Letter from the Special Issue Editor

Graph Neural Networks (GNNs) have propelled the field of graph-based machine learning, unlocking new and innovative applications in various domains, such as natural language processing, drug discovery, recommendation systems, and social network analysis. By leveraging the graph structure and node features, GNNs capture intricate relationships and dependencies in complex networks, resulting in more accurate predictions and a deeper understanding of the data. These advancements have led to significant breakthroughs in drug design, personalized recommendations, and community detection in social networks. Moreover, GNNs' ability to model and analyze structured data has opened up new avenues for advancing artificial intelligence. Particularly, integrating GNNs with large language models (LLMs) will elevate their capabilities by incorporating world knowledge from LLMs and enabling natural language querying of graph-structured data. These advancements are poised to reshape the landscape of GNN research, paving the way for exciting possibilities and future advancements.

Despite their promise, GNNs have limitations. These include challenges in generalizing to unseen graph structures, scalability issues with large-scale graphs, difficulties in handling heterophily, limited interpretability resulting in black-box behavior, complexities in data requirements and feature engineering, as well as concerns regarding over-smoothing and potential loss of discriminative information. In this special edition, seven carefully selected papers address these limitations and offer insights into improving GNNs.

Graph based machine learning has been centered on the premise of similar nodes have a stronger relationship. Heterophily breaks this assumption. The first article by **Zhu et al.**, titled "Heterophily and Graph Neural Networks: Past, Present, and Future," investigates the performance of GNNs on graphs exhibiting heterophily. The authors review various GNN designs proposed for handling heterophilous graphs and explore their connections to research objectives like robustness, fairness, and over-smoothing avoidance. They emphasize the need for tailored GNN designs specific to heterophily.

Explainable GNN models are often necessary for legal, regulatory, and compliance purposes. Two articles in this edition focus on the explainability of GNN models. **Kakkad et al.**'s "A Survey on Explainability of Graph Neural Networks" offers a comprehensive overview of explainability techniques for GNNs, categorizing them based on objectives, methodologies, and application scenarios. **Rex Ying**'s paper, "Generative Explanation for Graph Neural Networks: Methods and Evaluation," proposes a unified optimization framework for generative explanation methods, highlighting the shared characteristics and distinctions among these approaches.

Representation learning is an important topic in GNN research, and this edition features two articles that delve into this topic. First, **Han et al.** presents a graph contrastive learning (GCL) framework aimed at learning graph representations of homogeneous, heterogeneous, and hypergraphs. They discuss improvements in principled view generation, which contribute to generalizability, fairness, and interpretability. Next, **Seshadri**'s paper highlights the limitations of low-dimensional embeddings in learning representations. The work presents theoretical underpinnings showing how low-dimensional embeddings cannot capture the fine-grained community structure of real-world data.

Finally, **Wang et al.** presents the concept of "Customized Graph Neural Networks." They propose a novel framework, Customized-GNN, which generates sample-specific GNN models for individual graphs based on their structures. The authors show the effectiveness of this framework through comprehensive experiments on various graph classification benchmarks.

We believe these seven articles offer a sample of the ongoing work, recent advances, and existing limitations in the field of GNN research. By exploring various aspects of GNNs, such as performance on heterophilous graphs, explainability techniques, generative explanations, graph contrastive learning, limitations of low-dimensional embeddings, and customized GNN frameworks, these articles contribute to a deeper understanding of GNNs and their potential applications. Our special thanks to **Yoachen Xie** for their feedback on selected submissions and to **Nurendra Choudhary** for their role as the web publication chair for this edition.

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