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• **Supplementary File** •

Geometric deep learning: progress, applications and challenges

Wenming CAO, Canta ZHENG, Zhiyue YAN & Weixin XIE*

College of Electronics and Information Engineering, Shenzhen University, Shenzhen 518060*, China*

Appendix A Applications of geometric deep learning

Geometric deep learning has been widely explored in various fields. The recommendation system uses social networks or buying behaviors to provide users with accurate and fast services, such as friends, merchandise items, or personalized content, to improve their experience and create opportunities for attracting new users. The work in [1] encodes the users and the items with a graph neural network to predict rating scores in the recommendation. Besides, community detection and fraud detection in social networks are also popular in graph neural networks. Community detection is a common task in social network analysis to cluster nodes into multiple groups called communities. Graph neural networks can achieve both overlapping and non-overlapping community detection. Shchur et al. proposed the NOCD [2] model, which combines the Bernoulli Poisson probabilistic model with GCN, and achieves overlapping community detection. In past years, fraud or anomaly detection has attracted much attention in industry and academia. Its application directions include financial fraud detection, risk control, network navy identification, black and gray product identification, etc. Geniepath [3] proposes an adaptive graph convolutional network whose composition form is a homogeneous graph based on the Alipay account. In the neighbor dimension, it uses the attention mechanism to encode the neighbor's importance. In the network dimension, it uses the LSTM network to learn the optimal network depth.

Except for the above, geometric deep learning is also applied in many other fields such as computer vision, chemistry, biology, and knowledge graph. Three-dimensional data analysis has attracted more and more researchers' attention due to the emergence of new 3D technologies like VR(virtual reality). In this field, the three-dimensional shape data is modeled as a Riemannian manifold and discretized as a grid. There are two main application directions. One is to learn local descriptors and corresponding shapes. The other direction is to learn global descriptors and use them for the tasks in shape recognition. In chemistry and biology, researchers try to study the molecular structure using graph neural networks. A molecule can be treated as a graph whose nodes represent atoms and whose edges represent bonds. Molecular fingerprint and protein interface prediction are the two most popular types of research, which may be the key to reaching a level useful to the pharmaceutical industry. We have seen the initial results of this phenomenon. The knowledge graph is a typical type of non-Euclidean data that belongs to the homogeneous information network. The work [4] used GNN to solve the problem of entities outside the knowledge base in KBC settings. Research in knowledge graphs with geometric deep learning can better understand the relationship of the entities in the real world.

There are also many exciting types of research in image analysis. For example, [5] models the intermodality connections between two modalities through the cross-modal graph and proposed an adaptive cross-modal method with graph convolutional neural networks for RGB-D scene recognition. [6] utilized the graph model to preserve the spatial structure information and regional connectivity of the predicted category label map in semantic image segmentation. [7] combined hyperspectral image classification with graph learning and proposed the discriminant analysis with graph learning to capture the local manifold data and so on. Table 1 shows method characteristics in different applications.

Application filed	Example Method	Characteristic
Recommendation	[1].	Use heterogeneous GNNs to encode uses and items in a bipartite graph.
Community detection	[2].	Equivalent to node classification according to the graph structure.
Fraud detection	[3].	Equivalent to binary classification classification according to the node?s behavioral characteristics.
Computer vision	[5], [6], [7], [8].	Combine traditional methods for images or manifolds with graph learning to realize vision tasks like image segmentation according to connected information in images or manifolds.
Chemistry and biology	[9], [10].	Mainly contain graph pooling for molecular classification and graph generative networks for molecular design.
Knowledge graph	[4].	For multirelationship and multinode task in knowledge graph.

Table 1. Characteristic of methods in different applications.

* Corresponding author (email: wxxie@szu.edu.cn)

Appendix B More information about deeper architecture

Some methods have been proposed such as DeepGCNs [11] and DropEdge [12], which improve the performance in some datasets to a certain extent. The recent work [13] proposed GCNII, providing theoretical and empirical evidence that can effectively relieve the problem of over smoothing. It has proved to be the state-of-art so far.

Table 2 shows some recent deep GNN performance in the Cora dataset as the layers increases. As is shown, the typical graph neural networks like GCN get lower performance as the layers increase. GCNII [13] makes the best performance currently.

Dataset	method	Layers					
		2	4	8	16	32	64
Cora	GCN	81.1	80.4	69.5	64.9	60.3	28.7
	GCN(Drop [12])	82.8	82.0	75.8	75.7	62.5	49.5
	JKNet [14]	/	80.2	80.7	80.2	81.1	71.5
	JKNet(Drop)	/	83.3	82.6	83.0	82.5	83.2
	Incep [12]	/	77.6	76.5	81.7	81.7	80.0
	Incep(Drop)	/	82.9	82.5	83.1	83.1	83.5
	GCNII	82.2	82.6	84.2	84.6	85.4	85.5
	GCNII*	80.2	82.3	82.8	83.5	84.9	85.3

Table 2. Performances with different layers. cited from [13]

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