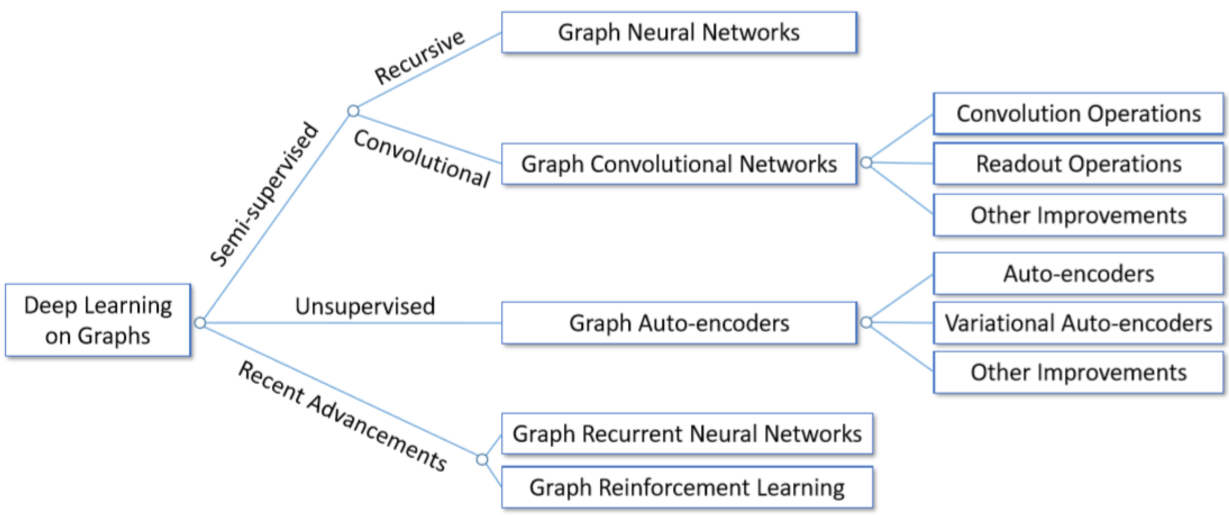
Graph Neural Network

`Graph embedding` 半监督 无监督

无监督学习



如图所示，图神经网络（GNN）在无监督学习方面主要是运用了基于Autoencoder的方法，通过link prediction任务和重构图任务进行无监督学习，从而让网络学习到图结构信息，让embedding中包含更丰富的信息。

近期相关研究：

Comparison of Different Graph Autoencoders (GAEs)

Method	Type	Objective	Scalability	Node Features	Other Improvements
SAE [75]	AE	L2-Reconstruction	Yes	No	-
SDNE [76]	AE	L2-Reconstruction + Laplacian Eigenmaps	Yes	No	-
DNGR [77]	AE	L2-Reconstruction	No	No	-
GC-MC [78]	AE	L2-Reconstruction	Yes	Yes	Convolutional Encoder
DRNE [79]	AE	Recursive Reconstruction	Yes	No	-
G2G [80]	AE	KL + Ranking	Yes	Yes	Nodes as distributions
VGAE [81]	VAE	Pairwise Probability of Reconstruction	No	Yes	Convolutional Encoder
DVNE [82]	VAE	Wasserstein + Ranking	Yes	No	Nodes as distributions
ARGA/ARVGA [83]	AE/VAE	L2-Reconstruction + GAN	Yes	Yes	Convolutional Encoder

详细介绍可请参考Deep Learning on Graphs: A Survey

半监督学习

半监督学习的工作很多，基本上大部分GNN都是半监督学习，总的来说，如果有部分标记的数据集用来做特定任务，半监督学习的效果一般比无监督学习的效果好，不过在无监督任务中也不是不能运用半监督学习的模型，正如下面会介绍到的一样，可以将Autoencoder的encoder和decoder部分替换为任意的半监督学习模型，增强最终效果。

在此列出一些已经实现了的近期GNN以供参考

- **SplineConv** from Fey *et al.*: SplineCNN: Fast Geometric Deep Learning with Continuous B-Spline Kernels (CVPR 2018)
- **GCNConv** from Kipf and Welling: Semi-Supervised Classification with Graph Convolutional Networks (ICLR 2017)
- **ChebConv** from Defferrard *et al.*: Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering (NIPS 2016)
- **NNConv** from Gilmer *et al.*: Neural Message Passing for Quantum Chemistry (ICML 2017)
- **ECConv** from Simonovsky and Komodakis: Edge-Conditioned Convolution on Graphs (CVPR 2017)
- **GATConv** from Veličković *et al.*: Graph Attention Networks (ICLR 2018)
- **SAGEConv** from Hamilton *et al.*: Inductive Representation Learning on Large Graphs (NIPS 2017)
- **GraphConv** from, *e.g.*, Morris *et al.*: Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks (AAAI 2019)
- **GatedGraphConv** from Li *et al.*: Gated Graph Sequence Neural Networks (ICLR 2016)
- **GINConv** from Xu *et al.*: How Powerful are Graph Neural Networks? (ICLR 2019)
- **ARMAConv** from Bianchi *et al.*: Graph Neural Networks with Convolutional ARMA Filters (CoRR 2019)
- **SGConv** from Wu *et al.*: Simplifying Graph Convolutional Networks (CoRR 2019)
- **APPNP** from Klicpera *et al.*: Predict then Propagate: Graph Neural Networks meet Personalized PageRank (ICLR 2019)
- **AGNNConv** from Thekumparampil *et al.*: Attention-based Graph Neural Network for Semi-Supervised Learning (CoRR 2017)
- **RGCNConv** from Schlichtkrull *et al.*: Modeling Relational Data with Graph Convolutional Networks (ESWC 2018)
- **SignedConv** from Derr *et al.*: Signed Graph Convolutional Network (ICDM 2018)

- **DNAConv** from Fey: Just Jump: Dynamic Neighborhood Aggregation in Graph Neural Networks (ICLR-W 2019)
- **EdgeConv** from Wang *et al.*: Dynamic Graph CNN for Learning on Point Clouds (CoRR, 2018)
- **PointConv** (including **Iterative Farthest Point Sampling**, dynamic graph generation based on **nearest neighbor** or **maximum distance**, and **k-NN interpolation**) from Qi *et al.*: PointNet: Deep Learning on Point Sets for 3D Classification and Segmentation (CVPR 2017) and PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space (NIPS 2017)
- **XConv** from Li *et al.*: PointCNN: Convolution On X-Transformed Points (official implementation) (NeurIPS 2018)
- **PPFConv** from Deng *et al.*: PPFNet: Global Context Aware Local Features for Robust 3D Point Matching (CVPR 2018)
- **GMMConv** from Monti *et al.*: Geometric Deep Learning on Graphs and Manifolds using Mixture Model CNNs (CVPR 2017)
- **HypergraphConv** from Bai *et al.*: Hypergraph Convolution and Hypergraph Attention (CoRR 2019)
- A **MetaLayer** for building any kind of graph network similar to the TensorFlow Graph Nets library from Battaglia *et al.*: Relational Inductive Biases, Deep Learning, and Graph Networks (CoRR 2018)
- **GlobalAttention** from Li *et al.*: Gated Graph Sequence Neural Networks (ICLR 2016)
- **Set2Set** from Vinyals *et al.*: Order Matters: Sequence to Sequence for Sets (ICLR 2016)
- **Sort Pool** from Zhang *et al.*: An End-to-End Deep Learning Architecture for Graph Classification (AAAI 2018)
- **Dense Differentiable Pooling** from Ying *et al.*: Hierarchical Graph Representation Learning with Differentiable Pooling (NeurIPS 2018)
- **Graclus Pooling** from Dhillon *et al.*: Weighted Graph Cuts without Eigenvectors: A Multilevel Approach (PAMI 2007)
- **Voxel Grid Pooling** from, *e.g.*, Simonovsky and Komodakis: Dynamic Edge-Conditioned Filters in Convolutional Neural Networks on Graphs (CVPR 2017)
- **Top-K Pooling** from Gao and Ji: Graph U-Net (ICLR 2019 submission) and Cangea *et al.*: Towards Sparse Hierarchical Graph Classifiers (NeurIPS-W 2018)
- **SAG Pooling** from Lee *et al.*: Self-Attention Graph Pooling (ICML 2019)
- **Local Degree Profile** from Cai and Wang: A Simple yet Effective Baseline for Non-attribute Graph Classification (CoRR 2018)
- **Jumping Knowledge** from Xu *et al.*: Representation Learning on Graphs with Jumping Knowledge Networks (ICML 2018)
- **Deep Graph Infomax** from Veličković *et al.*: Deep Graph Infomax (ICLR 2019)
- All variants of **Graph Auto-Encoders** from Kipf and Welling: Variational Graph Auto-Encoders (NIPS-W 2016) and Pan *et al.*: Adversarially Regularized Graph Autoencoder for Graph Embedding (IJCAI 2018)
- **RENet** from Jin *et al.*: Recurrent Event Network for Reasoning over Temporal Knowledge Graphs (ICLR-W 2019)
- **NeighborSampler** from Hamilton *et al.*: Inductive Representation Learning on Large Graphs (NIPS 2017)

推荐系统

请参考附件：**推荐系统.pdf**

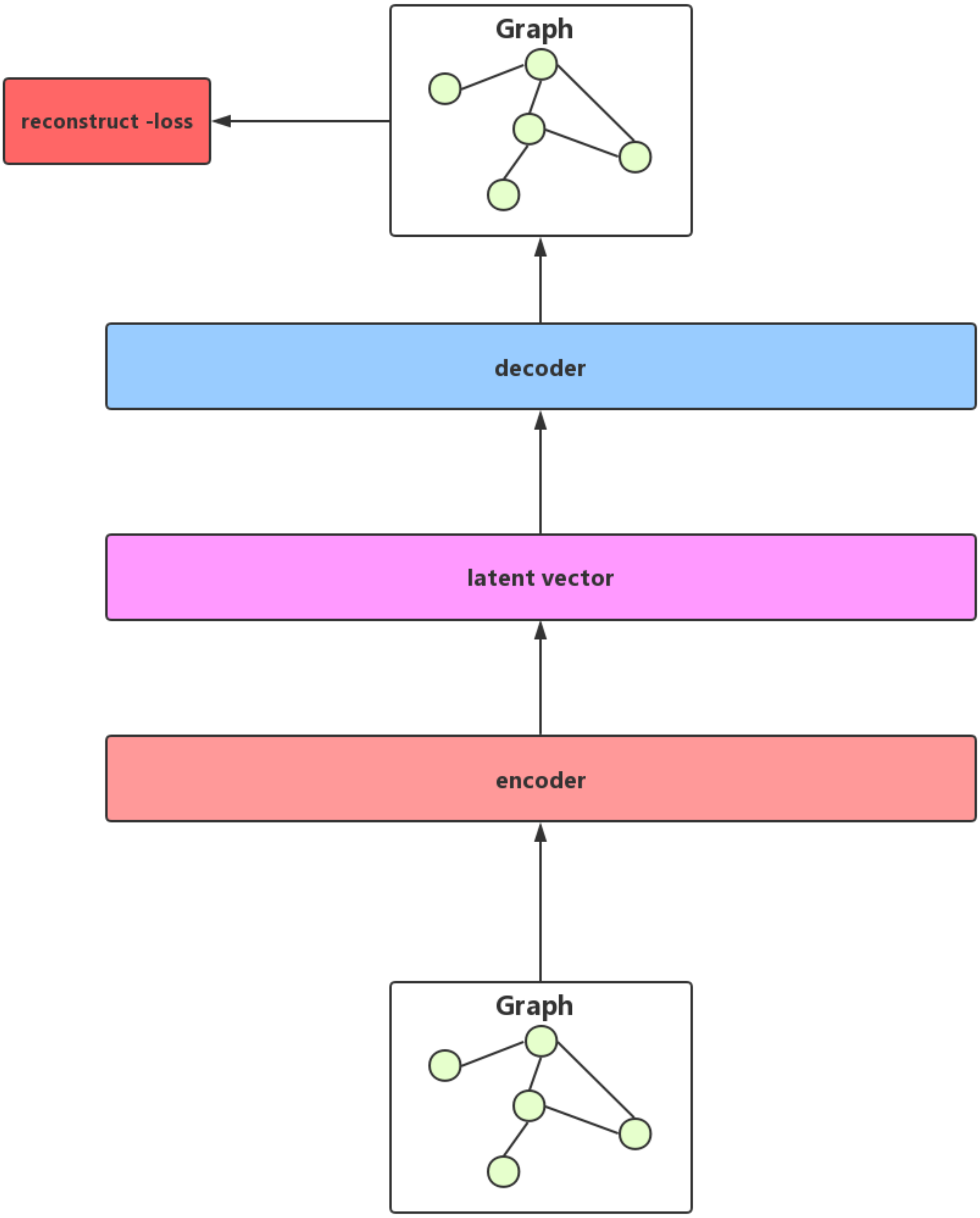
GNN实际应用

TABLE 3
Applications of graph neural networks.

Area	Application	Algorithm	Deep Learning Model	References
Text	Text classification	GCN	Graph Convolutional Network	[1], [23], [48] [2], [22], [46]
		GAT	Graph Attention Network	[68]
		DGCNN	Graph Convolutional Network	[106]
		Text GCN	Graph Convolutional Network	[107]
		Sentence LSTM	Graph LSTM	[62]
	Sequence Labeling (POS, NER)	Sentence LSTM	Graph LSTM	[62]
	Sentiment classification	Tree LSTM	Graph LSTM	[60]
	Semantic role labeling	Syntactic GCN	Graph Convolutional Network	[108]
	Neural machine translation	Syntactic GCN	Graph Convolutional Network	[109], [110]
		GGNN	Gated Graph Neural Network	[38]
	Relation extraction	Tree LSTM	Graph LSTM	[111]
		Graph LSTM	Graph LSTM	[44], [112]
		GCN	Graph Convolutional Network	[113]
	Event extraction	Syntactic GCN	Graph Convolutional Network	[114], [115]
	AMR to text generation	Sentence LSTM	Graph LSTM	[116]
		GGNN	Gated Graph Neural Network	[38]
	Multi-hop reading comprehension	Sentence LSTM	Graph LSTM	[117]
	Relational reasoning	RN	MLP	[96]
		Recurrent RN	Recurrent Neural Network	[118]
		IN	Graph Neural Network	[4]
Image	Social Relationship Understanding	GRM	Gated Graph Neural Network	[119]
	Image classification	GCN	Graph Convolutional Network	[120], [121]
		GGNN	Gated Graph Neural Network	[122]
		DGP	Graph Convolutional Network	[35]
		GSNN	Gated Graph Neural Network	[123]
	Visual Question Answering	GGNN	Gated Graph Neural Network	[119], [124], [125]
	Object Detection	RN	Graph Attention Network	[126], [127]
	Interaction Detection	GPNN	Graph Neural Network	[128]
		Structural-RNN	Graph Neural Network	[42]
	Region Classification	GCNN	Graph CNN	[129]
	Semantic Segmentation	Graph LSTM	Graph LSTM	[63], [130]
		GGNN	Gated Graph Neural Network	[131]
		DGCNN	Graph CNN	[132]
		3DGNN	Graph Neural Network	[133]
Science	Physics Systems	IN	Graph Neural Network	[4]
		VIN	Graph Neural Network	[91]
		GN	Graph Networks	[3]
	Molecular Fingerprints	NGF	Graph Convolutional Network	[51]
		GCN	Graph Convolutional Network	[99]
	Protein Interface Prediction	GCN	Graph Convolutional Network	[5]
	Side Effects Prediction	Decagon	Graph Convolutional Network	[134]
	Disease Classification	PPIN	Graph Convolutional Network	[135]
Knowledge Graph	KB Completion	GNN	Graph Neural Network	[6]
	KG Alignment	GCN	Graph Convolutional Network	[136]
Combinatorial Optimization		structure2vec	Graph Convolutional Network	[7]
		GNN	Graph Neural Network	[137]
		GCN	Graph Convolutional Network	[138]
		AM	Graph Attention Network	[139]
Graph Generation		NetGAN	Long short-term memory	[140]
		GraphRNN	Rucurrent Neural Network	[137]
		Regularizing VAE	Variational Autoencoder	[141]
		GCPN	Graph Convolutional Network	[142]
		MolGAN	Relational-GCN	[143]

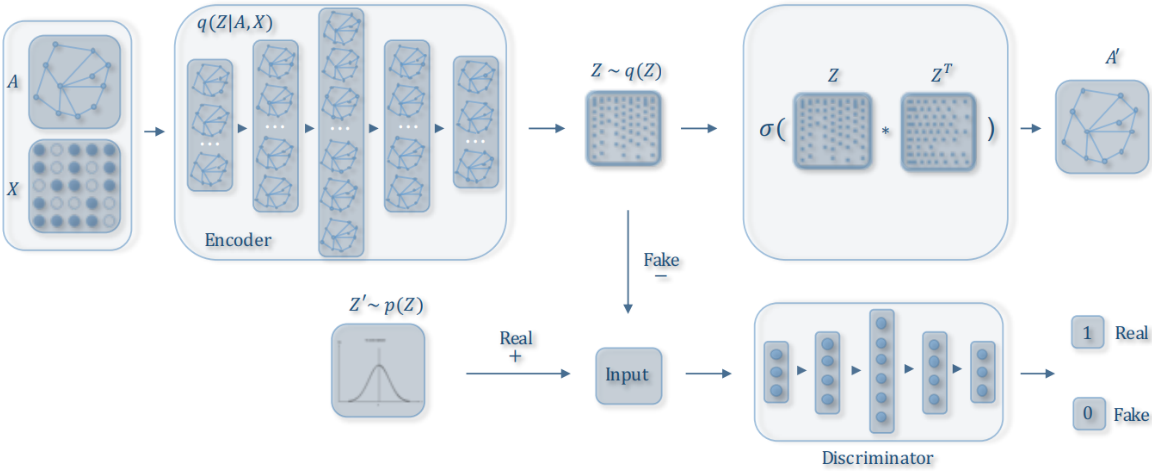
本次任务模型框架

GAE&VGAE



其中encoder和decoder都可以在上面提到的半监督模型中任意选择

ARGA&ARVGA



其中encoder、decoder和discriminator都可以在上面提到的半监督模型中任意选择

实验效果展示

聚类图示

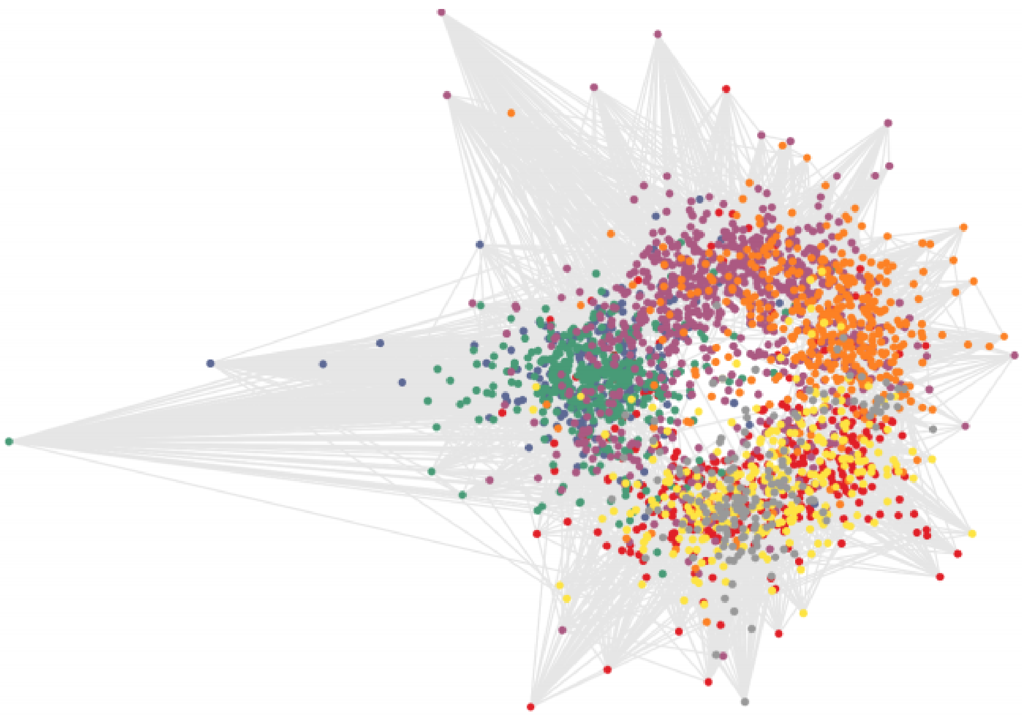


Figure 1: Latent space of unsupervised VGAE model trained on Cora citation network dataset [1]. Grey lines denote citation links. Colors denote document class (not provided during training). Best viewed on screen.

Figure 3: The Cora data visualization comparison. From left to right: embeddings from our ARGA, VGAE, GAE, DeepWalk, and Spectral Clustering. The different colors represent different groups.

指标对比

无监督聚类指标

聚类方法	指标名	指标值	Embedding
K-means	time	2.830502986907959	no
K-means	time	0.11931586265563965	**yes**
K-means	roc	0.5019011406844107	no
K-means	roc	0.9399882619387965	**yes**
K-means	mean_auc	0.6679340937896071	no
K-means	mean_auc	0.9431105716088222	**yes**
K-means	adjusted_rand_score	0.15276087390029897	no
K-means	adjusted_rand_score	0.48880056899221924	**yes**
K-means	adjuested_mutual_info_score	0.22946117234356792	no
K-means	adjuested_mutual_info_score	0.5309173000431427	**yes**
K-means	homogeneity_score	0.23236101031528184	no
K-means	homogeneity_score	0.5350186592750334	**yes**
K-means	completeness_score	0.27652318331984904	no
K-means	completeness_score	0.5326231454058572	**yes**
K-means	v_measure_score	0.2525258479451513	no
K-means	v_measure_score	0.5338182148816589	**yes**
K-means	fowlkes_mallows_score	26.055423707030968	no
K-means	fowlkes_mallows_score	40.97070549672973	**yes**
K-means	silhouette_score	-0.0027151608373969793	no

K-means	silhouette_score	0.1821691393852234	**yes**
K-means	calinski_harabaz_score	40.67669021359497	no
K-means	calinski_harabaz_score	540.7332549271462	**yes**

半监督分类指标

由于使用的数据集是带部分标签的，所以也可以进行半监督分类任务，结果如下：

- **分类能力较弱的分类器（KNN）：**

```
Original:
              precision    recall  f1-score   support

      class0       0.18      0.29      0.22       130
      class1       0.18      0.34      0.24        91
      class2       0.32      0.67      0.43       144
      class3       1.00      0.00      0.01       319
      class4       0.23      0.44      0.30       149
      class5       0.00      0.00      0.00       103
      class6       0.08      0.03      0.04        64

    accuracy                           0.23      1000
   macro avg       0.28      0.25      0.18      1000
weighted avg       0.44      0.23      0.16      1000

--------------------------------------------------



Embedded:
              precision    recall  f1-score   support

      class0       0.64      0.66      0.65       130
      class1       0.73      0.85      0.79        91
      class2       0.78      0.96      0.86       144
      class3       0.87      0.67      0.76       319
      class4       0.75      0.81      0.77       149
      class5       0.78      0.71      0.74       103
      class6       0.61      0.78      0.68        64

    accuracy                           0.76      1000
   macro avg       0.74      0.78      0.75      1000
weighted avg       0.77      0.76      0.76      1000
```

- **分类能力较强的分类器（XGBoost）：**

```
Original:
              precision    recall  f1-score   support
```

```
      class0       0.43      0.38      0.40       130
      class1       0.56      0.66      0.61        91
      class2       0.73      0.71      0.72       144
      class3       0.67      0.55      0.60       319
      class4       0.55      0.67      0.60       149
      class5       0.53      0.53      0.53       103
      class6       0.38      0.56      0.46        64

    accuracy                           0.58      1000
   macro avg       0.55      0.58      0.56      1000
weighted avg       0.59      0.58      0.58      1000

--------------------------------------------------


Embedded:
              precision    recall  f1-score   support

      class0       0.61      0.72      0.66       130
      class1       0.61      0.84      0.70        91
      class2       0.89      0.83      0.86       144
      class3       0.87      0.62      0.73       319
      class4       0.64      0.74      0.68       149
      class5       0.78      0.76      0.77       103
      class6       0.58      0.81      0.68        64

    accuracy                           0.73      1000
   macro avg       0.71      0.76      0.73      1000
weighted avg       0.75      0.73      0.73      1000
```

可拓展性

本次项目使用了划分子图的方法，可以在超大型图上进行mini-batch训练，理论上可支持所有图的数据

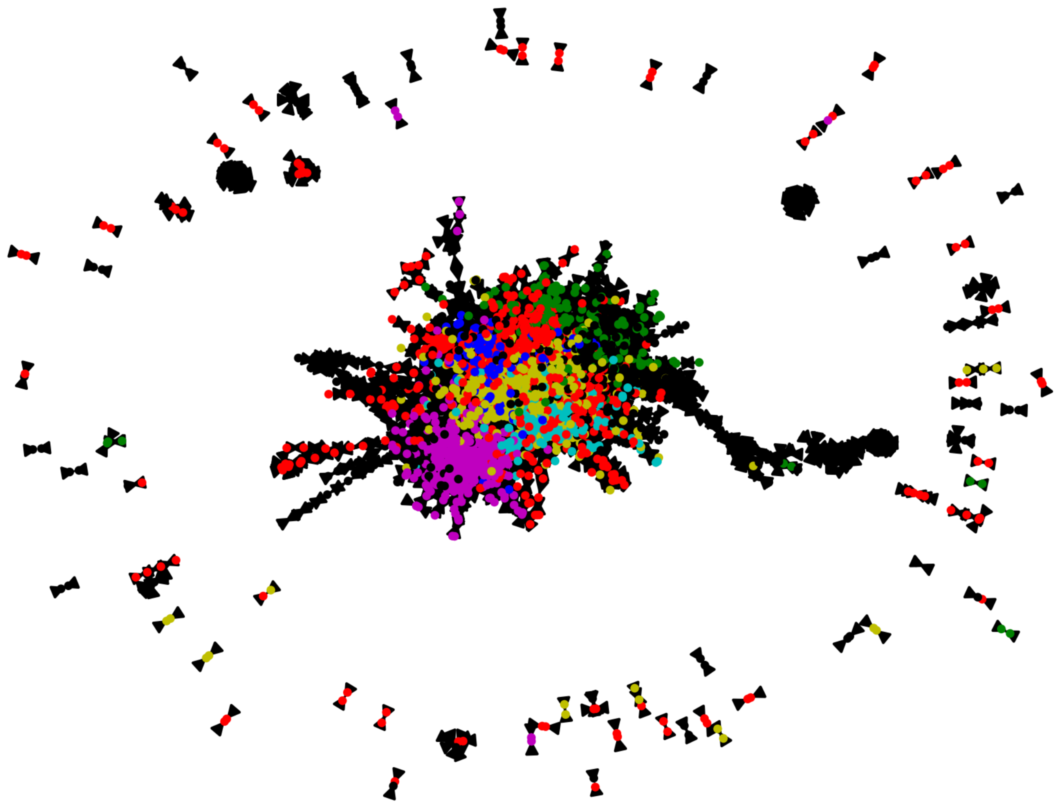
> 经测试，本算法可以在Reddit数据集上运行，效果与小数据集相当
> Reddit数据集大小：
> **node**:232965
> **edge**:114615892
> **feature**:602

可视化

本项目自带可视化函数，分为两类：

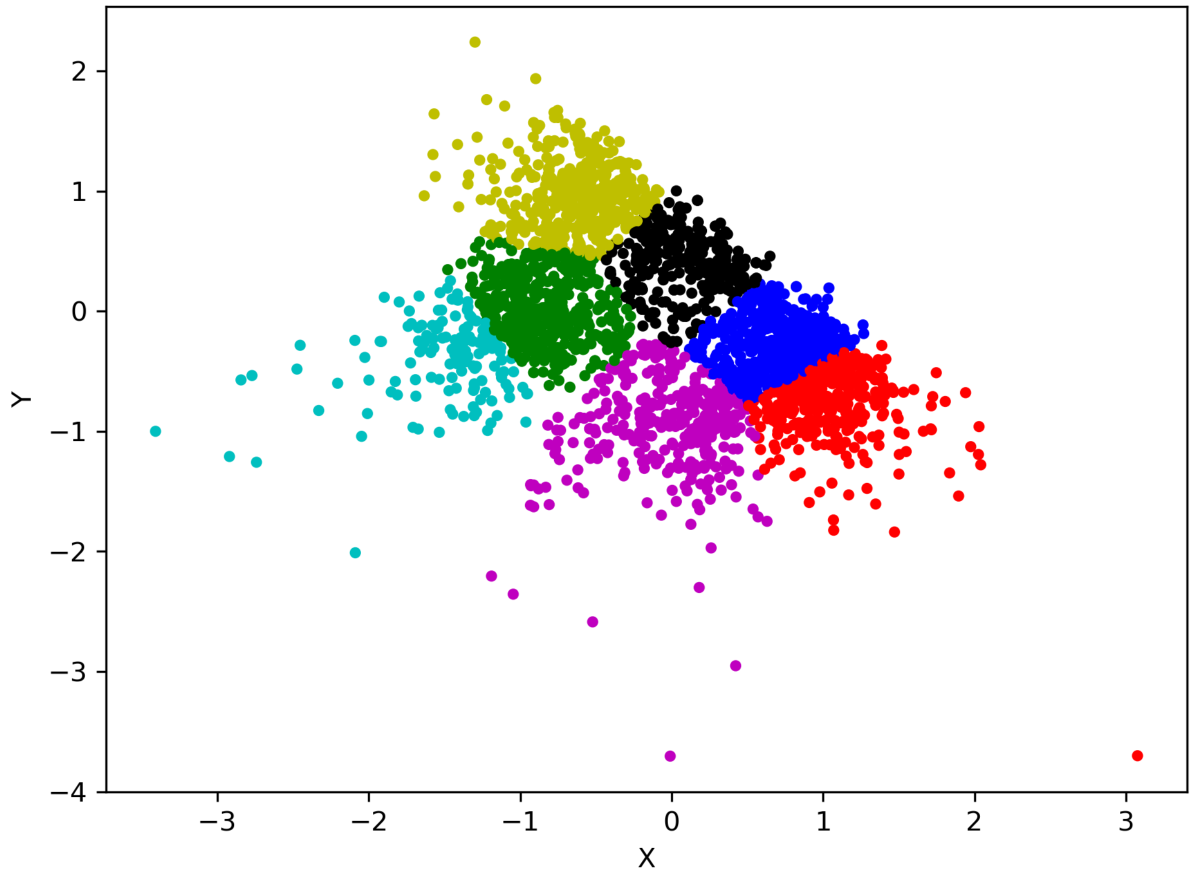
- Graph的可视化（带标签）
- 将Embedding压缩到2或3维时聚类效果可视化

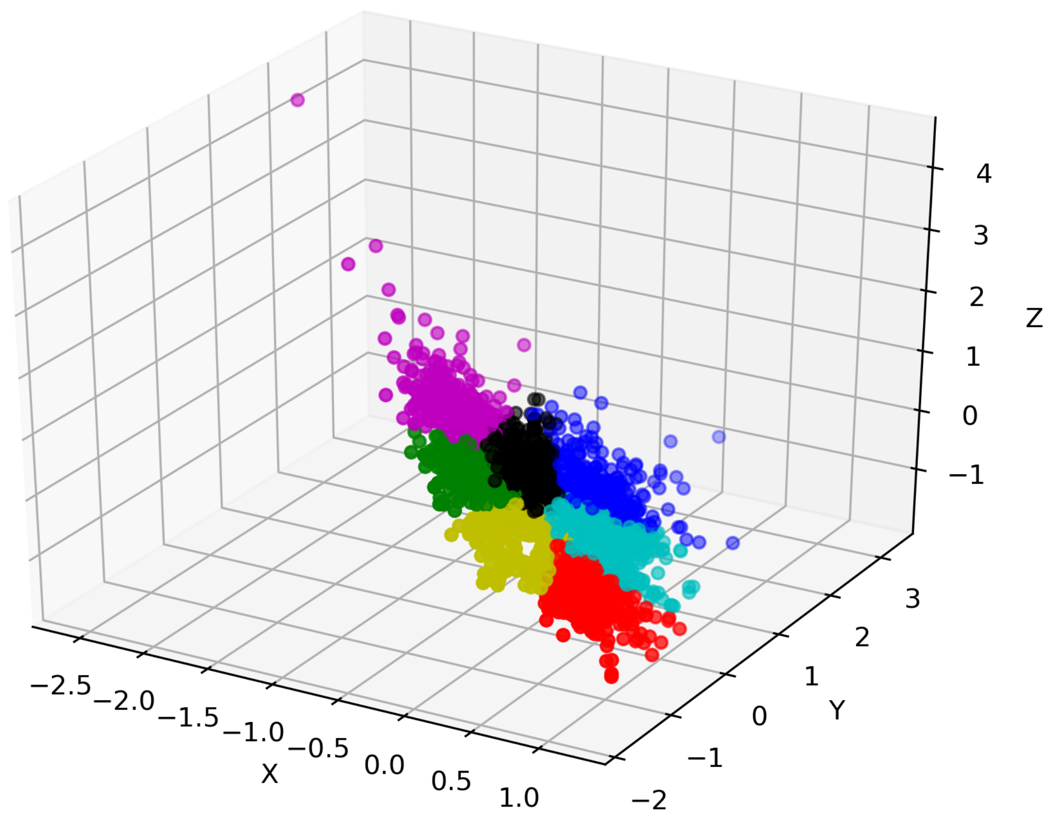
Graph可视化



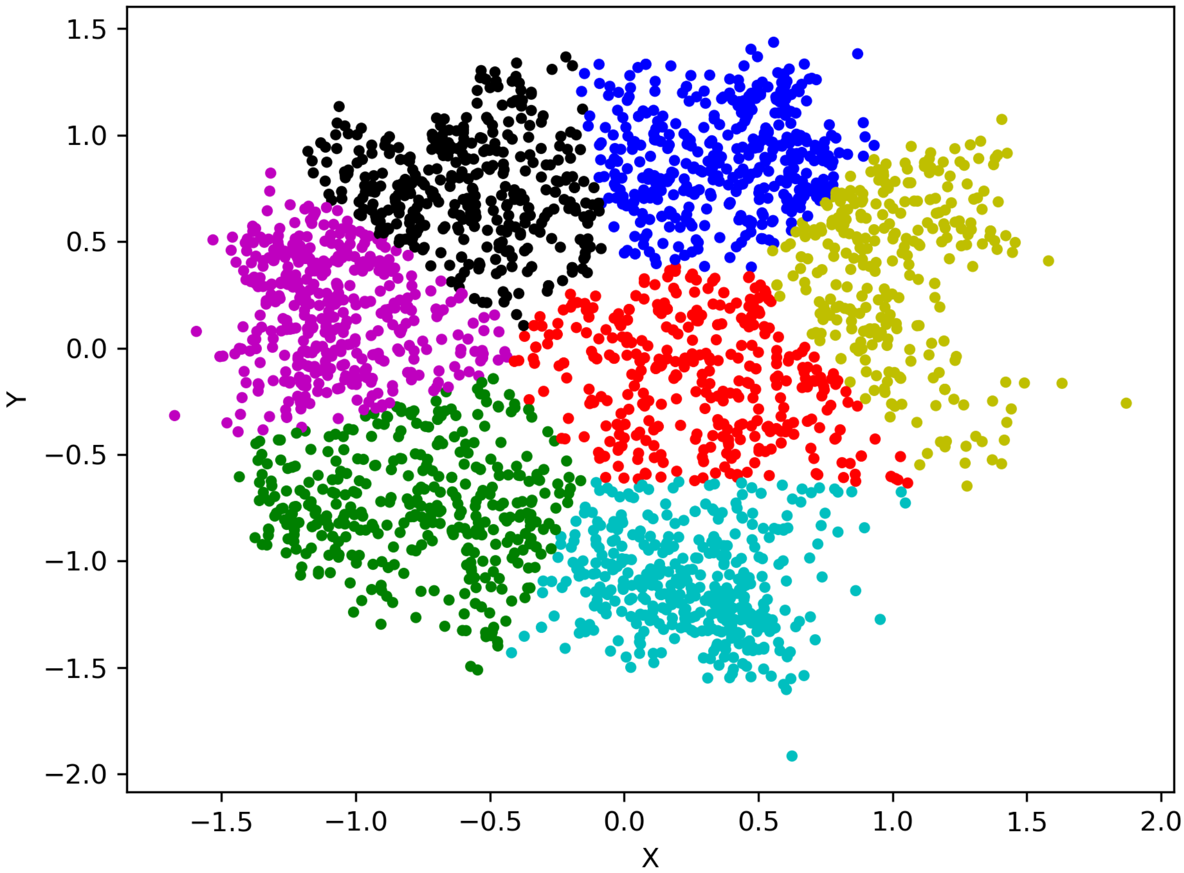
Embedding可视化

GAE+GCN

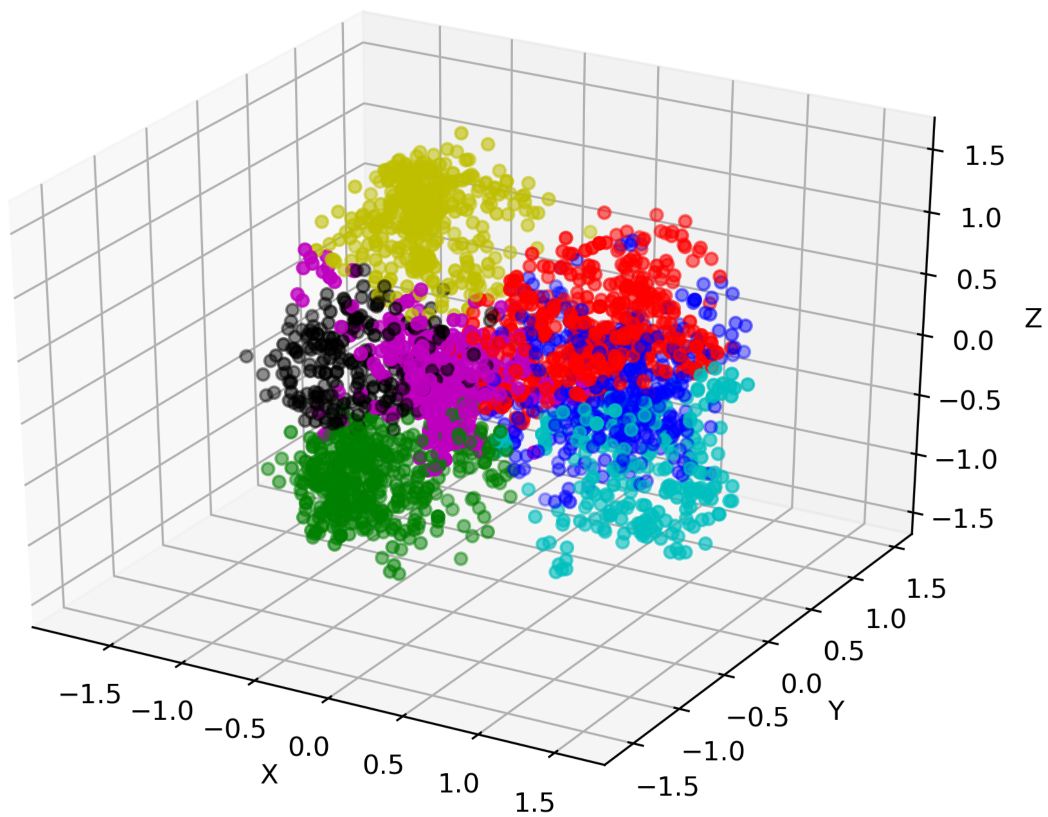




GAE+GAT



1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
Y
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
X



1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
Z
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
X
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
Y