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LLM Output and Analysis: Applications and Evaluation of Graph Neural Networks

1. Introduction

Graph Neural Networks (GNNs) are a powerful class of neural networks that deal with graph-structured data. [1] Unlike traditional neural networks, GNNs are capable of addressing graph-structured problems. It is because in GNN, entities (nodes) and their relationships (edges) form a non-Euclidean space. The unique ability to process data with complex connections enables GNNs to solve a wide range of problems in fields like social networks, molecular chemical reactions, and natural language processing (NLP).

1. Applications and Target Users

GNNs can be applied in several fields, including Natural Language Processing, social networks, citation networks, molecular biology, chemistry, physics, and NP-hard combinatorial optimization problems. [2] Users in these fields include:

Data Scientists and Social Scientists. Social Media data and Interpersonal relationships tend to be complicated and connected. Those working with network-based data, such as social networks, leverage GNNs for tasks like node classification, link prediction, and graph classification. [3]

Chemists and Biologists. Chemical reactions and biological processes, like protein reactions and gene expressions have specific paths and patterns. Hence, the data obtained is likely to have connections with each other. In these cases, GNNs can perform better naturally than other kinds of neural networks. They are crucial for molecular property prediction, drug discovery, and protein interaction studies by modeling atomic and molecular structures as graphs. [4]

NLP and Knowledge Graph Practitioners. GNNs power question-answering systems, content summarization, and text classification by modeling words or documents as graphs to capture semantic relationships. [5]

To sum up, GNNs have their applications in diverse fields requiring a strong ability to analyze graph-structured data, and playing pivotal roles in domains like social networking, healthcare, and Machine Learning research.

1. Outcome of ChatGPT About the GNN

When querying ChatGPT about Graph Neural Networks, it provided several valuable insights and detailed information below.

* 1. Graph Data Representation:

Graphs represent data in nodes (entities) and edges (relationships). Examples include social networks (people and their connections), molecules (atoms and bonds), and citation networks (papers and references).

Traditional neural networks (CNNs, RNNs) struggle with irregular graph structures because they expect data in fixed-size grid formats.

* 1. Reason for Invention:

Many real-world problems involve graph-structured data. Standard neural networks cannot effectively capture relationships and dependencies in non-Euclidean spaces, like graphs. GNNs were invented to generalize deep learning to this complex data type.

They allow us to process relational data, improving tasks like node classification, link prediction, and graph classification.

* 1. What Makes GNNs Special:

Relational Learning: GNNs excel at learning the structure of relationships between entities (nodes). They aggregate information from neighbors, making them powerful for tasks where relationships matter, such as predicting molecular properties.

Permutation Invariance: Unlike traditional methods, GNNs are invariant to the ordering of nodes, making them ideal for graph data where node positions aren't fixed.

Generalization: GNNs generalize well to various types of graphs and can work on variable-sized inputs, making them versatile across domains like chemistry, biology, social networks, and recommendation systems.

ChatGPT’s outcome showcased comprehensive and accurate descriptions of GNN applications and capabilities, emphasizing its ability to process complex relational data better than traditional neural networks.

1. Analysis of the Outcome from ChatGPT

ChatGPT provides a well-rounded overview of Graph Neural Networks (GNNs), covering various domains and applications. It explains both technical aspects, such as graph convolution, and high-level use cases like drug discovery and fraud detection. The model’s ability to convey GNN concepts in a simple and clear manner makes it accessible to non-experts, while its versatility allows it to address different levels of expertise, from introductory topics to advanced issues like over-smoothing in deeper architectures.

However, there are some limitations to its explanations. While the breadth of information is strong, the depth is sometimes lacking, particularly in theoretical foundations and cutting-edge research trends. For instance, more focus could be given to advanced architectures such as Graph Attention Networks (GATs) and Graph Isomorphism Networks (GINs). Additionally, the model rarely presents critical views, omitting discussions on scalability, overfitting, and handling noisy graph structures, which are important considerations for researchers.

Despite these limitations, ChatGPT proves effective for summarizing technical topics like GNNs, providing a useful starting point for exploration. It offers insight into general applications, helping narrow down areas for further study. However, given the rapid advancements in the field, cross-validation with recent literature is necessary to ensure up-to-date and accurate information.

For the next step of GNN, A more detailed exploration of GNN limitations, such as over-smoothing and performance issues on large graphs, is also needed. Finally, conducting empirical studies on real-world tasks like node classification and link prediction will help assess the practical performance of GNN models and guide future research.

1. List of Papers

After searching the Internet, I have found several articles about GNN foundations and their applications in academics. *Understanding and bridging the gaps in current GNN performance optimizations* [6] can help me better understand what GNN is and its basic algorithms; *GNNLab: a factored system for sample-based GNN training over GPUs* [7] will lead me through the implementation of such networks and let me see the results; *Deep learning for fake news detection: A comprehensive survey* [8] gives me an application field in fake news detection where I decided to research deeper in this course.

By focusing on these papers, I will deepen my understanding of GNN architectures and their practical applications, and I will go further to find myself progressing in graph neural network.

1. Reference

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[4] H. Cai, H. Zhang, D. Zhao, J. Wu, and L. Wang, “FP-GNN: a versatile deep learning architecture for enhanced molecular property prediction,” Briefings in Bioinformatics, vol. 23, no. 6, Sep. 2022, doi: <https://doi.org/10.1093/bib/bbac408>

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