Topological Features for Graph Representations

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Graphs have been used as a powerful tool for representing various structured and complex data, including social networks, knowledge graphs, and protein–protein interaction networks, etc. in the field of machine learning [1]. For example, to encode a social network as a graph, nodes represent individual users, while edges represent the relationships between nodes, such as friends or colleagues. However, extracting effective representations from a given graph is always a challenge. Precisely, a graph representation can convert high-dimensional, sparse graph-structured data into low-dimensional, dense vectors.

Designing expressive graph representations is a central topic in graph-structured data. For a representation to be truly effective, it must assign distinct representations to non-isomorphic graphs; otherwise, non-isomorphic graphs may exhibit similar features, leading to confusion and ambiguous tasks. For example, the classic Weisfeiler–Lehman (WL) test assesses the expressive power of graph representations, which finds real applications in graph neural networks. However, typical message-passing neural networks were pointed out its limited expressiveness [2, 3]. On the other hand, applying higher-order WL variants [3] has demonstrated enhanced expressive capabilities while suffering from severe computation costs.

Very recently, Zhang et al. [4] revealed that most existing graph representations cannot effectively distinguish the presence of cut vertices or edges, resulting in a challenge to identify complex graph structures. They thus introduced the Generalized Distance Weisfeiler-Lehman (GD-WL) to better represent the topology features of a graph by encoding the distance information (e.g., shortest path distance or resistance distance) to represent topological structures more effectively.

In this study, we consider more topological features, such as centrality measures, to better understand the topology characteristics of given graphs. We aim to quantify the similarity between nodes across different graphs, by extracting topological features and conducting pairwise graph alignment. We believe the approach could pave the way for distinguishing two highly similar but non-isomorphic graphs.

Keywords: graph isomorphism, topological feature, centrality, graph representation

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