Chapter 10
Future Research Directions

Abstract Heterogeneous Graph (HG) representation has made great progress in recent years, which clearly shows that it is a powerful and promising graph analysis paradigm. However, it is still a young and promising research field. In this chapter, we first make a summarization of this book and then illustrate some advanced topics, including challenging research issues, and explore a series of possible future research directions. One major potential direction is exploring fundamental ways to keep intrinsic structures or properties in HG. And another direction is to integrate the techniques widely used or newly emerged in machine learning to further enhance the applicability of HG on more key fields. We will illustrate more fine-grained potential works along with these two directions.

10.1 Introduction

Heterogeneous Graph (HG) representation has significantly facilitated the HG analysis and related applications. This book conducts a comprehensive study of the state-of-the-art HG representation methods. Thorough discussions and summarization of the reviewed methods, along with the widely used benchmarks and resources, are systematically presented. Then, in part one of this book, we present the advanced HG representation techniques. Particularly, we first introduce several classical structure-preserved HG methods. These methods preserve the heterogeneous structure by most fundamental elements in HG, including meta-path, relation, and network schema. Then attribute information is introduced to enrich the characteristics of nodes. Heterogeneous Graph Neural Networks (HGNN) naturally provide an alternative way to integrate attributes with structural information. Besides static heterogeneous graphs, we introduce dynamic HGNN methods, which mainly focus on updating node representation in an efficient way or learning node representations while considering sequential evolution. In part two, the necessity of HG to fuse abundant heterogeneous interactions is comprehensively displayed in several prevalent applications. The recommendation is one of such prevalent applications, as the interactions of users and items can be naturally built as an HG. Particularly, three advanced HG based recommendation methods are presented to show the effectiveness of integrating heterogeneous information. Another interesting application is using HG to overcome data sparsity problems in text mining. We summarize the methods, which utilize the powerful capabilities of HG to integrate extra information, to demonstrate the superiority of HG representation methods in text mining. More importantly, one of the unique characteristics of this book is that we not only summarise the methods invented based on public academic data, but also the methods deployed on real-world systems. These methods further promote the application of the HG methods towards industrial production. We hope that this book can provide a clean sketch and key technique summarization on HG representation, which could help both the interested readers as well as the researchers that wish to continue working in this area.

In this chapter, we point out some promising research directions on HG representation. Preserving HG structures and properties is deemed as one of the most fundamental ways to encode heterogeneous information. More fundamental but largely ignored methods are pointed out by us, such as motif/network-schema preserved methods, and dynamic and uncertainty properties of HG captured methods, etc. Besides shallow methods, deep GNN is a developing topic in recent years. Self-supervised learning and pre-training are emerged topics in GNN. And we point out that they are also worth exploring in HGNN. Moreover, to further deepen the reliability of HG representation methods in more key fields, it is important to integrate extra knowledge to make HG representation methods more fair, robust, explainable, and stable. Last but not least, we believe that exploring more potential industrial applications of HG representation methods holds great promising in the further.

10.2 Preserving HG Structures

The basic success of HG representation builds on the HG structure preservation. This also motivates many HG representation methods to exploit different HG structures, where the most typical one is meta-path [9, 32]. Following this line, meta-graph structure is naturally considered [43]. However, HG is far more than these structures. Selecting the most appropriate meta-path is still very challenging in the real world. An improper meta-path will fundamentally hinder the performance of HG representation method. Whether we can explore other techniques, e.g., motif [44, 16] or network schema [45] to capture HG structure is worth pursuing. Moreover, if we rethink the goal of traditional graph representation, i.e., replacing the structure information with the distance/similarity in a metric space, a research direction to explore is whether we can design a HG representation method which can naturally learn such distance/similarity rather than using pre-defined meta-path/meta-graph.

10.3 Capturing HG Properties

As mentioned before, many current HG representation methods mainly take the structures into account. However, some properties, which usually provide additional useful information to model HG, have not been fully considered. One typical property is the dynamics of HG, i.e., a real world HG always evolves over time. Despite that the incremental learning on dynamic HG is proposed [39], dynamic HG representation is still facing big challenges. For example, [2] is only proposed with a shallow model, which greatly limits its representation ability. How can we learn dynamic HG representation in deep learning framework is worth pursuing. The other property is the uncertainty of HG, i.e., the generation of HG is usually multi-faceted and the node in a HG contains different semantics. Traditionally, learning a vector representation usually cannot well capture such uncertainty. Gaussian distribution may innately represent the uncertainty property [18, 47], which is largely ignored by current HG representation methods. This suggests a huge potential direction for improving HG representation.

10.4 Deep Graph Learning on HG Data

We have witnessed the great success and large impact of GNNs, where most of the existing GNNs are proposed for homogeneous graph [19, 35]. Recently, HGNNs have attracted considerable attention [38, 42, 11, 7].

One natural question may arise that what is the essential difference between GNNs and HGNNs. More theoretical analysis on HGNNs are seriously lacking. For example, it is well accepted that the GNNs suffer from over-smoothing problem [20], so will heterogeneous GNNs also have such problem? If the answer is yes, what factor causes the over-smoothing problem in HGNNs since they usually contain multiple aggregation strategies [38, 42]. Moreover, some researchers have derived the generalization bounds for GNNs [31, 30] and analyzed the key factors dominating the generalization error. Hence, a natural question is arisen. What is the key factors influencing the generalization ability of HG representation methods? Metapath or the aggregation function?

In addition to theoretical analysis, new technique design is also important. One of the most important directions is the self-supervised learning. It uses the pretext tasks to train the neural networks, thus reducing the dependence on manual labels. [22]. Considering the actual demand that label is insufficient, self-supervised learning can greatly benefit the unsupervised and semi-supervised learning, and has shown remarkable performance on homogeneous graph representation [36, 33, 26, 41]. Therefore, exploring self-supervised learning on HG representation is expected to further facilitate the development of this area.

Another important direction is the pre-training of HGNNs [15, 28]. Nowadays, HGNNs are designed independently, i.e., the proposed method usually works well for some certain tasks, but the transfer ability across different tasks is ill-considered.

When dealing with a new HG or task, we have to train a HG representation method from scratch, which is time-consuming and requires large amounts of labels. In this situation, if there is a well pre-trained HGNN with strong generalization that can be fine-tuned with few labels, the time and label consumption can be reduced.

10.5 Making HG Representation Reliable

Except from the properties and techniques in HG, we are also concerned about the ethical issues in HG representation, such as fairness, robustness and interpretability. Considering that most methods are black boxes, making HG representation reliable is an important future work.

Fair HG Representation. The representations learned by methods are sometimes highly related to certain attributes, e.g., age or gender, which may amplify the societal stereotypes in the prediction results [4, 10]. Therefore, learning fair or de-biased representations is an important research direction. There are some researches on the fairness of homogeneous graph representation [4, 29]. However, the fairness of HG is still an unsolved problem, which is an important research direction in the further.

Robust HG Representation. Also, the robustness of HG representation, especially the adversarial attacking, is always an important problem [24]. Since many real world applications are built based on HG, the robustness of HG representation becomes an urgent yet unsolved problem. What is the weakness of HG representation and how to enhance it to improve the robustness need to be further studied.

Explainable HG Representation. Moreover, in some risk aware scenarios, e.g., fraud detection [14] and bio-medicine [6] , the explanation of models or representations is important. A significant advantage of HG is that it contains rich semantics, which may provide eminent insight to promote the explanation of heterogeneous GNNs. Besides, the emerging disentangled learning [25, 23], which divides the representation into different latent spaces to improve the interpretability, can also be considered. Learning post-explanation model for GNNs has attracted attention in recent years [27]. Then it is necessary to develop a post-explanation model for HGNNs to explain the prediction mechanism of these methods.

Stable HG Representation. Furthermore, most HG representation methods assume the training graph and testing graph are drawn from same distribution. However, this assumption is easily to be violated, as distribution shifts may arise from different environments that are common in real-world data collections pipelines, such as locations, times, experimental conditions, etc [13]. For considering the generalization ability of HG representation methods, it is necessary to improve the stability of HG representation methods under unknown testing environments. Causal variables and relations are deemed to be invariant across environments. Recently, some literatures aimed to discovery such variables in representation learning [1]. It will be a promising direction to marry causal learning with HG representation methods to enhance the stability of HG representation methods on agnostic environments.

10.6 Technique Deployment in Real-world Applications

Many HG-based applications have stepped into the era of graph representation. This survey has demonstrated the strong performance of HG representation methods on E-commerce and cybersecurity. Exploring more capacity of HG representation on other areas holds great potential in the future. For example, in software engineering area, there are complex relations among test sample, requisition form, and problem form, which can be naturally modeled as HG. Therefore, HG representation is expected to open up broad prospects for these new areas and become promising analytical tool. Another area is the biological systems, which can also be naturally modeled as a HG. A typical biological system contains many types of objects, e.g., gene expression, chemical, phenotype, and microbe. There are also multiple relations between gene expression and phenotype [34]. HG structure has been applied to biological system as an analytical tool, implying that HG representation is expected to provide more promising results. For another area, transportation prediction, the data usually consists of heterogeneous objects, such car, traffic light, etc, and exists in a spatiotemporal format, so it is natural to model such complex data with HG while considering the spatiotemporal information.

In addition, since the complexity of HGNNs are relatively large and the techniques are difficult to parallelize, it is difficult to apply the existing HGNNs to large-scale industrial scenarios. For example, the number of nodes in E-commerce recommendation may reach one billion [46]. Therefore, successful technique deployment in various applications while resolving the scalability and efficiency challenges will be very promising.

10.7 Others

Last but not least, there are also some important future work that cannot be summarized in the previous sections. Therefore, we carefully discuss them in this section.

Hyperbolic Heterogeneous Graph Representation. Some recent researches point out that the underlying latent space of graph may be non-Euclidean, but in hyperbolic space [5]. Some attempts have been made towards hyperbolic graph/heterogeneous graph representation, and the results are rather promising [8, 21, 40]. However, how to design an effective hyperbolic heterogeneous GNNs is still challenging, which can be another research direction.

Heterogeneous Graph Structure Learning. Under the current HG representation framework, HG is usually constructed beforehand, which is independent on the HG representation. This may result in that the input HG is not suitable for the final task. HG structure learning can be further integrated with HG representation, so that they can promote each other.

Heterophily Heterogeneous Graph Representation. Current HG representation methods focus on the leverage of network homophily. Due to recent research on homogeneous networks that study learning network representation on Heterophily network [3, 48], it would be interesting to find heterophily HG and explore how to generalize design principles and paradigms used in heterophily homogeneous network representation to HG representation.

Connections with Knowledge Graph. Knowledge graph representation has great potential on knowledge reasoning [17]. However, knowledge graph representation and HG representation are usually investigated separately. Recently, knowledge graph representation has been successfully applied to other areas, e.g., recommender system [12, 37]. It is worth studying that how to combine knowledge graph representation with HG representation, and incorporate knowledge into HG representation.

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