GIDN: A Lightweight Graph Inception Diffusion Network for High-efficient Link Prediction

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Abstract

In this paper, we propose a Graph Inception Diffusion Networks (GIDN) model. This model generalizes graph diffusion in different feature spaces, and uses the inception module to avoid the large amount of computations caused by complex network structures. We evaluate GIDN model on Open Graph Benchmark (OGB) datasets, reached an 11% higher performance than AGDN on ogbl-collab dataset.

1 Introduction

Currently, many implementations of semantic applications rely on knowledge graphs, where new knowledge is inferred from existing knowledge. e.g., recommendation computing [1, 2] and search engines [3, 4]. Knowledge graphs map real-world entities and relationships between entities into triples [5], denoted
as (head entity, relation, tail entity), e.g., (Turing, BornIn, England), indicating that Turing was born in England. Knowledge graphs have gained great achievement in many fields, such as natural language processing [6, 7], deep learning [12], and graph processing [9, 10].

Even though large-scale Knowledge Graphs currently contain more than a billion triples, these datasets are still incomplete [8], meaning that they are missing a large number of valid triples. Knowledge graph embedding, also known as link prediction, can effectively complement these datasets [11, 13]. For example, it is known that cephalosporins and alcohol together can cause a disulfiram-like reaction, and cefpirome is a cephalosporin, so it is inferred that cefpirome and alcohol cannot be taken together. Knowledge graph embedding aims to encode real-world entities and relationships as a low-dimensional vector that can be efficiently stored and computed, and contain semantic-level information [14].

Due to the rapid development of artificial intelligence, knowledge graphs that meet the need for data processing and understanding are receiving increasing attention. The main approach of some well-designed knowledge graph models is to map entities and relations into and reason in a continuous space. For example, TransE [15] interprets relations as translations of entities in low dimensions, modeling the inversion and composition patterns. RotatE [16] treats relations as rotations from source entities to target entities in complex spatial vectors, enabling modeling and inference of various relational patterns. There are also methods in symbolic space where models are based on symbolic logic rules, such as Markov logic networks [17]. Recently, researchers have proposed to combine neural methods and symbolic methods to make models with better capacity and interpretability, such as pLogicNet [18] and NBFNet [19].

2 Related Work

2.1 Graph Neural Networks

To address the drawbacks of heuristic techniques, graph neural networks provide heuristics that can learn appropriate features from the networks themselves in the link prediction task [35–37]. SEAL [26] fixes multiple flaws of WLNM, not only replacing the fully connected neural network in WLNM with a graph neural network, but also allowing learning from latent and explicit node features, thereby absorbing multiple types of information. Because some information is lost when computing feature vectors at the pooling layer, LGLP [34] proposes to learn features directly from target links instead of closed subgraphs. And in order for the graph convolutional layer to effectively learn edge embeddings from the graph, LGLP modifies the original bounding subgraph into the corresponding line graph. SEAL needs to operate on each subgraph, which doesn’t work very well on large graphs. NBFNet [19] explicitly captures the path between two nodes for link prediction while achieving relatively low time complexity.
2.2 Shallow Embedding Technique

Inspired by the word2vec [20], Perozzi et al. [21] proposes a graph mining approach combining random walk [22] and word2vec algorithm to learn the hidden information and social representation of a graph. Tang et al. [23] puts forward an algorithm whose target function preserves both local and global structure of a graph, resulting in greater efficiency and effectiveness. Grover et al. [24] improves the random walk method in Deepwalk [21], makes it possible to reflect the characteristics of both depth-first and breadth-first sampling, thus improving the effectiveness of network embedding. However, one limitation of these works is that too many parameters are associated in the model, which significantly reduces the computational speed.

2.3 Logic Rule Induction Methods

The heuristic technology is calculated according to the characteristics of the graph structure, and the key is to calculate the similarity calculation score for the neighborhood of the two target nodes [29, 30]. As shown in Figure 1, according to the maximum number of neighbor hops used in the calculation process, the heuristic methods can be divided into three groups, including first-order, second-order and higher-order heuristics. Zhang et al. [25] proposed Weisfeiler-Lehman Neural Machine(WLNM) to extract a subgraph for each target link domain as an adjacency matrix, and train a fully connected neural network on these adjacency matrices to learn a link prediction model. Studies have shown that higher-order heuristics such as rooted PageRank [31] and Simrank [32] have better performance than lower-order heuristics [27, 33]. However, the increase in the number of grid hops means higher computational costs and memory consumption. Moreover, the lack of heuristics has poor applicability to different types of networks [28, 30], which means complex computation is required to find the appropriate heuristic for different networks.

3 Method

Encapsulating the representation of graph diffusion can provide a better basis for prediction than the graph itself. Graph diffusion is the use of a matrix for each prediction target in a graph to represent the information in its proximity. For example, for node n, its H-hop node is the node reached by jumping H times from node n. The i-th row of the matrix is the neighborhood information of the i-hop of node n. Standard graph diffusion operations rely on extensive tensor calculations, which require expensive storage space and running time. Graph Diffusion Networks model uses a combination of small-hop nodes and learnable generalised weighting coefficients to achieve multi-layer generalised graph diffusion in different feature spaces, while also ensuring moderate complexity and running time.

If the depth of the network is increased, the network will become computationally complex. The Inception module is able to capture rich features while
avoiding the computational effort associated with an overly deep network, making it more adaptable to training with a large number of samples.

Data augmentation can expand the dimension of training data. In graph structure, data augmentation mainly focuses on nodes and edges. Random walk is a method removing the edges between nodes who have different labels and building connections for the nodes with the same labels.

4 Evaluation

We conduct experiments on the ogbl-collab dataset [39]. We run the model 10 times and record the mean ± standard deviation of Hits@50. The results are shown in Table 1. Our method reaches better performance than AGDN [38], and higher ceiling than PLNLP [40].

| Method | ogbl-collab(Hits@50) |
|--------|----------------------|
| AGDN   | 0.4480 ± 0.0542      |
| PLNLP  | 0.7059 ± 0.0029      |
| GIDN   | 0.7096 ± 0.0055      |

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