Knowledge Graph Completion based on Hyperbolic Graph Contrastive Attention Network

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***Abstract*—Knowledge graph completion technology is important for the integrity of knowledge graph. However, the feature mining of knowledge graph is not sufficient due to the lack of hierarchical and neighborhood information. To solve such issues, this paper proposes a knowledge graph completion method based on the Hyperbolic Graph Contrastive ATtention network(HyGCAT). HyGCAT embedded the knowledge graph into the hyperbolic space with constant negative curvature to capture the complex hierarchical relations between entities with less memory. Meanwhile, HyGCAT uses the attention mechanism to learn the latent representations of neighborhood entities. Furthermore, HyGCAT strengthens the correlation between representations of entities and neighbor subgraphs through contrastive learning. The proposed method can improve the performance of link prediction for knowledge graphs completion significantly.**

Keywords—knowledge graph, hyperbolic space, attention network, contrastive learning , knowledge graph completion

I. Introduction

Knowledge graph is a semantic network that reveals the relationships between entities in the world. The structured knowledge in a knowledge graph is usually organized into triples (v_h, r, v_t), which are head entities, relations and tail entities. In recent years, knowledge graphs has been widely used in the field of industrial artificial intelligence. However, with the continuous growth of industrial knowledge, most of the knowledge stored by knowledge graphs is sparse and incomplete. In order to complete the knowledge system, finding all true triples manually will be costly. As a result, how to complete the knowledge automatically in the evolving knowledge graphs becomes an important challenge.

Generally, knowledge graph completion uses an encoder-decoder framework as Figure 1 shows. The encoders based on GCN[1](graph convolutional neural network) generate representations of entities and relations in the knowledge graph to predict the adjacency tensor. When recovering the graph structure, the decoder based on KGE(knowledge graph embedding) can predict the missing links in the original graph to complete the knowledge graph. KGE is the common method for decoding due to its simplicity and effectiveness. KGE embeds entities and relations into knowledge graphs as low-dimensional representations. It defines a score function on the embedding space to measure the rationality of triples. Generally , triples with a higher score will be regarded as more credible.

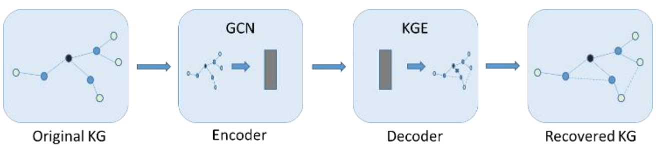

Fig. 1. Encode-decoder framework for knowledge graph completion

Although knowledge graph completion is becoming more and more important, the existing methods have some problems. Knowledge networks in the real world are often characterized by multi-hierarchical structures, especially in large-scale knowledge graph. Existing knowledge graph completion methods embed independent triples into a continuous low-dimensional vector space in Euclidean space. The entities and relations are inferred by the vectors in Euclidean space. The missing elements in knowledge triples are predicted by neural network model. Nevertheless, the hierarchical relations between entities in this space are missing. The hierarchical relation is important to large-scale knowledge mapping for storing high-level represents.

Hyperbolic space is a embedding space with negative constant curvature. The curvature at any position in this space is a negative constant. Compared with the graph in Euclidean space, the graph in hyperbolic space has unique expressive representation. As shown in Figure 2, the knowledge graph can expand exponentially in hyperbolic space and polynomially in Euclidean space. It can better capture the hierarchical structure of graph data because of its distribution pattern. Meanwhile, considering a large-scale knowledge graph, the hyperbolic graph can save redundant embedding space.

Moreover, most existing knowledge graph completion methods treat triples independently as simple link prediction problems. It will lose the information from neighborhoods of entities that is likely to ignore the latent feature contained in

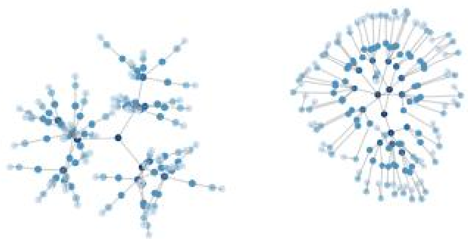

Fig. 2. Knowledge distribution in Euclidean space (left) and hyperbolic space (right)

neighbor entities.

All neighbors share the same weight during neighborhood aggregation in GCN. In order to improve the feature learning from neighbors, we use GAT (Graph Attention Network) [2] to model the neighborhood structure of each central entity through the attention mechanism. The weights of neighbor entities will depend on the importance of the node feature. Therefore, attention networks can comprehensively capture the neighborhood features of each central entity.

Meanwhile, contrastive learning has been widely used in graph representation learning recently. The positive sample and the negative sample will be obtained by data augmentation. Contrastive learning mainly aims to capture the statistical relevance of positive and negative samples by training encoders. We change the the neighbor structure of the central entity by node dropping and edge perturbation to generate negative samples. Contrasting these samples can enhance the strong relevance to important information from neighbor domain.

This paper proposes a knowledge graph completion method based on the hyperbolic graph contrastive attention network(HyGCAT). It consolidates the hierarchical modeling capability of hyperbolic geometry and the structure learning capability of graph contrastive attention network to learn embedded representation on knowledge graphs. At the encoder stage of knowledge graph completion, this paper uses graph attention mechanism to capture the relationship between neighbors and the central entity. The entities and neighbors feature from graph neural network in Euclidean space will be embedded in hyperbolic space. In addition, the contrastive module will further strengthen the links between entities and their neighbors. At last, the KGE method will recover the graph by these representations to complete the knowledge graph.

II. Hyperbolic Representation Learning and Graph Contrastive Learning - A Preliminary Work

Hyperbolic space is one of the most potential space researches recently. The curvature of hyperbolic space is a negative constant and it is zero in Euclidean space. Previous studies have shown that hyperbolic space is better than Euclidean space when modeling knowledge graph data of tree hierarchy with multi-relations. In recent years, many studies have attempted to embed a variety of hierarchical data into hyperbolic space including graph representation learning and recommendation systems. Chami et al.[3] aggregates the expressive ability of GCN and hyperbolic geometry to learn the representation of nodes in scale-free or hierarchical graphs. This paper shows that the GCN in hyperbolic space can learn hierarchical structures and performs well even when the dimensions are low. The MuRP model from Balazevic et al.[4] embeds hierarchical multi-relation data into the Poincare sphere of hyperbolic geometry. Multi-relation knowledge graph data is embedded into the hyperbolic space for link prediction. Hyperbolic is also widely used in NLP due to its special embedding. Sun et al.[5] proposes a hyperbolic relational graph neural network for KG embedding. The hyperbolic transformation is used to capture knowledge associations with the hierarchical relationship.

Graph contrastive learning is the state-of-the-art method in unsupervised graph representation learning recently. The graph contrastive learning method DGI proposed by Petar et al[6]. It maximizes the information between local structure and global context to find the satisfying results. The graphical mutual information proposed by Peng[7] et al. can maximize the mutual information between the original features of an entity and its 1-hop neighbors. It obtain the optimal results in inductive node classification and link prediction tasks. GraphCL[8] maximizes the consistency between two augmented views of the same graph through the contrast loss in the latent space. However, there has been little research on the contrastive learning in knowledge graph completion nowadays.

III. Method Overview

In this section, the framework of HyGCAT will be introduced. The overview of HyGCAT is shown in Figure 3.

Firstly, the input of the framework is the knowledge graph in the Euclidean space. The entities and relations are embedded into hyperbolic space to obtain hyperbolic embedded vectors. In various hyperbolic spaces, the Poincare sphere model is most suitable for representation learning because it can be adjusted using gradient optimization. Points in Euclidean tangent space are mapped to hyperbolic space according to the exponential mapping in Poincare sphere model.

Random walk is often used in entities sampling. In order to better extract the hierarchical relationship in the

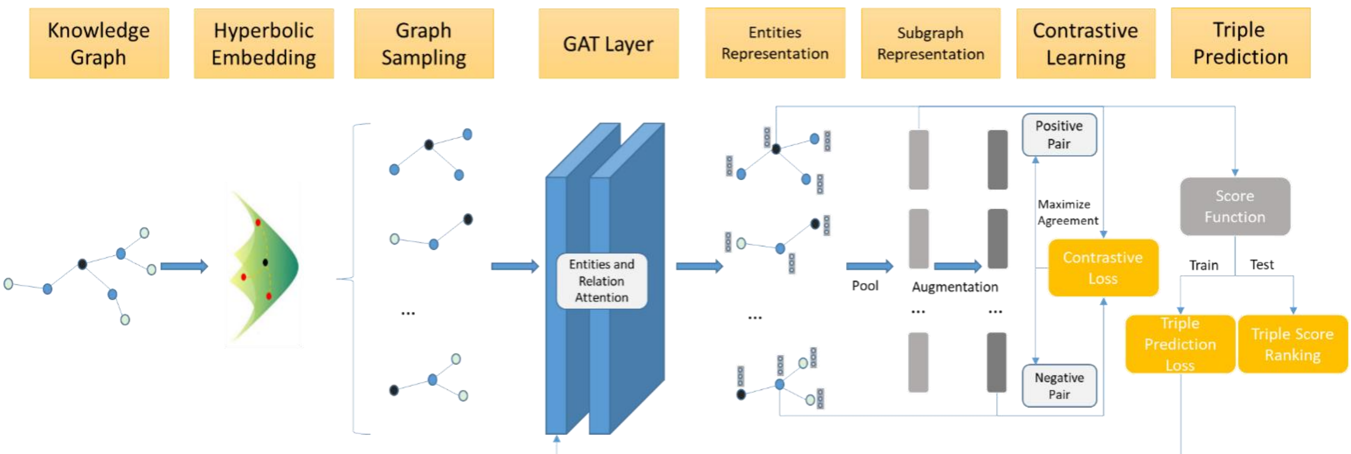

Fig. 3. The overview of Hyperbolic Graph Contrastive ATtention network(HyGCAT)

subsequent hyperbolic space, the Diffusion Sampler is adopted as the entities sequence sampling method. The diffusion process on the graph can be used to create the vertex sequence with the hierarchical information and tree topology of the input graph.

After completing entities sampling, the coding layer uses GAT network as graph neural network for training. We can transform the sampled entities and subgraphs into vector representations in hyperbolic space. GAT treats different neighbor nodes differently by measuring the correlation between the central entities and its neighbor nodes. It applies the importance as a weight to aggregate the central entities and neighbor structure information. As a result, it can describe the central node more accurately and improve the expression ability of the representation model. In this stage, HyGCAT uses two attention layers for relations attention and entities attention. These layers are respectively used to generate the embedded vector and the attention of neighbor triples for the fusion of neighborhood information. In addition, HyGCAT uses the pooling algorithm to aggregate the neighbor vectors which can generate the vector representation of the neighbor subgraph.

In the phase of graph contrastive learning, HyGCAT uses node dropping and edge perturbation for data augmentation using the vectors in hyperbolic space. Then we can generate the negative representation samples of entities and neighbor subgraphs corresponding to real entities and subgraphs. By comparing the positive relationships with the negative relationships, the contrastive loss can be adjusted under different combinations. The contrastive learning stage can strengthen the association between the central entity and the positive neighbor subgraph while the association between the central entity and the negative samples is weakened.

Finally, knowledge triples are predicted in the decoder stage. Various of existing knowledge graph embedding models can be used as the decoder. The decoder uses the generated representations to predict the adjacency vectors. Since there is a bijection between the adjacency vector and the graph structure, the prediction can be regarded as a recovery of the original knowledge graph structure. When recovering the knowledge graph structure, the decoder can predict the missing links in the original graph which can complete the knowledge graph. MuRP can embed multiple graph data with the Poincare sphere model in hyperbolic space. In the previous stage the operation was in hyperbolic space similarly that MuRP model will be used as decoder in HyGCAT. MuRP transforms the entity embedding by learning relation specific parameters through Mobius matrix-vector multiplication and Mobius addition. The prediction results are scored by the score function in MuRP. The loss of triplet prediction is obtained in the training stage while the predicted score of each triplet is obtained in the test stage. Then the decoder can recover the graph though predictions to complete the knowledge graph.

IV. CONCLUSION

In general, this paper proposes a knowledge graph completion method named HyGCAT. The main contributions of this paper are summarized as follows:

1) Different from the previous link prediction methods based on Euclidean space, HyGCAT embedded the knowledge graph into hyperbolic space at the start of knowledge graph completion. It solved the problems including the lack of hierarchical information and large space usage of complex knowledge graphs by using the characteristics of hyperbolic space graphs such as hierarchical representation and exponential diffusion.

2) Considering the weak knowledge mining ability of neighbor subgraph in knowledge graph completion, this paper strengthens the correlation between the representation of the central entity and the neighbor subgraph through contrastive learning. We improve the mining effect of important information from neighbor entities through attention mechanism which can improve the overall learning effect for edge knowledge.

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