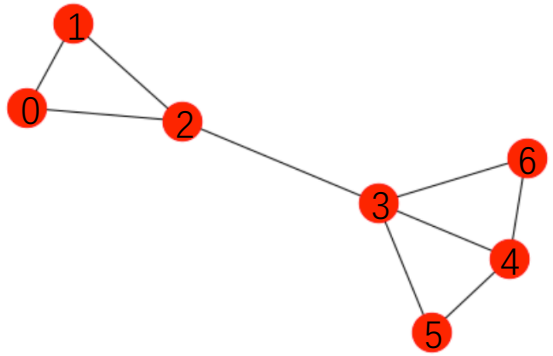
$H^{(l+1)}$ A $H^{(l)}$

第0节点表示



图卷积网络

Graph Convolutional Network



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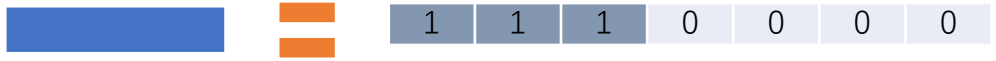
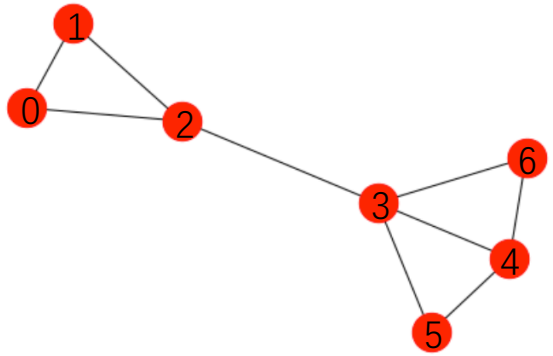


图卷积网络

Graph Convolutional Network



$AH^{(l)}$ 公式的物理含义是什么

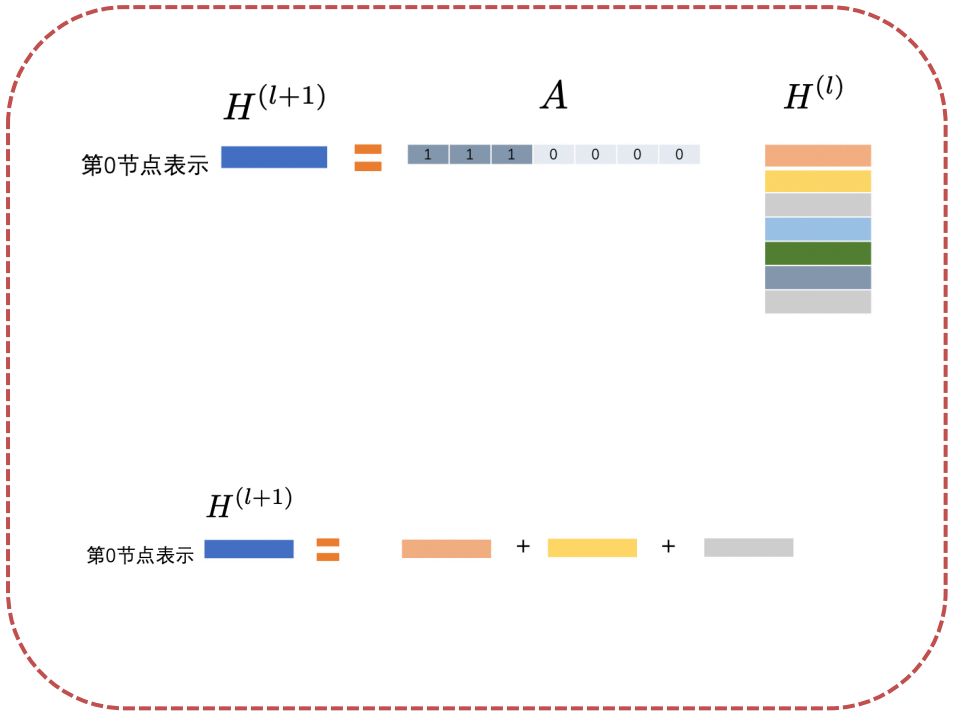
$H^{(l+1)}$

第0节点表示 

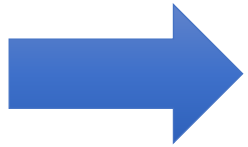
图卷积网络

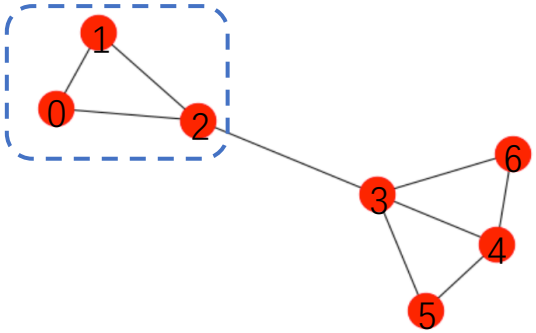
Graph Convolutional Network

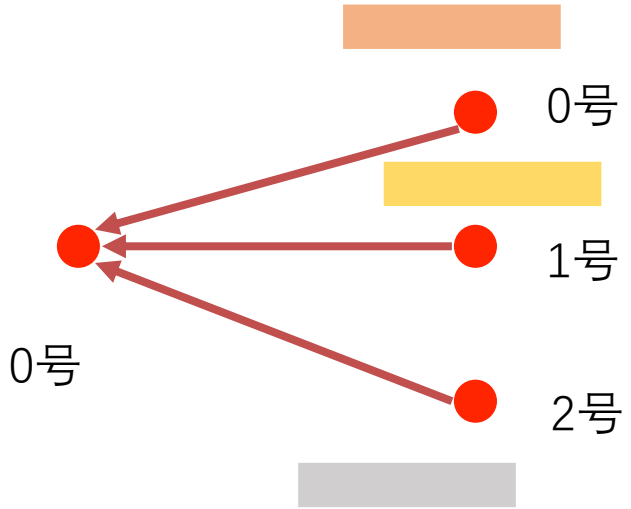
$AH^{(l)}$ 公式的物理含义是什么



消息传递
Message Passing

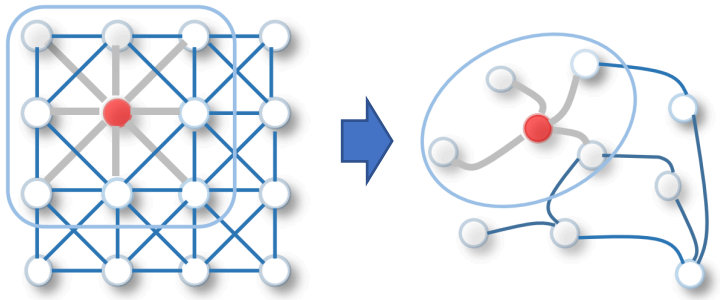




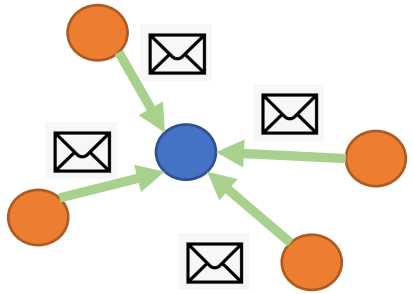


图卷积网络

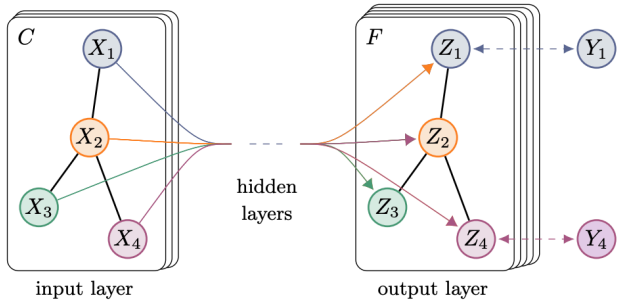
Graph Convolutional Network



如何从**图像卷积**，类比到**图结构卷积**



怎么用**消息传递**方式实现图卷积网络

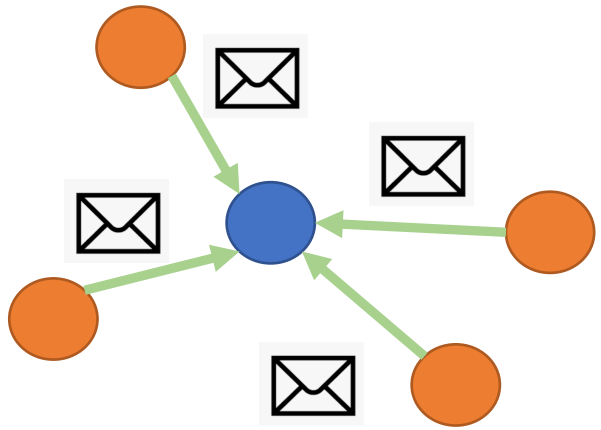


怎么用多层图网络完成**节点分类任务**

参考文献: SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS (ICLR 2017)

图卷积网络

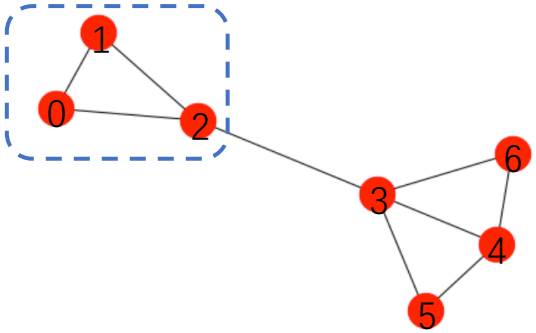
Graph Convolutional Network



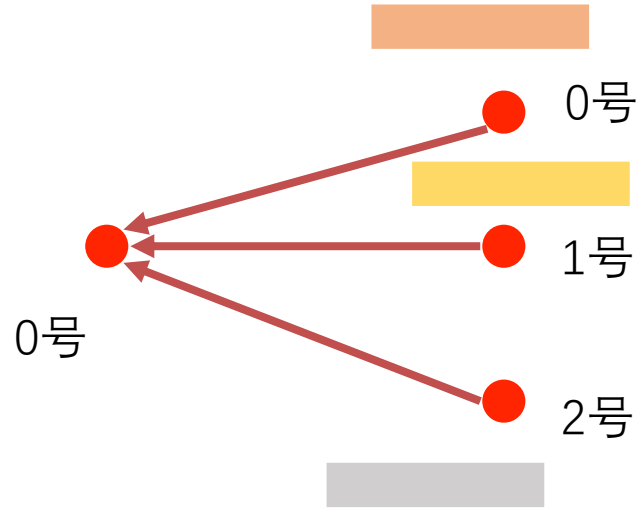
怎么用**消息传递**方式实现图卷积网络

图卷积网络

Graph Convolutional Network



消息传递
Message Passing

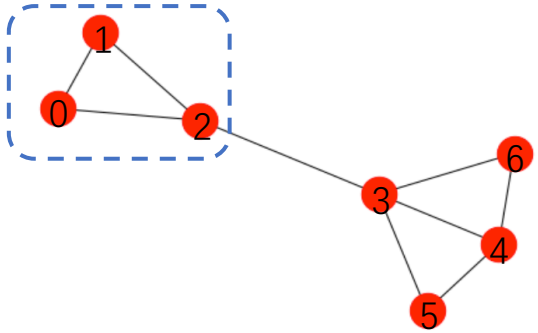


发送Send

1. 边上的源节点，往目标节点发送特征

图卷积网络

Graph Convolutional Network



消息传递
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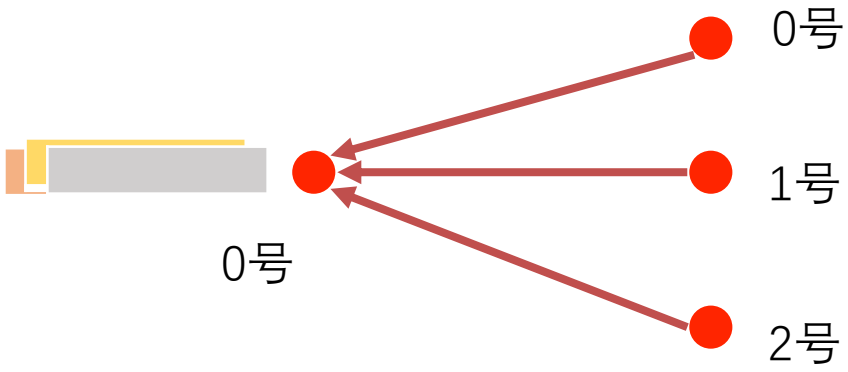
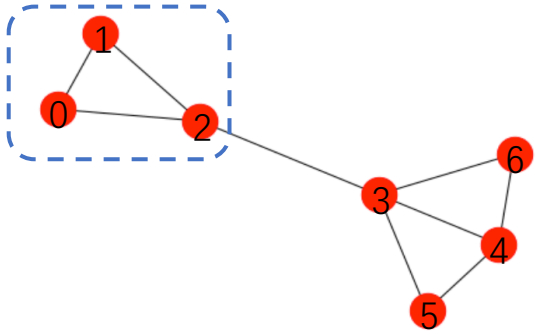


接收Recv

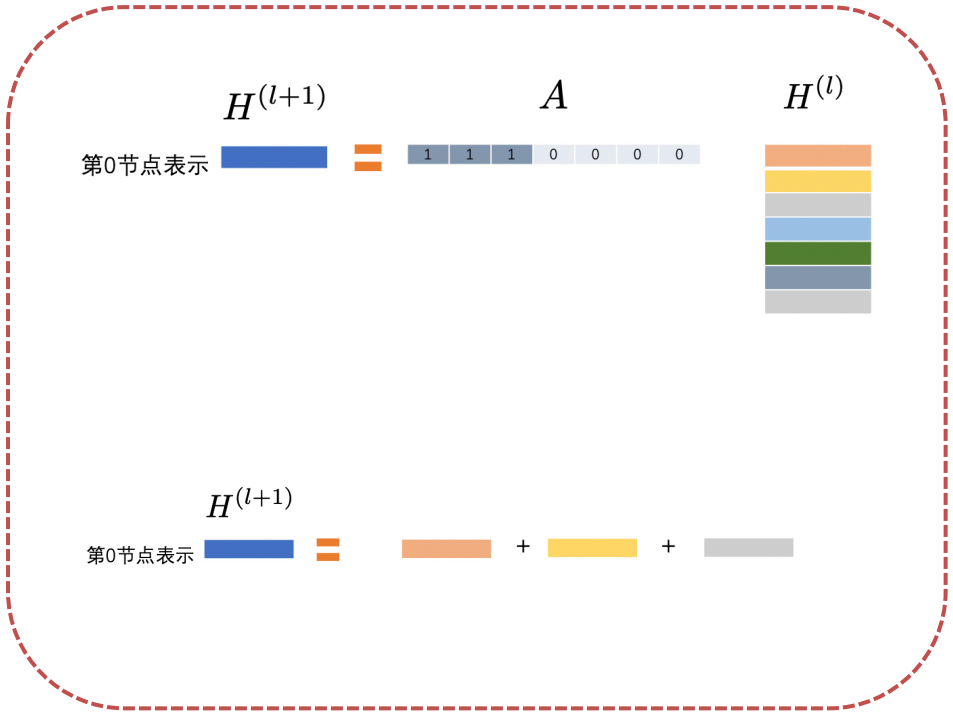
2. 目标节点对收到的特征进行聚合

图卷积网络

Graph Convolutional Network



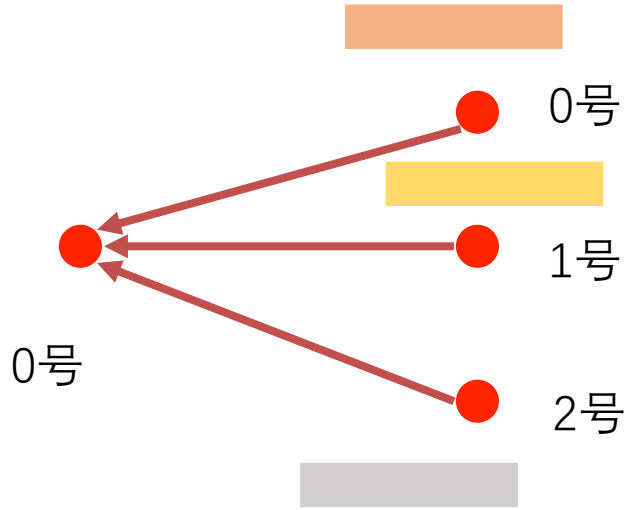
$AH^{(l)}$ 公式的物理含义是什么



消息传递
Message Passing

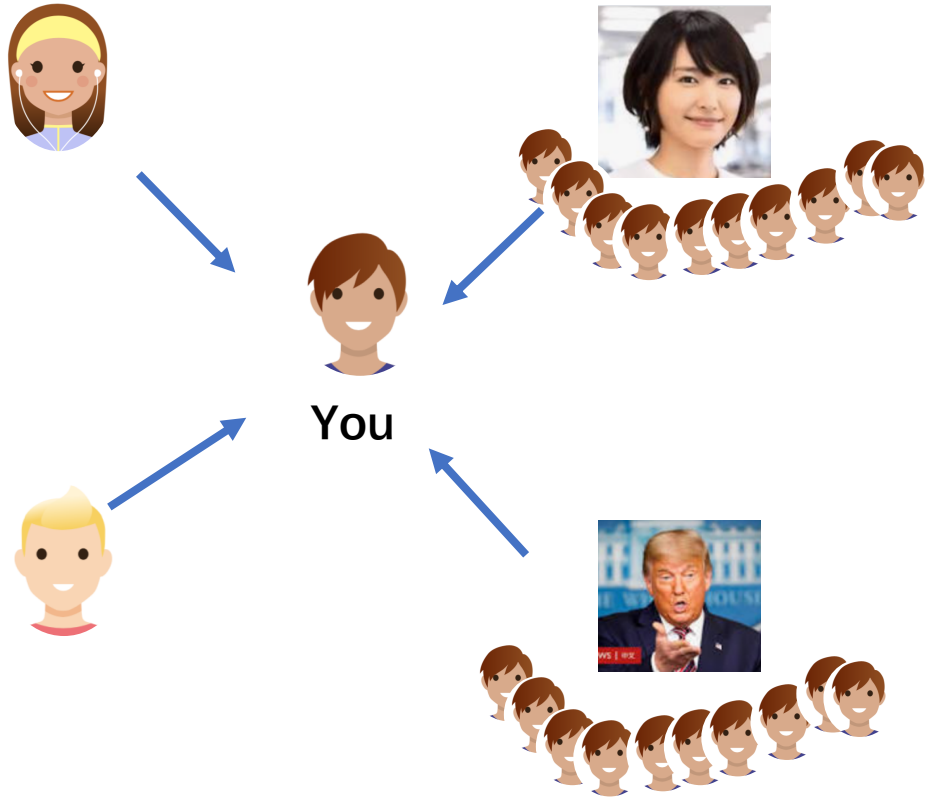
发送SEND 源节点发送特征给目标节点

接收RECV 目标节点接收特征并统计



图卷积网络

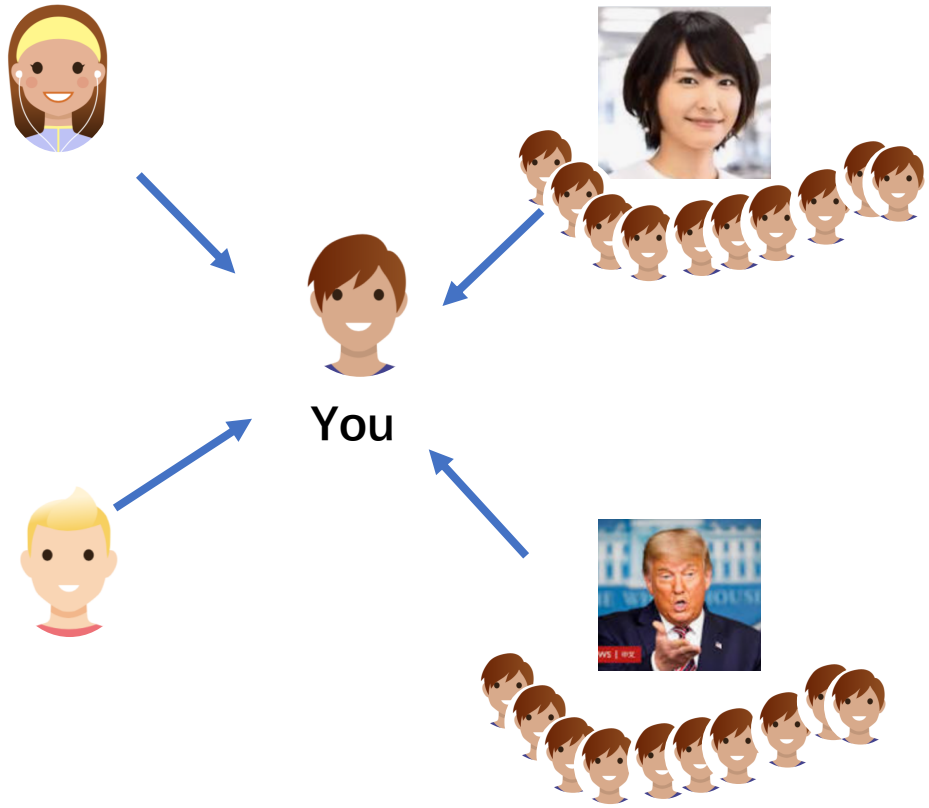
$AH^{(l)}$ 将邻居的特征接收、聚合



是否所有的人对自己的评价都是有用的？

图卷积网络

$AH^{(l)}$ 将邻居的特征接收、聚合

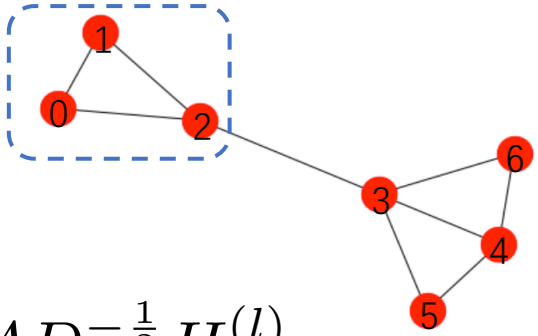


是否所有的人对自己的评价都是有用的？

如何衡量邻居的重要性 **度**

图卷积网络

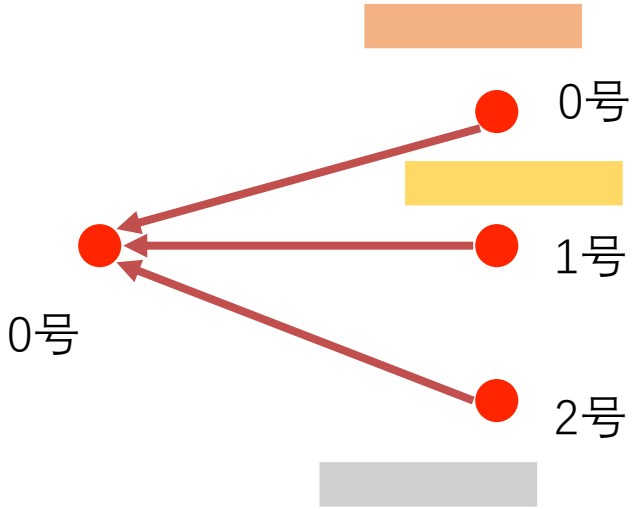
Graph Convolutional Network

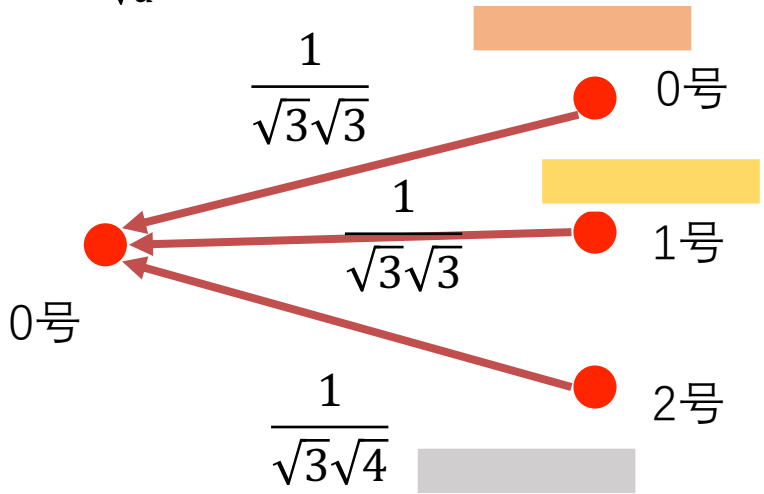


给边加权

$AH^{(l)}$ → $D^{-\frac{1}{2}}AD^{-\frac{1}{2}}H^{(l)}$

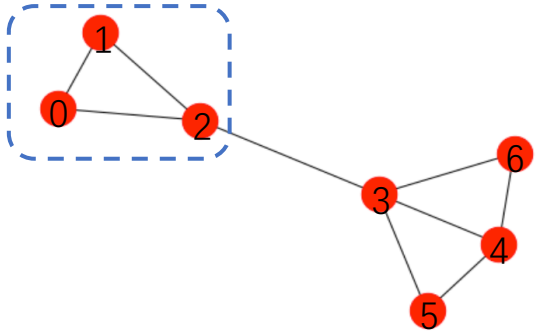
d越大，信息量越小，$\frac{1}{\sqrt{d}}$越小



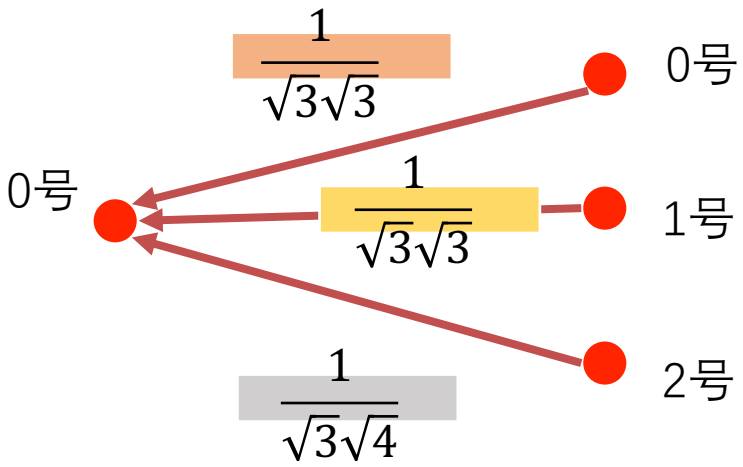


图卷积网络

Graph Convolutional Network



$$D^{-\frac{1}{2}}AD^{-\frac{1}{2}}H^{(l)}$$

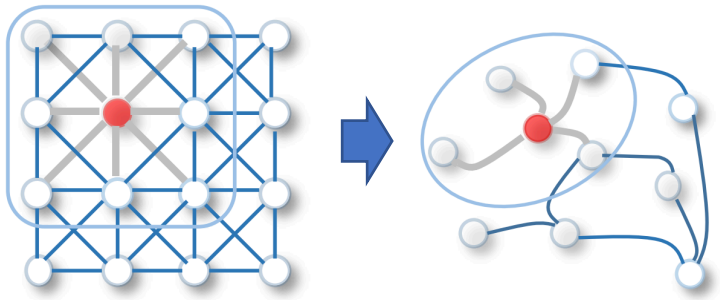


在PGL中Message Passing实现

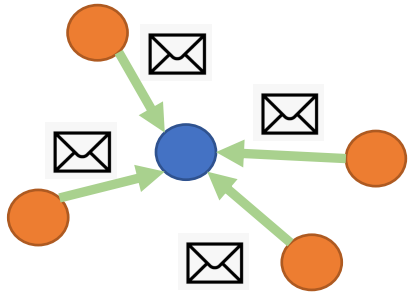
```
from paddle.fluid.layers import sequence_pool as pool

# 发送函数，从发送源src到发送目标点dst
def send(src_feat, dst_feat, edge_feat):
    return src_feat["norm"] * dst_feat["norm"] * src_feat["h"]

# 接收函数，从发送源src到发送目标点dst
def recv(message):
    return pool(message, "sum")
```

图卷积网络

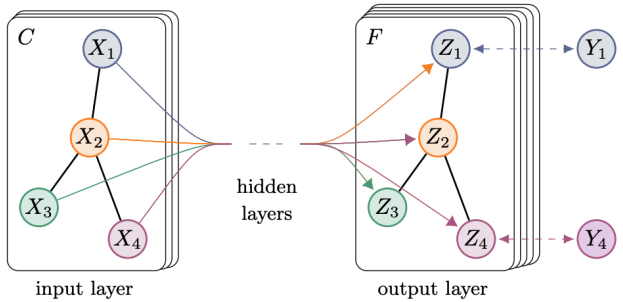
Graph Convolutional Network



如何从**图像卷积**，类比到**图结构卷积**



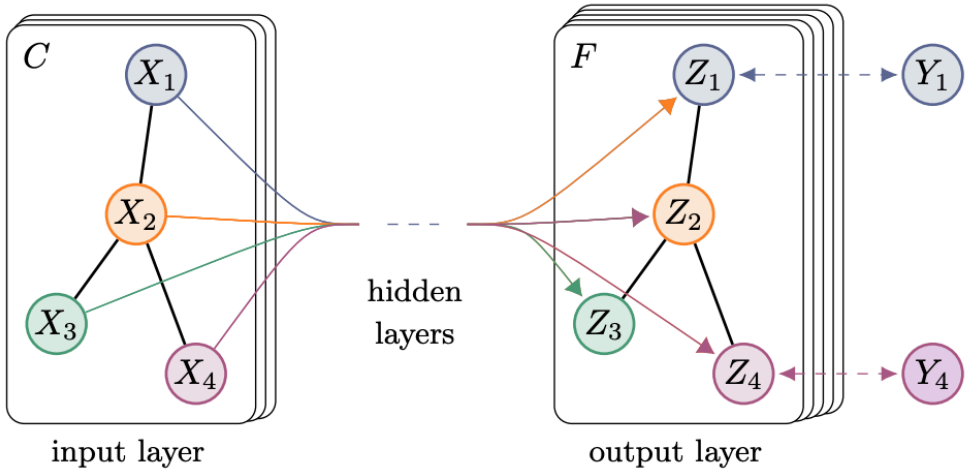
怎么用**消息传递**方式实现图卷积网络



怎么用多层图网络完成**节点分类任务**

图卷积网络

Graph Convolutional Network



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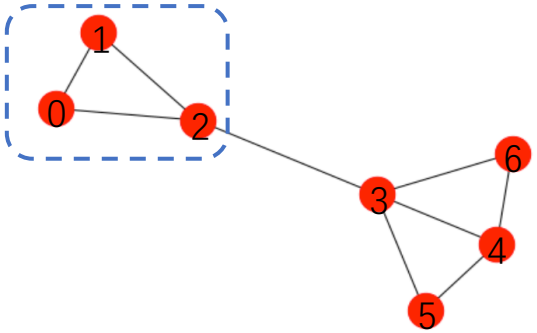
图卷积网络

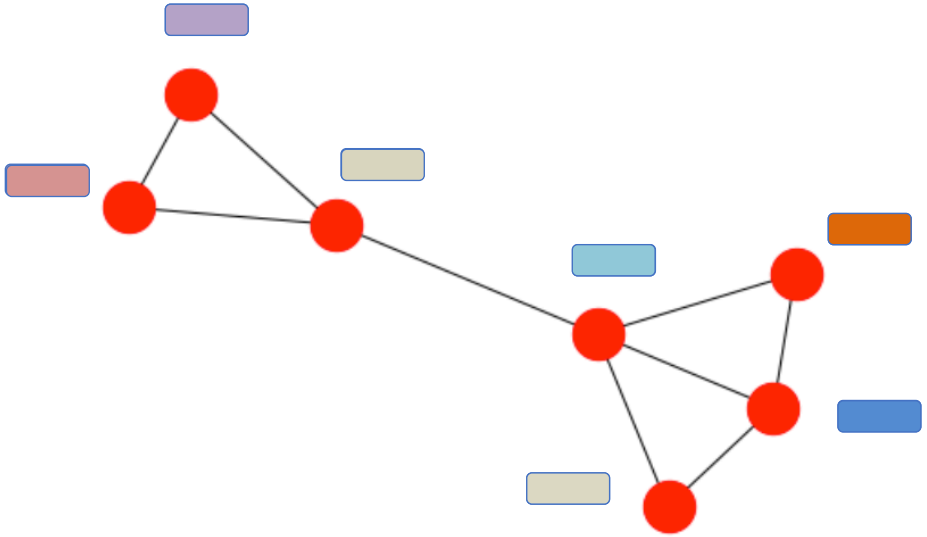
Graph Convolutional Network



GCN算法全流程

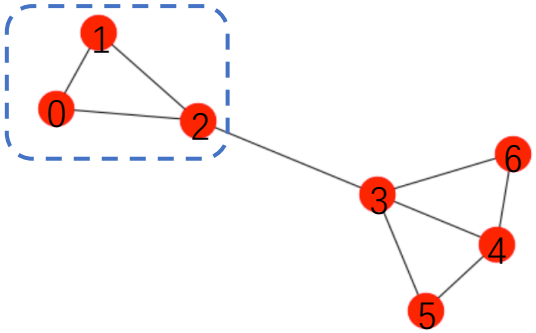
$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

第一步： $\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}$ 节点间进行特征传递



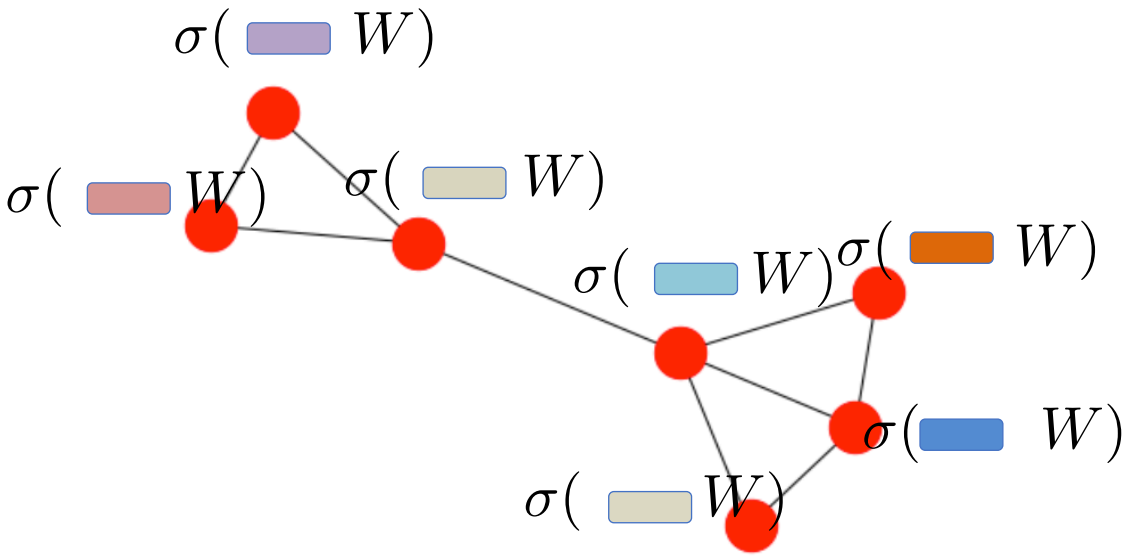
图卷积网络

Graph Convolutional Network



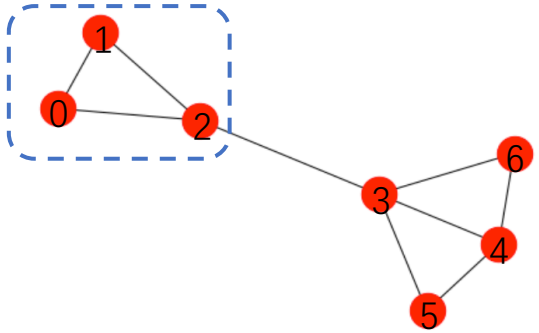
GCN算法全流程 $$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

第二步： 对每一个节点过一层DNN



图卷积网络

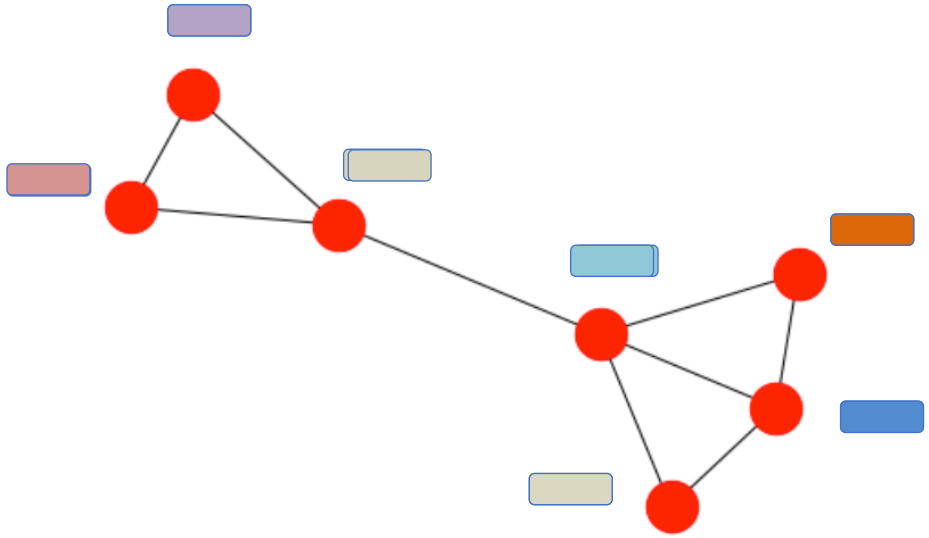
Graph Convolutional Network

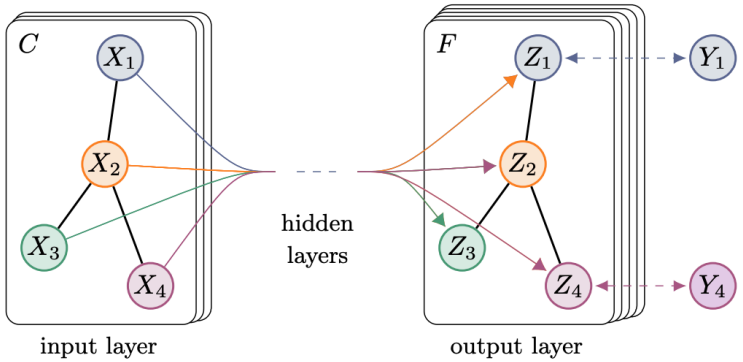


GCN算法全流程

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

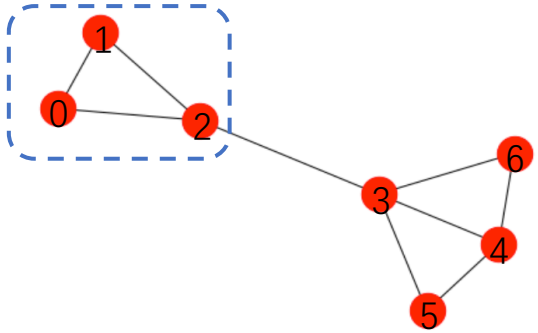
重复L次，步骤1和步骤2，实现多层图卷积网络





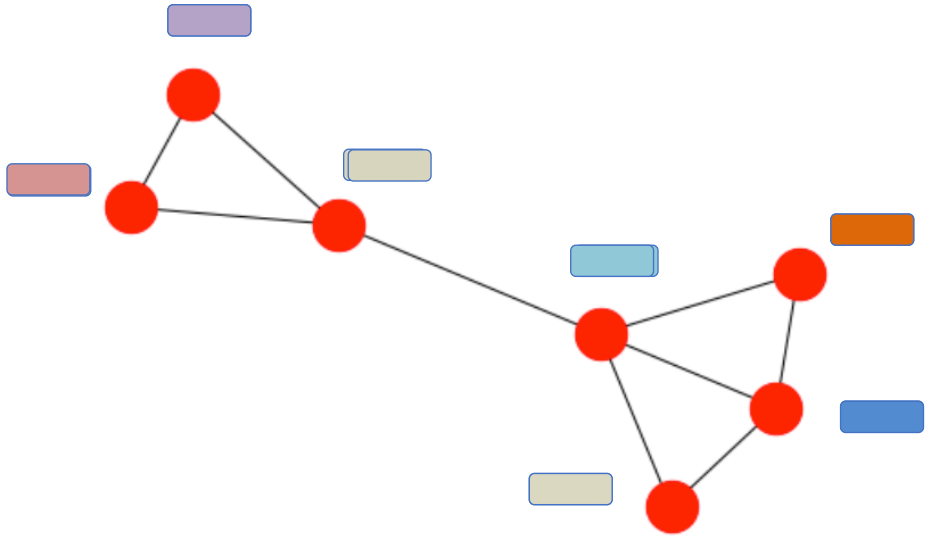
图卷积网络

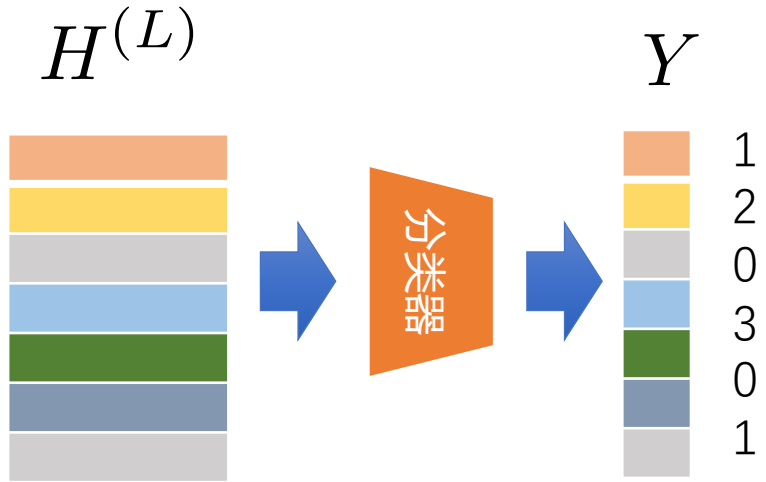
Graph Convolutional Network



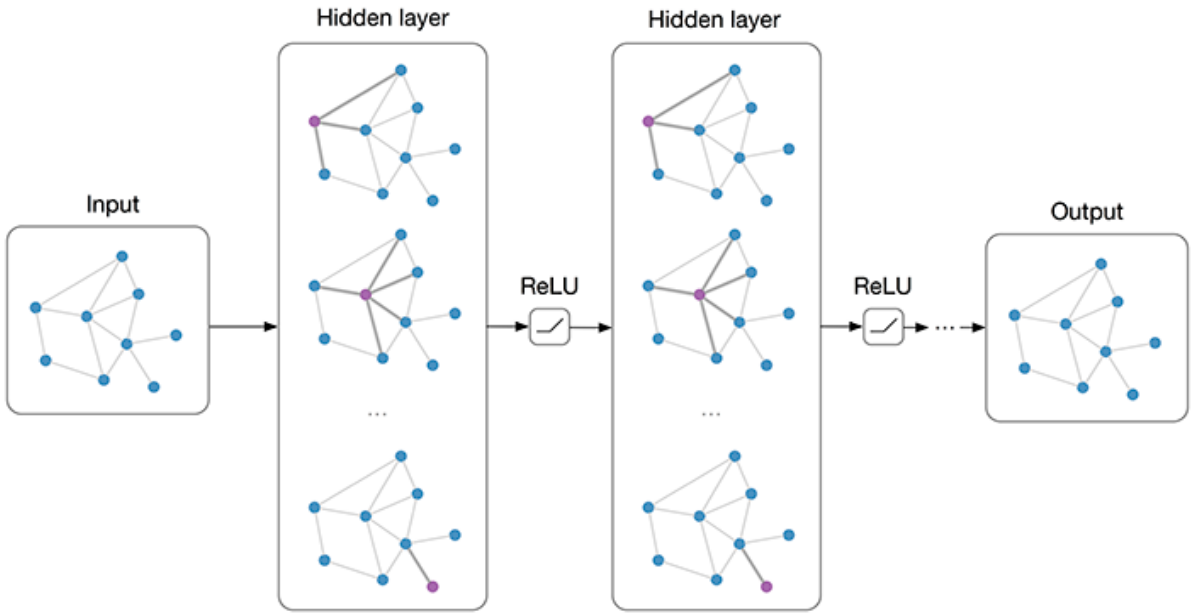
GCN算法全流程 $$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right)$$

获取的最终表示 $H^{(L)}$ 作为最终节点表示



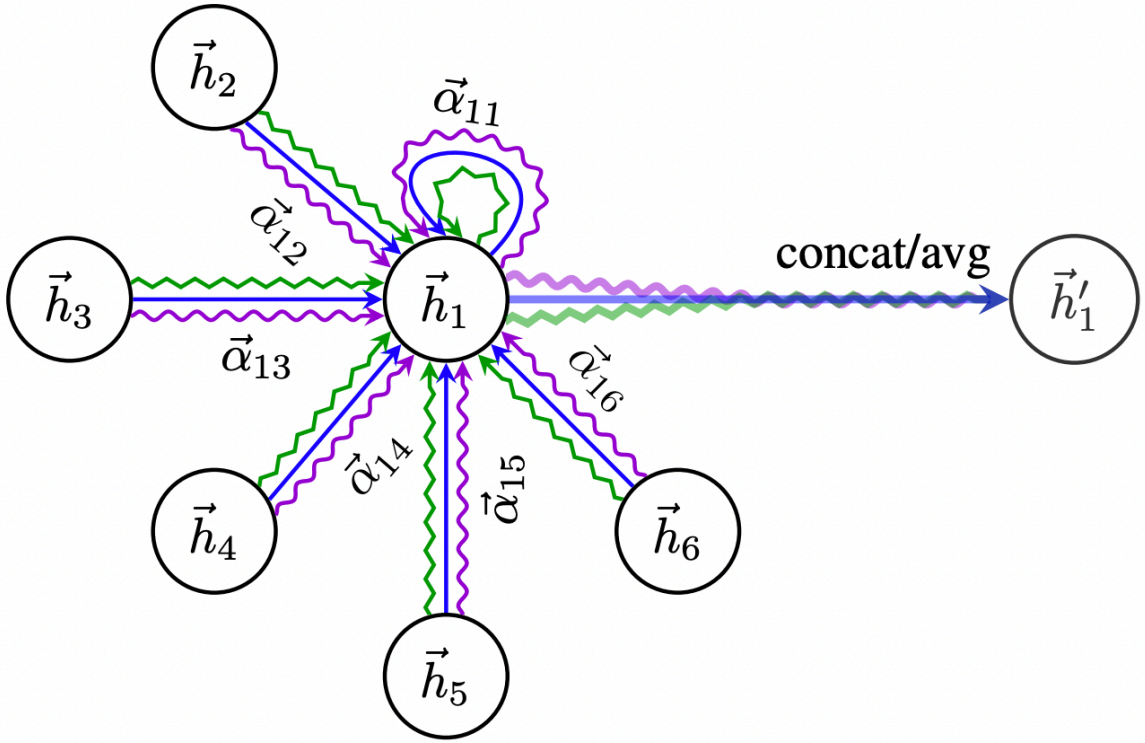


图卷积网络多种形式



图卷积网络（GCN）

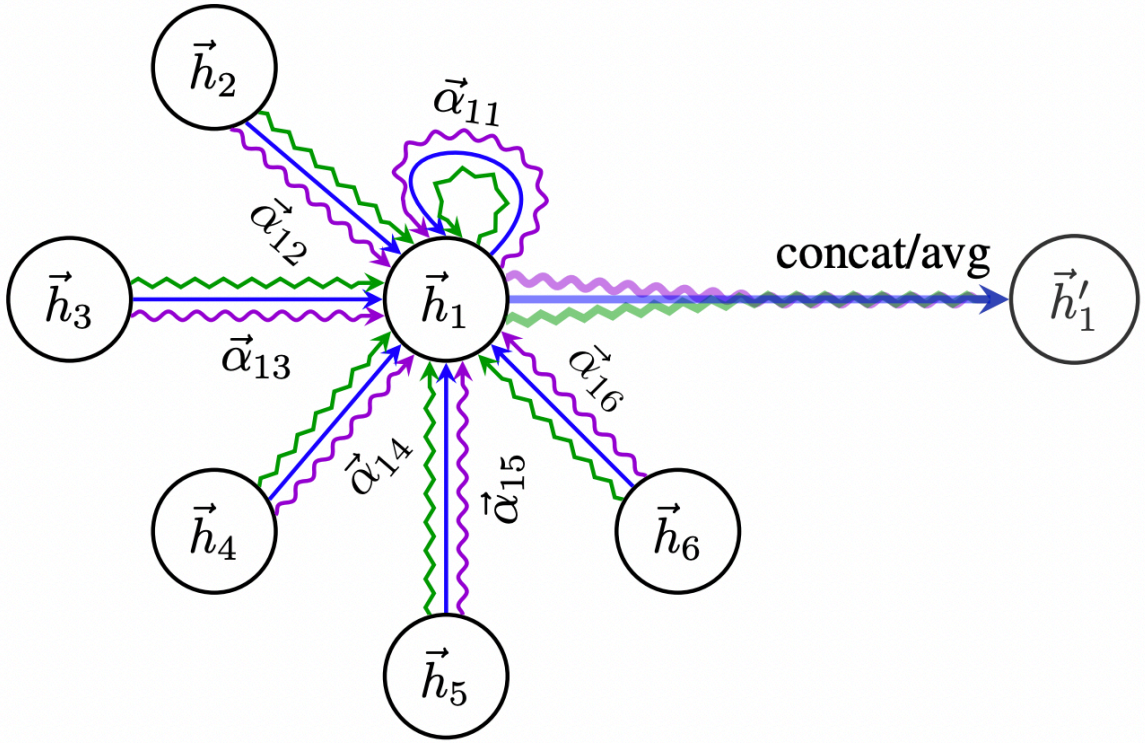
Kipf, Thomas N and Welling, Max
Semi-Supervised Classification with Graph Convolutional Networks
ICLR 2017



图注意力网络（GAT）

Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò and Yoshua Bengio
Graph Attention Networks,
ICLR 2018

图卷积网络多种形式



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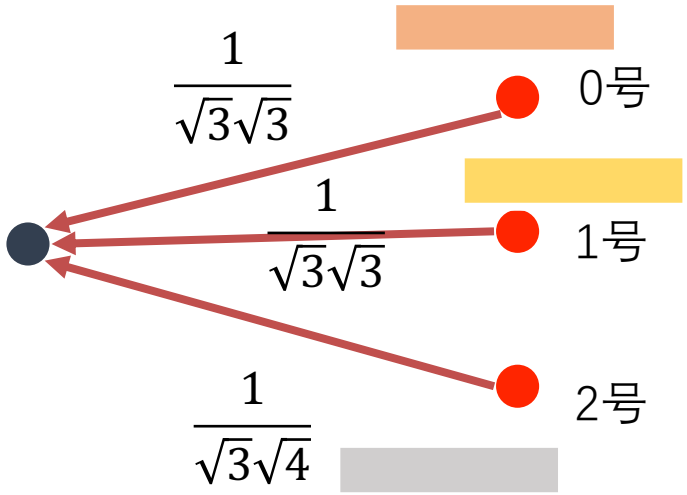
图注意力网络

Graph Attention Network

$$D^{-\frac{1}{2}}AD^{-\frac{1}{2}}H^{(l)}$$

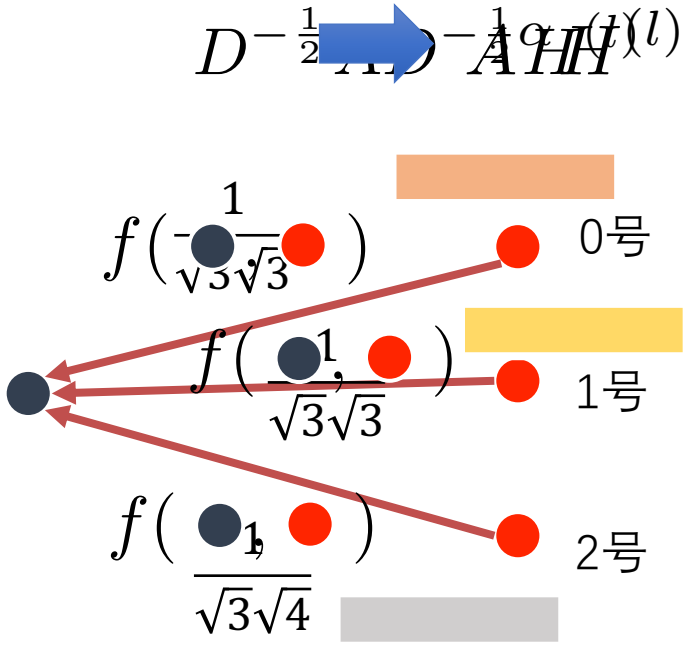


GCN中边的权重：

- 与节点的度相关
- 不可学习

图注意力网络

Graph Attention Network



GCN中边的权重：

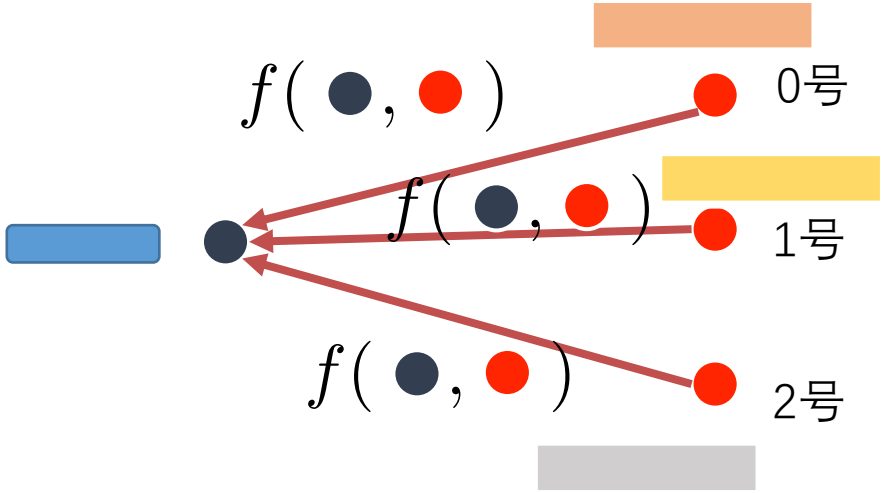
- 与节点的度相关
- 不可学习

GAT中的边权重 $f(\bullet, \bullet)$

- 权重变成节点间的函数
- 权重与两个节点相关性有关
- 可学习

图注意力网络

Graph Attention Network



attention计算方法

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

特征聚合计算方法

$$\vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

图注意力网络

Graph Attention Network

飞桨

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特征聚合计算方法

$$\vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

单头GAT消息传递在PGL中Message Passing实现

```
from paddle.fluid.layers import sequence_pool as pool
from paddle.fluid.layers import sqeuence_softmax as edge_softmax
import paddle.fluid.layers as L
...
# 发送函数，从发送源src到发送目标点dst
def send(src_feat, dst_feat, edge_feat):
    src_weight = L.fc(src_feat["h"], size=1, name="a1_weight")
    dst_weight = L.fc(dst_feat["h"], size=1, name="a2_weight")
    weight = L.leaky_relu(src_weight + dst_weight, alpha=0.2)
    # 计算每一条边的源节点以及目标节点相关性
    return {"weight": weight, "h":  src_feat["h"]}

# 接收函数，从发送源src到发送目标点dst
def recv(message):
    # 对相关性进行softmax 归一化
    alpha = edge_softmax(message["weight"])
    hidden = pool(alpha * message["h"], "sum")
    return hidden
```

图注意力网络

Graph Attention Network

飞桨

attention计算方法

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

特征聚合计算方法

$$\vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

多头 Attention 特征聚合方法

$$\vec{h}'_i = \Big\Vert_{k=1}^{K}\sigma\left(\sum_{j\in\mathcal{N}_i}\alpha_{ij}^k\mathbf{W}^k\vec{h}_j\right)$$

```
for head_no in range(n_heads):
    # 请完成单头的GAT的代码
    single_output = single_head_gat(graph_wrapper,
                                    node_feature,
                                    hidden_size,
                                    name="head_%s" % (head_no) )
    heads_output.append(single_output)
```

作业部分代码

num_nodes * feature_size -> num_heads * num_nodes * hidden_size

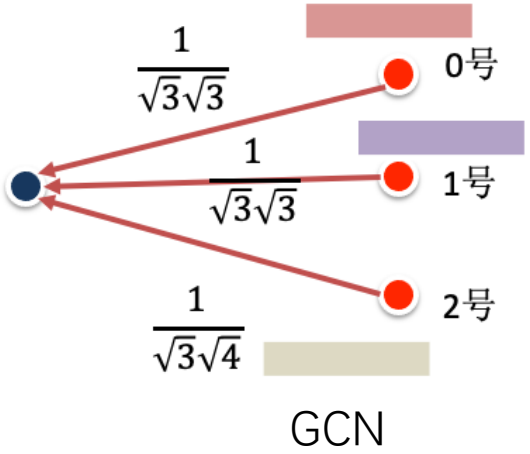
Message Passing

GCN、GAT都是基于邻居聚合的模型

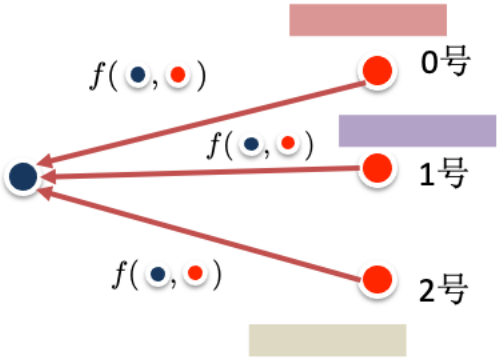
称为 **Spatial (空间) GNN**

大部分的Spatial GNN都可以用Message Passing实现

- **消息的发送**
- **消息的接收**



GCN



GAT

Message Passing

基于消息传递的 Graph Neural Network的通用公式

$$h_l^{(t)}(v) = f(h_l^{(t-1)}, \mathcal{F}\{h_l^{(t-1)}(u)|u \in N(v)\})$$

多层MLP

F可以是聚合函数
通常是Mean/Max/Sum

邻居消息发送

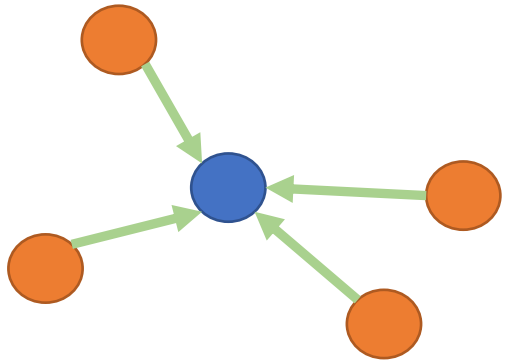
Message Passing

$$h_l^{(t)}(v) = f(h_l^{(t-1)}, \mathcal{F}\{h_l^{(t-1)}(u)|u \in N(v)\})$$

Message Passing流程

1. 邻居的发送信息

2. F可以看作是目标接收信息的方式



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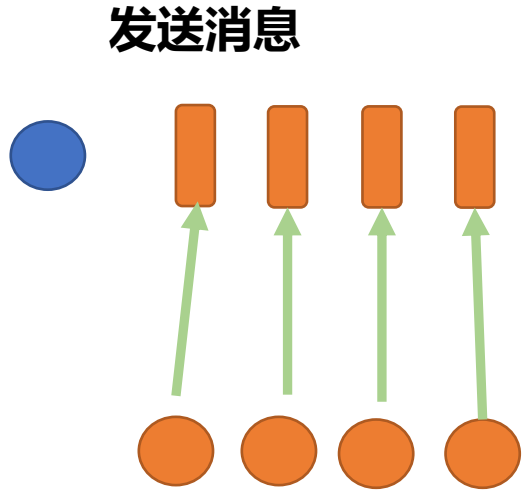

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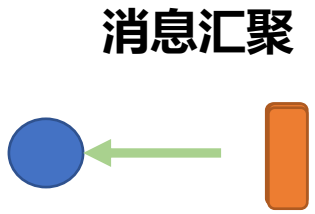
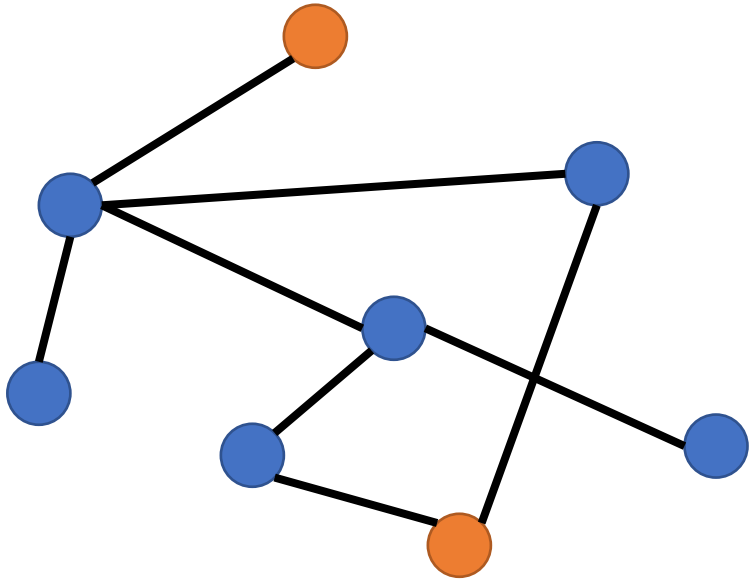


GCN: F = 基于度的加权求和
GAT: F = 基于 Attention 的 加权求和

Message Passing

$$h_l^{(t)}(v) = f(h_l^{(t-1)}, \mathcal{F}\{h_l^{(t-1)}(u) | u \in N(v)\})$$

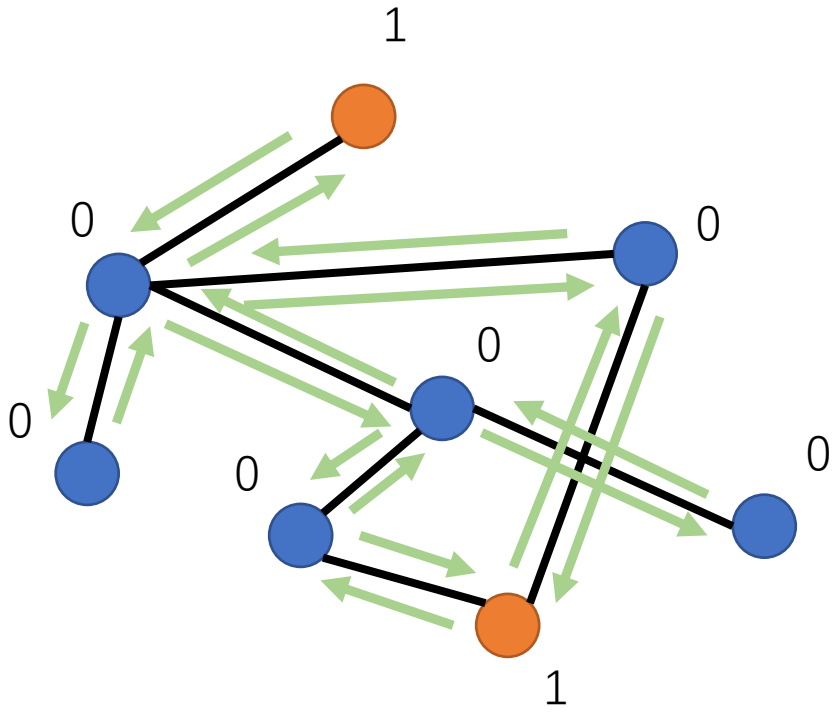


用Message Passing的范式解决问题

1. 哪些点的邻居存在橙色点（包括自己）
2. 每个节点附近平均有多少个橙色点（包括自己）
3. 哪些点的半径为2范围内存在橙色点 (包括自己)

Message Passing

$$h_l^{(t)}(v) = f(h_l^{(t-1)}, \mathcal{F}\{h_l^{(t-1)}(u) | u \in N(v)\})$$



1. 哪些点的邻居存在橙色点（包括自己）

$\mathcal{F}$ 为求Max

Message Passing

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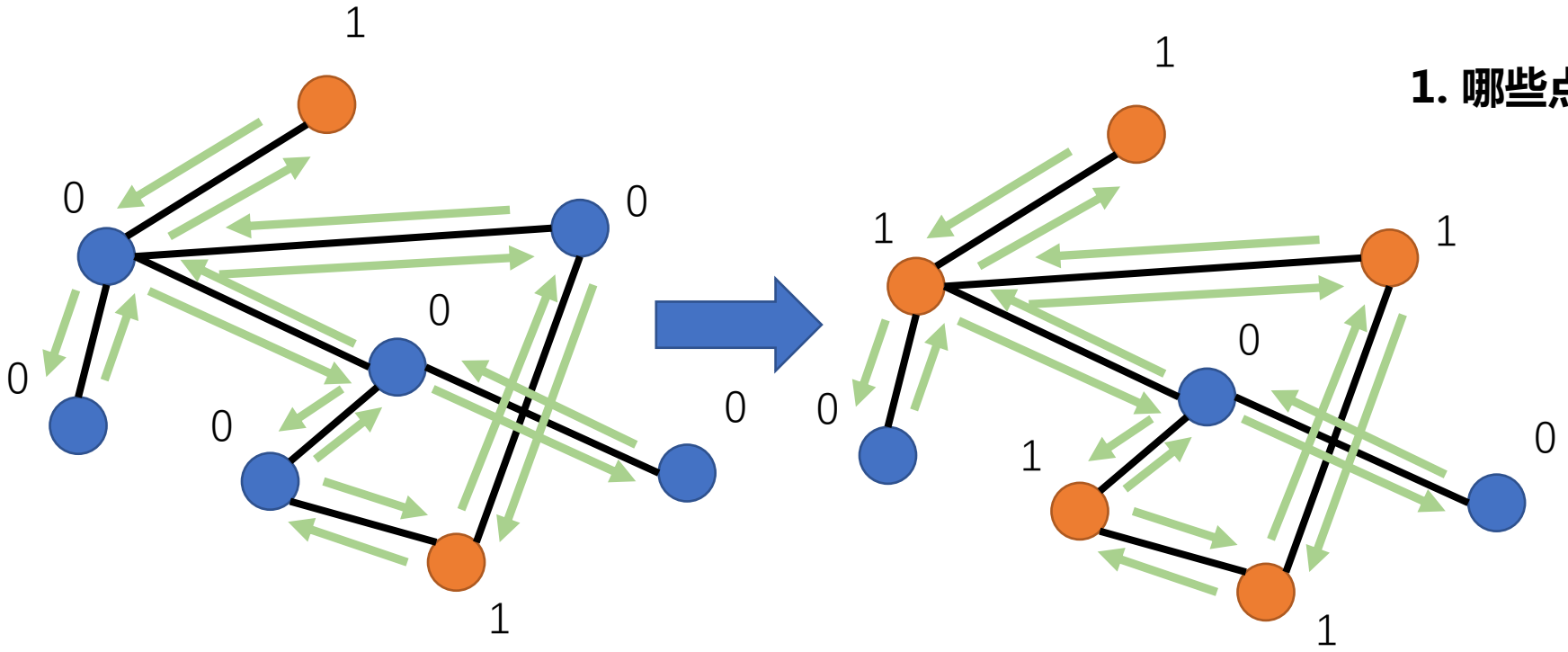

1. 哪些点的邻居存在橙色点（包括自己）

$\mathcal{F}$ 为求Max

邻居节点有1的有5个

Message Passing

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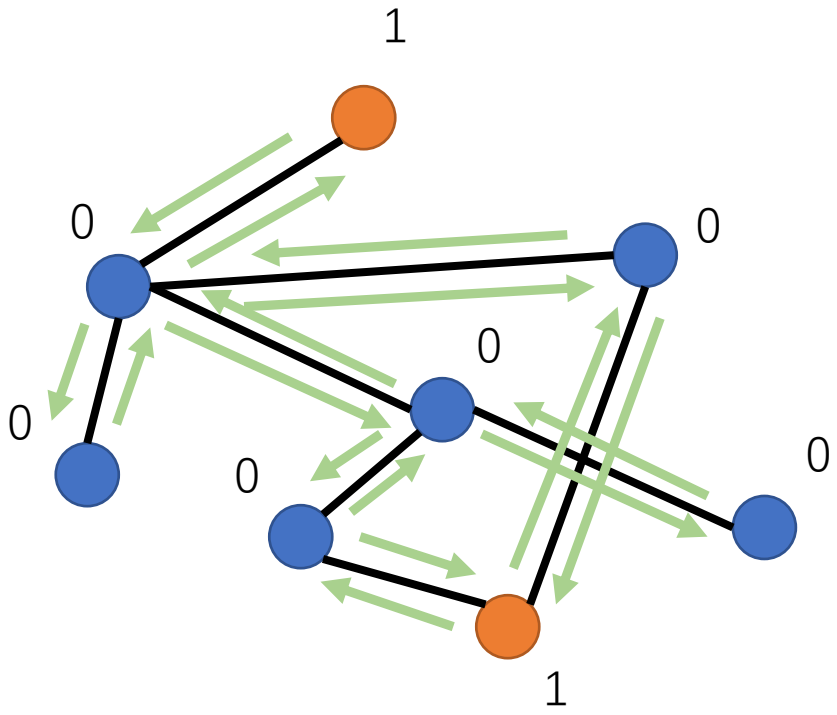

2. 每个节点附近平均有多少个橙色点(包括自己)

$\mathcal{F}$ 为求均值Mean

Message Passing

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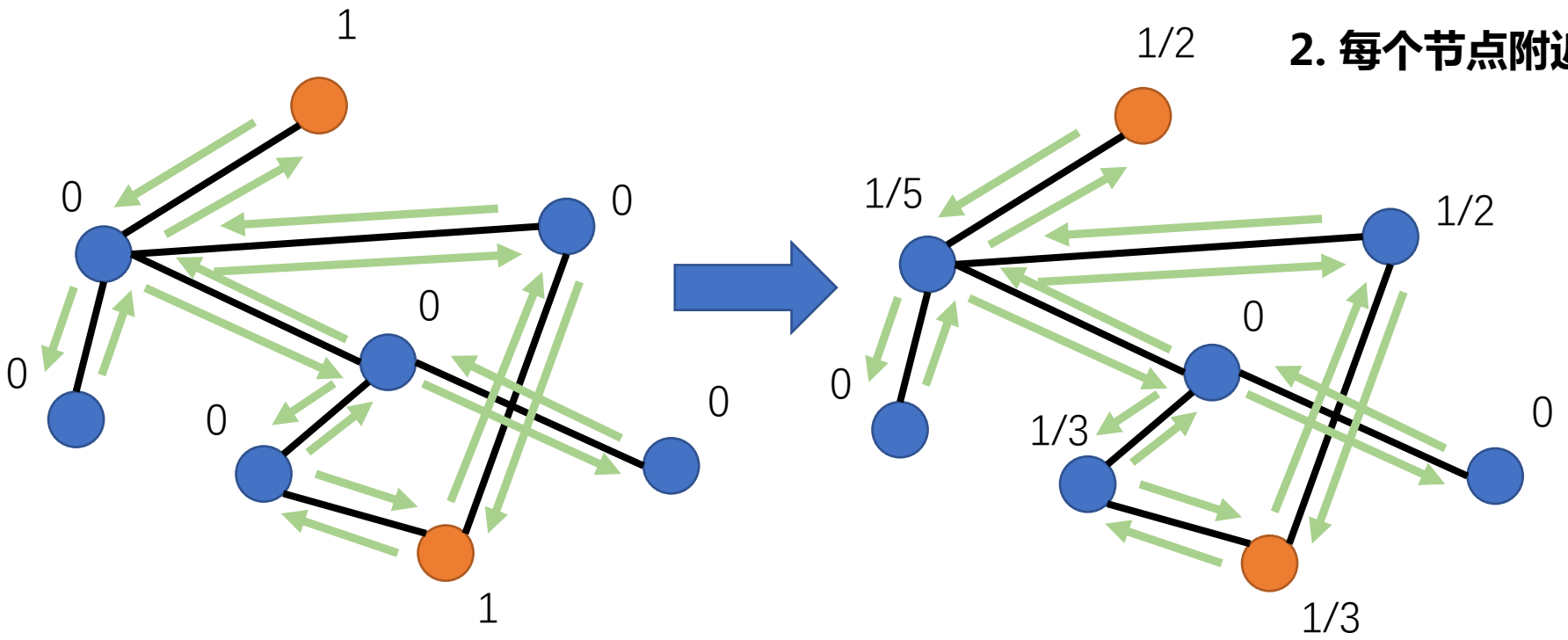

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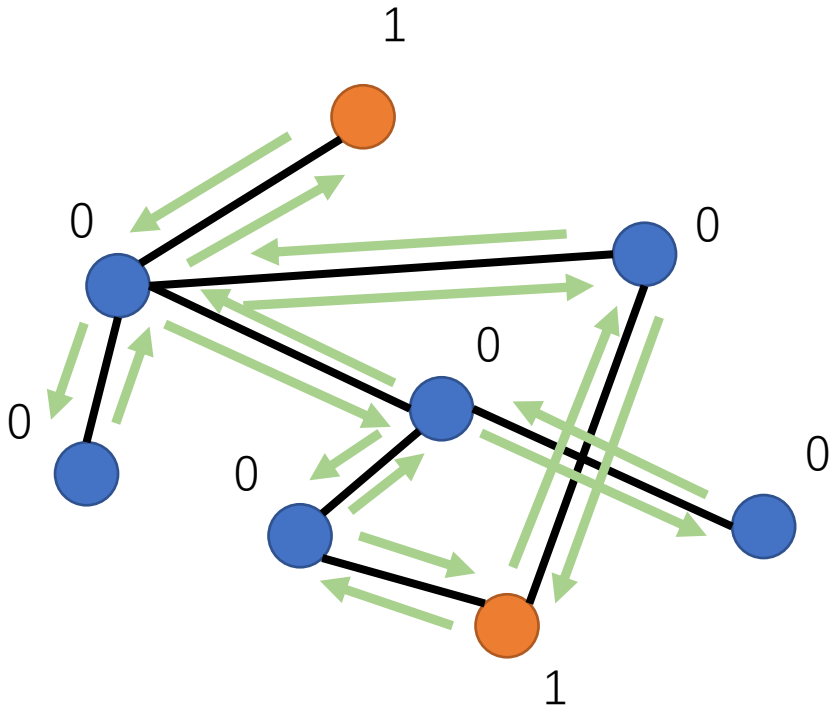

3. 哪些点的半径为2范围内存在橙色点(包括自身)

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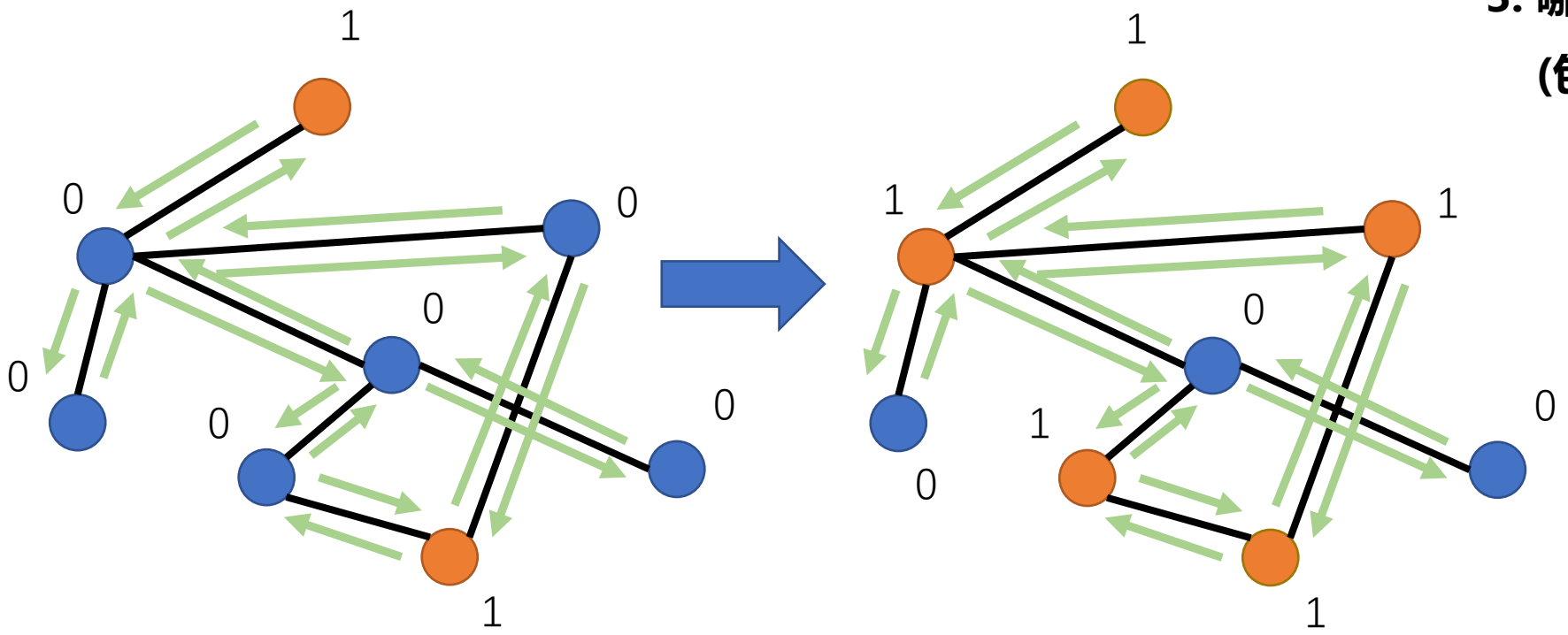

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$\mathcal{F}$ 为求Max

第一次迭代

1. 一阶邻居有橙色点

Message Passing

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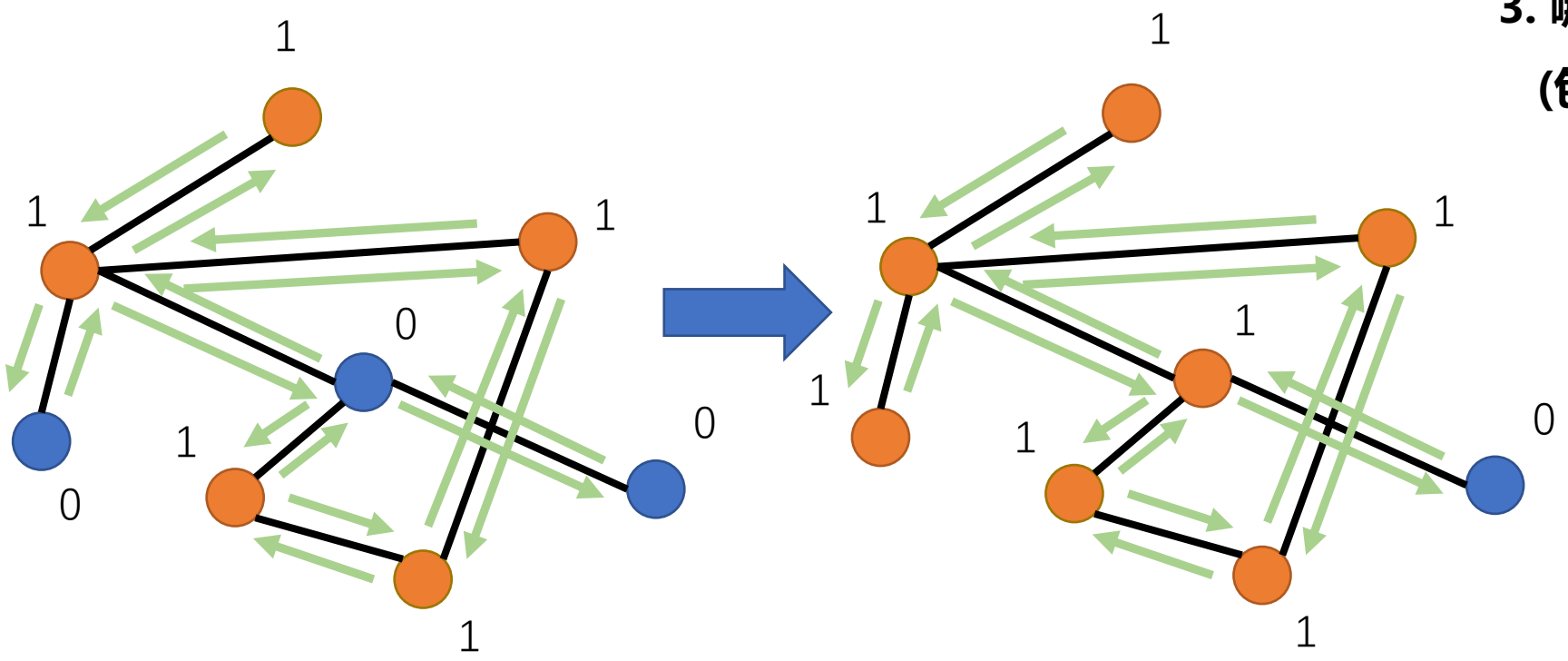

3. 哪些点的半径为2范围内存在橙色点（包括自身）

$\mathcal{F}$ 为求Max

第一次迭代

1. 一阶邻居有橙色点

第二次迭代

2. 二阶邻居有橙色点

Message Passing

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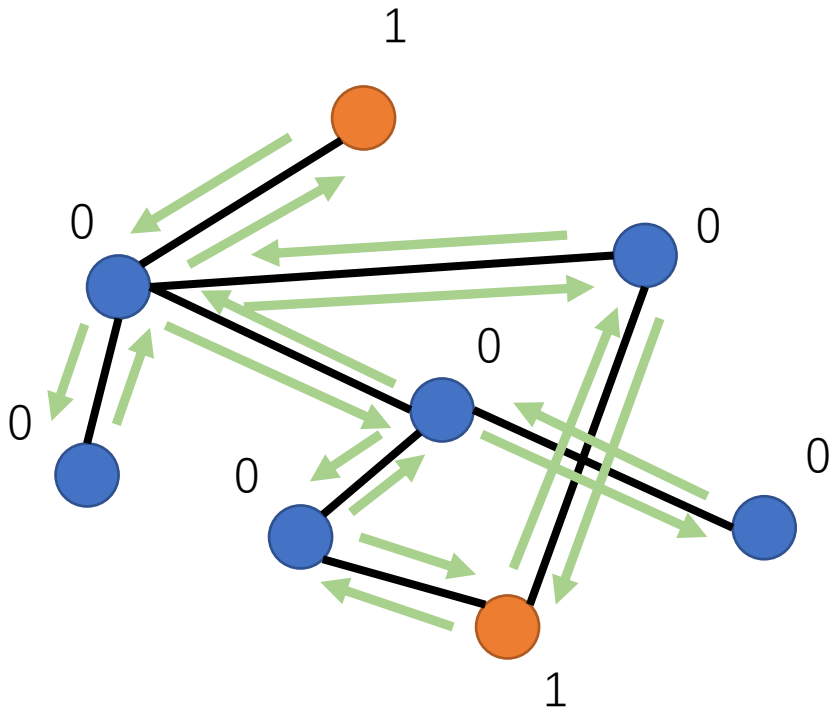

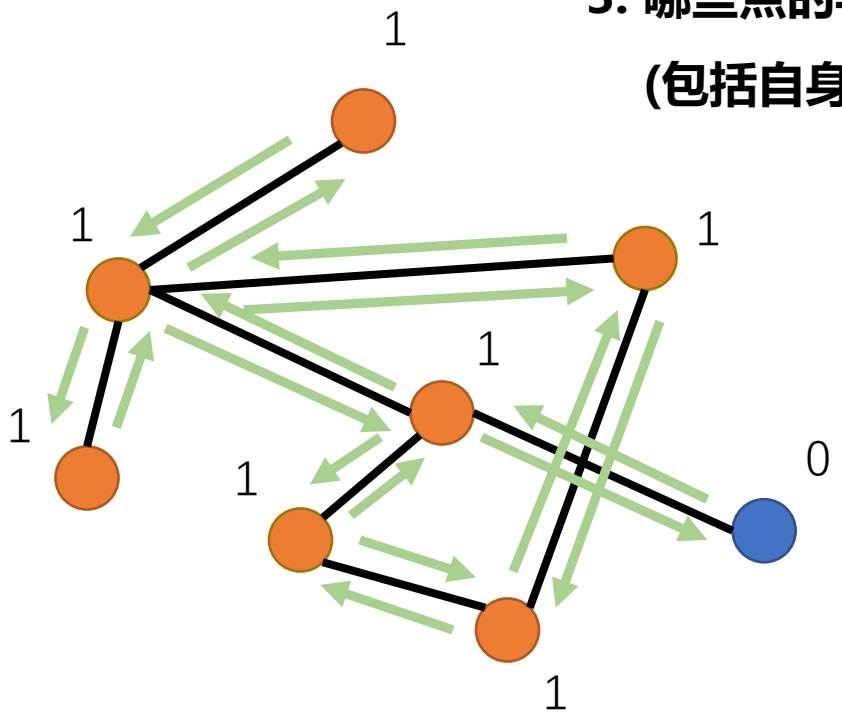

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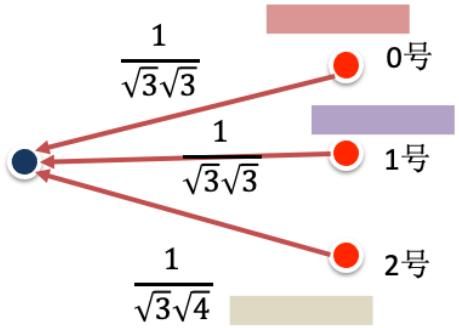
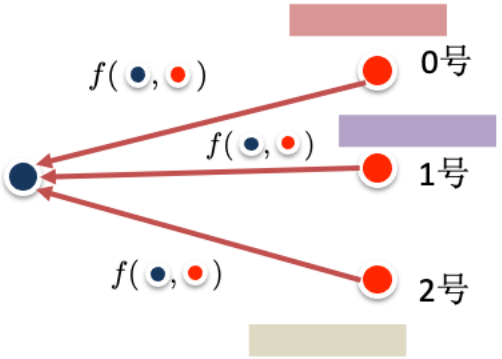
总结

1. GCN算法介绍



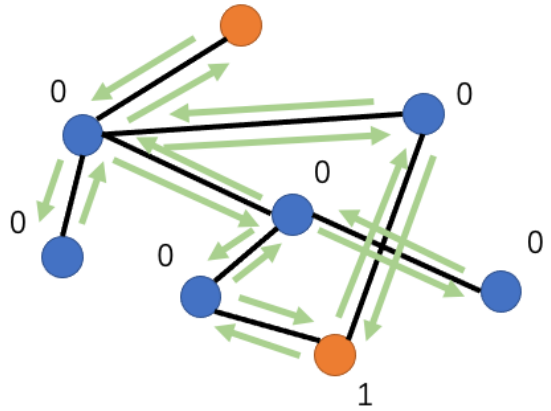
GCN

2. GAT算法介绍



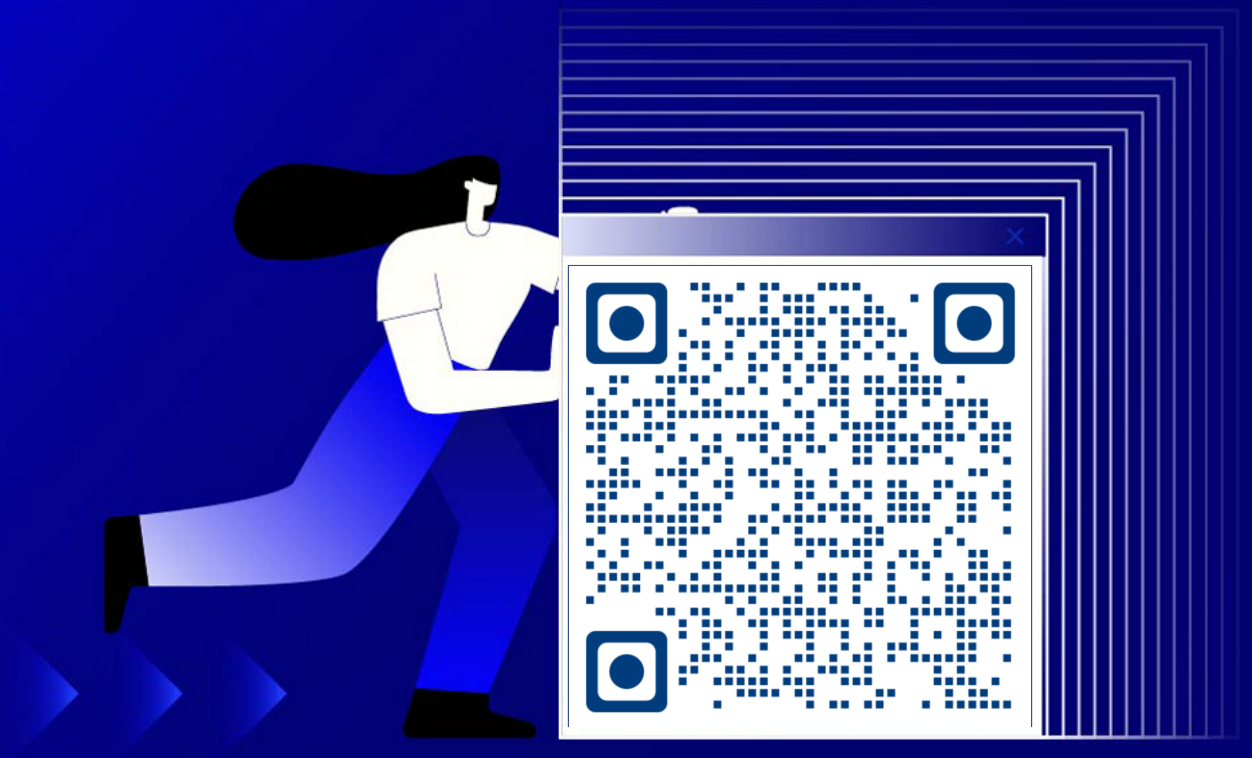
GAT

3. Message Passing 消息传递算法



课后作业

实现 GAT 模型的消息传递接口



PGL github

谢谢观看