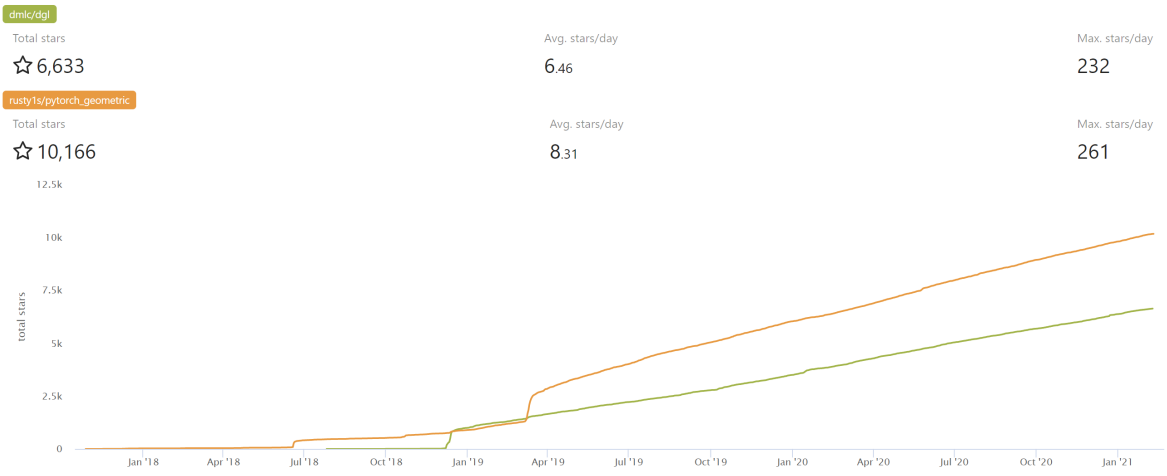
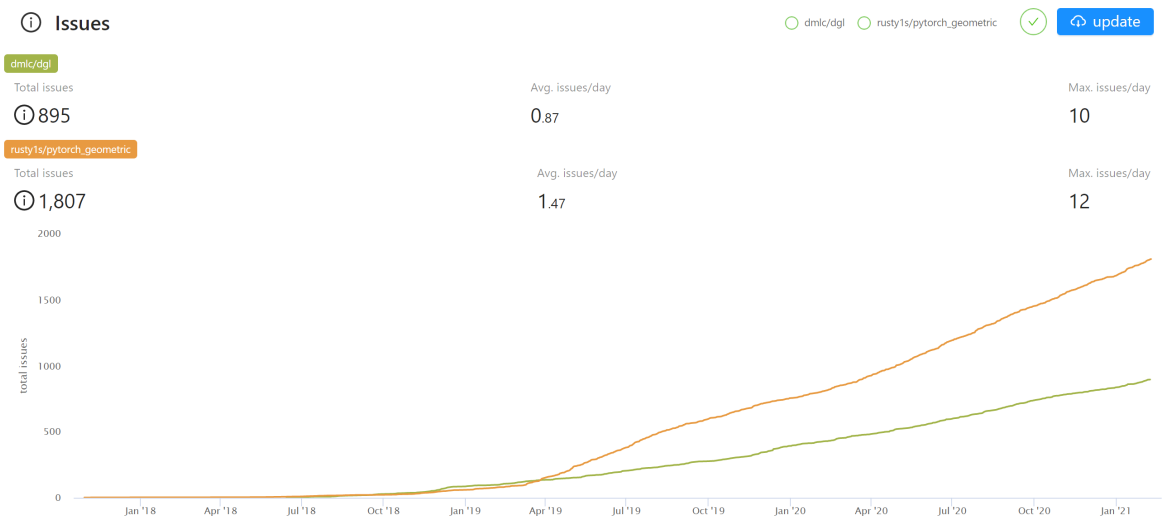
GNN intro

Created time	@Feb 9, 2021 9:32 PM
Link	
Summary	Coding introduction to GNN
Type	Article

Outline

- ▼ Popular packages
  - ▼ PyTorch geometric vs DGL

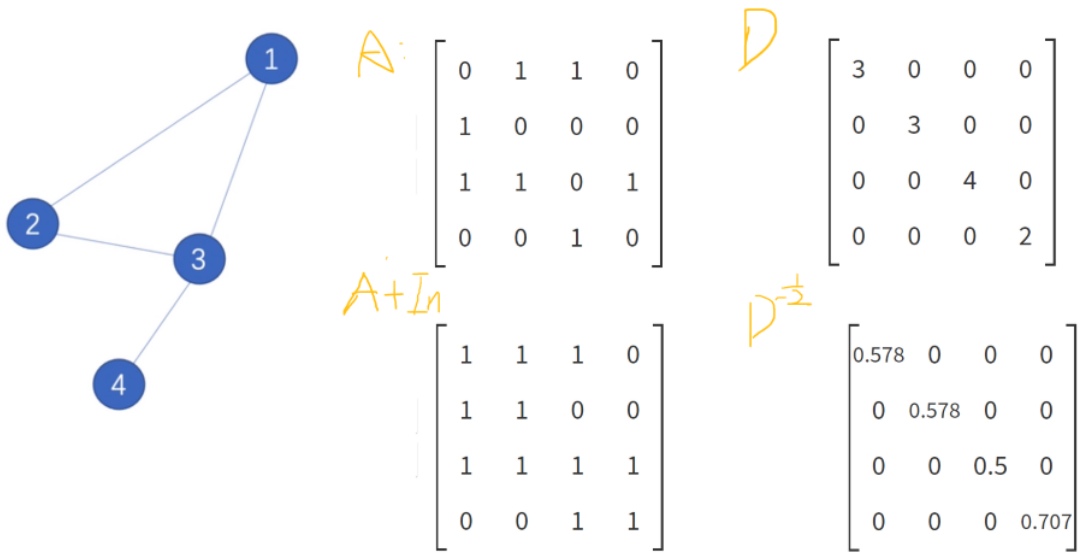




▼ GCN

MP-GNN的中心思想是通过非线性变换从局部节点邻域中反复聚集信息来学习有意义的节点嵌入。

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



$\tilde{A} = A + I_N$:

```
[[1. 1. 1. 0.]
 [1. 1. 1. 0.]
 [1. 1. 1. 1.]
 [0. 0. 1. 1.]]
```

$\tilde{D}^{-\frac{1}{2}}$:

```
[[0.57735027 0.         0.         0.        ]
 [0.         0.57735027 0.         0.        ]
 [0.         0.         0.5        0.        ]
 [0.         0.         0.         0.70710678]]
```

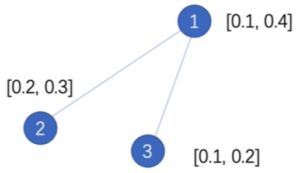
$\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$:

```
[[0.57735027 0.         0.         0.        ]
 [0.         0.57735027 0.         0.        ]
 [0.         0.         0.5        0.        ]
 [0.         0.         0.         0.70710678]]
 •
[[1. 1. 1. 0.]
 [1. 1. 1. 0.]
 [1. 1. 1. 1.]
 [0. 0. 1. 1.]]
 •
[[0.57735027 0.         0.         0.        ]
 [0.         0.57735027 0.         0.        ]
 [0.         0.         0.5        0.        ]
 [0.         0.         0.         0.70710678]]
```

=

```
[[0.33333333 0.33333333 0.28867513 0.        ]
 [0.33333333 0.33333333 0.28867513 0.        ]
 [0.28867513 0.28867513 0.25       0.35355339]
 [0.         0.         0.35355339 0.5       ]]
```

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



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

$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0.1 & 0.4 \\ 0.2 & 0.3 \\ 0.1 & 0.2 \end{bmatrix} = \begin{bmatrix} 0.3 & 0.5 \\ 0.1 & 0.4 \\ 0.1 & 0.4 \end{bmatrix} = \begin{matrix}[[0.2+0.1, 0.3+0.2] \\ [0.1 \quad , 0.4 \quad] \\ [0.1 \quad , 0.4 \quad]]\end{matrix}$$

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

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 0.1 & 0.4 \\ 0.2 & 0.3 \\ 0.1 & 0.2 \end{bmatrix} = \begin{bmatrix} 0.4 & 0.9 \\ 0.3 & 0.7 \\ 0.2 & 0.6 \end{bmatrix} = \begin{matrix}[[0.1+0.2+0.1, 0.4+0.3+0.2] \\ [0.1+0.2 \quad , 0.4+0.3 \quad] \\ [0.1+0.1 \quad , 0.4+0.2 \quad]]\end{matrix}$$

Resources

Name	Tags	Description	Links
GNN learning repo	Code	Collected by Cankun	https://github.com/Wang-Cankun/learn-gnn
PyTorch geometric	Tool	PyTorch based; Stanford CS224W course example	https://github.com/rusty1s/pytorch_geometric
OGB	Tool	Open Graph Benchmark, Datasets; Created by Jure Leskovec	https://ogb.stanford.edu/
SEMI-SUPERVISED CLASSIFICATION WITH GRAPH CONVOLUTIONAL NETWORKS	Paper	Original GCN paper (2016)	https://arxiv.org/pdf/1609.02907.pdf
Graph Neural Networks (GNN) using Pytorch Geometric	Video	PyTorch Geometric basic tutorial from CS224W 2019 class	https://www.youtube.com/watch?v=-UjytpbqX4A
Untitled			