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Generalizing graph neural network across graphs and time

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ABSTRACT

Graph-structured data widely exist in diverse real-world scenarios, analysis of these graphs can uncover valuable insights about their respective application domains. However, most previous works focused on learning node representation from a single fixed graph, while many real-world scenarios require representations to be quickly generated for unseen nodes, new edges, or entirely new graphs. This inductive ability is essential for high-throughtput machine learning systems. However, this inductive graph representation problem is quite difficult, compared to the transductive setting, for that generalizing to unseen nodes requires new subgraphs containing the new nodes to be aligned to the neural network trained already. Meanwhile, following a message passing framework, graph neural network (GNN) is an inductive and powerful graph representation tool. We further explore inductive GNN from more specific perspectives: (1) generalizing GNN across graphs, in which we tackle with the problem of semi-supervised node classification across graphs; (2) generalizing GNN across time, in which we mainly solve the problem of temporal link prediction; (3) generalizing GNN across tasks; (4) generalizing GNN across locations.

CCS CONCEPTS

• **Information systems** → **Data mining**; • **Computing methodologies** → Neural networks.

KEYWORDS

Graph-structured data, graph neural network, inductive

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1 INTRODUCTION

Graph-structured data widely exist in diverse real-world scenarios, such as social networks, e-commerce graphs, citation graphs, and biological networks. Analysis of these graphs can uncover valuable insights about their respective application domains [1]. And effective analytics can bring benefits for lots of applications, *i.e.*, node classification, node recommendation, link prediction and so on. For instance, by analysing a graph of social network (*e.g.*, Facebook/Twitter/Wechat), we can classify users, recommend friends, and predict whether an interaction will happen between two users.

Although graph analytics is beneficial and essential, most existing graph analytics approaches suffer the high space and computation cost. To conduct the expensive graph analytics, lots of approaches have been proposed, including the new space-efficient graph storage [6], the distributed graph data processing framework (*e.g.*, GraphX [3], GraphLab [8]), and so on.

Additionally, graph representation learning provides an effective way to the graph analytics problem. To be more specific, graph representation learning transforms a graph into a low dimensional space in which the graph information is preserved as much as possible. After representing a graph into a set of low dimensional vectors, the downstream graph algorithms can then be computed efficiently.

However, most previous works focused on learning node representation from a single fixed graph, while many real-world scenarios require representations to be quickly generated for unseen nodes, new edges, or entirely new graphs. This inductive ability [4] is essential for high-throughtput machine learning systems, operating on evolving graphs and constantly meeting unseen nodes (*e.g.*, posts on Wikipedia, users and items on Amazon). Besides, an inductive approach can also facilitates generalization across graphs with the same form of features: for instance, one can train a neural network on protein-protein interaction graphs derived from a model organism, and then easily produce node representations for graphs from the new organisms, by using the trained model.

This inductive graph representation problem is quite difficult, compared to the transductive setting, for that generalizing to unseen nodes requires new subgraphs containing the new nodes to be aligned to the neural network trained already. Meanwhile, following a message passing framework, in which each node receives, maps and aggregates messages from its neighboring nodes in multiple layers to generate its own embedding vector, graph neural network (GNN) [12] is an inductive and powerful graph representation tool. And my main exploration is improving the generalization of GNNs.

2 PRESENTED WORK

Generalizing GNN across graphs. For semi-supervised node classification [5] across graphs, recent graph neural networks (GNNs) integrate node features with network structures, thus enabling inductive node classification models that can be applied to new nodes or even new graphs in the same feature space. However, inter-graph differences still exist across graphs within the same domain. Thus, training just one global model (e.g., a state-of-the-art

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GNN) to handle all new graphs, whilst ignoring the inter-graph differences, can lead to suboptimal performance. In this work, we study the problem of inductive node classification across graphs. Unlike existing one-model-fits-all approaches, we propose a novel meta-inductive framework called MI-GNN [11] to customize the inductive model to each graph under a meta-learning paradigm. That is, MI-GNN does not directly learn an inductive model; it learns the general knowledge of how to train a model for semi-supervised node classification on new graphs. To cope with the differences across graphs, MI-GNN employs a dual adaptation mechanism at both the graph and task levels. More specifically, we learn a graph prior to adapt for the graph-level differences, and a task prior to adapt for the task-level differences conditioned on a graph. Extensive experiments on five real-world graph collections demonstrate the effectiveness of our proposed model.

Generalizing GNN across time. For temporal link prediction [2], in which a future edge containing old or new nodes will be predicted. However, most existing works resort to taking discrete snapshots of the temporal graph, or are not inductive to deal with new nodes, or do not model the exciting effects which is the ability of events to influence the occurrence of another event. In this work, We propose TREND [10], a novel framework for temporal graph representation learning, driven by TempoRal Event and Node Dynamics and built upon a Hawkes process-based graph neural network (GNN). TREND presents a few major advantages: (1) it is inductive due to its GNN architecture; (2) it captures the exciting effects between events by the adoption of the Hawkes process; (3) as our main novelty, it captures the individual and collective characteristics of events by integrating both event and node dynamics, driving a more precise modeling of the temporal process. Extensive experiments on four real-world datasets demonstrate the effectiveness of our proposed model.

3 ONGOING AND PROPOSED RESEARCH

Generalizing GNN across tasks. Web text classification is a fundamental research problem with many real-world applications, such as predicting the topics of online articles and the categories of e-commerce product descriptions. However, the so-called low-resource text classification, given no or few labeled samples, presents a serious concern for supervised learning. Meanwhile, many Web texts are inherently grounded on a network structure, such as a hyperlink/citation network for online articles, and a user-item purchase network for e-commerce products. These graph structures capture rich semantic relationships, which can potentially augment low-resource text classification. In this work, we propose a novel model called Graph-Grounded Pre-training and Prompt tuning (G2P2) to address low-resource Web text classification in a two-pronged approach: During pre-training, we propose three *graph interaction-based contrastive strategies*; during testing, we explore prompt tuning with *graph contexts-based initialization*. Extensive experiments on four real-world datasets demonstrate the strength of G2P2 in zero- and few-shot text classification in Web applications.

Generalizing GNN across locations. The social networks in different locations show different structures and semantics. There is a need to make different GNNs for different graphs. Meanwhile, graphs in real world tend to have large scales, *e.g.*, having more than one million nodes or edges. Hence, that training different GNNs for different graphs is not practical. In this work, we resort to the prompt learning [7] and designs customized prompts for graphs in different locations. Without training on each graphs, we still can get different GNNs by integrating different prompts with just one GNN.

4 RESEARCH ISSUES FOR DISCUSSION

Firstly, how do we design prompts for different downstream tasks, *e.g.*, node classification, graph classification to align them with the pre-trained GNN? Since the label-free pre-training task, like link prediction, is often different from downstream tasks, there is a gap between them.

Secondly, how do we design pre-training strategy as well as corresponding prompts for graph anomaly detection [9] in different locations? Anomaly detection is different from the common node classification task, *e.g.*, linked normal and abnormal nodes should have different embeddings in anomaly detection while linked nodes tend to get similar embeddings in common cases. Besides, graphs in different locations prefer different GNNs.

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REFERENCES

[1] Hongyun Cai, Vincent W Zheng, and Kevin Chen-Chuan Chang. 2018. A comprehensive survey of graph embedding: Problems, techniques, and applications. *TKDE* 30, 9 (2018), 1616–1637.
[2] Aswathy Divakaran and Anuraj Mohan. 2020. Temporal link prediction: A survey. *New Generation Computing* 38, 1 (2020), 213–258.
[3] Joseph E Gonzalez, Reynold S Xin, Ankur Dave, Daniel Crankshaw, Michael J Franklin, and Ion Stoica. 2014. {GraphX}: Graph Processing in a Distributed Dataflow Framework. In *11th USENIX symposium on operating systems design and implementation (OSDI 14)*. 599–613.
[4] Will Hamilton, Zhitao Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. In *NeurIPS*. 1024–1034.
[5] Thomas N Kipf and Max Welling. 2017. Semi-supervised classification with graph convolutional networks. In *ICLR*.
[6] Pradeep Kumar and H Howie Huang. 2016. G-store: high-performance graph store for trillion-edge processing. In *SC'16: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*. IEEE, 830–841.
[7] Pengfei Liu, Weizhe Yuan, Jinlan Fu, Zhengbao Jiang, Hiroaki Hayashi, and Graham Neubig. 2021. Pre-train, prompt, and predict: A systematic survey of prompting methods in natural language processing. *arXiv preprint arXiv:2107.13586* (2021).
[8] Yucheng Low, Joseph Gonzalez, Aapo Kyrola, Danny Bickson, Carlos Guestrin, and Joseph M Hellerstein. 2012. Distributed GraphLab: A Framework for Machine Learning and Data Mining in the Cloud. *Proceedings of the VLDB Endowment* 5, 8 (2012).
[9] Xiaoxiao Ma, Jia Wu, Shan Xue, Jian Yang, Chuan Zhou, Quan Z Sheng, Hui Xiong, and Leman Akoglu. 2021. A comprehensive survey on graph anomaly detection with deep learning. *IEEE Transactions on Knowledge and Data Engineering* (2021).
[10] Zhihao Wen and Yuan Fang. 2022. TREND: TempoRal Event and Node Dynamics for Graph Representation Learning. In *Proceedings of the ACM Web Conference 2022*. 1159–1169.
[11] Zhihao Wen, Yuan Fang, and Zemin Liu. 2021. Meta-Inductive Node Classification across Graphs. In *Proceedings of the International ACM SIGIR Conference on Research and Development in Information Retrieval*. 1219–1228.
[12] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. 2020. A comprehensive survey on graph neural networks. *IEEE TNNLS* 32 (2020), 4–24. Issue 1.