Guest Editorial Emerging Trends and Advances in Graph-Based Methods and Applications

I. Motivations and Objectives

THE integration of graph structures in diverse domains has recently garnered substantial attention, presenting a paradigm shift from classical euclidean representations. This new trend is driven by the advent of novel algorithms that can capture complex relationships through a class of neural architectures: the Graph Neural Networks (GNNs) [1], [2]. These networks are adept at handling data that can be effectively modeled as graphs, introducing a new representation learning paradigm. The significance of GNNs extends to several domains, including computer vision [3], [4], natural language processing [5], chemistry/biology [6], physics [7], traffic networks [8], and recommendation systems [9].

Despite their success, several challenges persist in proving the effectiveness of graph-based solutions compared to vector-based algorithms in certain domains, hence prompting the exploration of novel algorithms of deep learning on graphs [2]. Indeed, scalability is a major bottleneck in the use of graphs in practical applications, as most proposed algorithms have been primarily designed for sparse graphs. However, much effort has been devoted to addressing scalability issues, including heuristic methods, approximate solutions, and the use of massively parallel and distributed architectures. Moreover, the shift from euclidean space representations to graph-based paradigms poses notable challenges in terms of computing adaptability, which require exploration. Even memory usage considerations, such as inefficiencies in managing allocated memory with large sparse matrices representing graphs and the lack of a locality principle in memory access, significantly impact the performance of most graph algorithms. These problems have raised the question of whether this inefficiency is intrinsic to the graph-based representation or whether it stems from inadequacies in the algorithmic models designed for such data structures.

To address these concerns, the exploration of novel algorithms and models that incorporate deep learning in graphs has emerged as a promising avenue. In particular, learning graph representations including deep graph embeddings, CNN generalizations to graph-structured data [4], and neural message-passing approaches [3] have recently witnessed a surge in research and interest. The purpose of this special section is to provide a platform for exploring graph-based methods and learning approaches across applications, fostering discussions on techniques, achievements, and open challenges. We hope that this special section will serve as a catalyst for continued research in this area, with the aim of promoting the establishment of reliable and efficient solutions that significantly advance the state of the art.

II. Contributions

Contributions submitted to this special section can be broadly grouped into four major categories, namely *Graph Representation Learning*, *Drug Repurposing and Network Biology*, *Action Segmentation and Computer Vision* and *Other Applications*.

Graph Representation Learning. This category gathers the contributions dealing with the problem of learning meaningful and informative representations of graph-structured data able to capture the inherent properties and relationships of the graph, eventually enabling downstream machine learning tasks, such as node classification, link prediction, or graph classification, to be performed more effectively.

In this group, we have the work titled *HDGCN: Dual-channel graph convolutional network with higher-order information for robust feature learning* by He et al. It proposes HDGCN, a dual-channel Graph Convolutional Network for robust feature learning, able to incorporate higher-order information. The model extracts features from higher-order positive and negative graphs, alongside conventional GCN features. A feature fusion function transforms node features into edge features, and a fractional staggered negative sampling method improves topological feature capture. Extensive experiments demonstrate HDGCN's state-of-the-art performance in pairwise link prediction, higher-order structure prediction, and node classification across various real-world datasets. The paper emphasizes HDGCN's robustness in handling diverse tasks and attributes.

In the contribution titled *Graph Reconfigurable Pooling for Graph Representation Learning*, Li et al. propose RecPool, a novel approach for graph representation learning, that addresses tasks such as graph classification, link prediction, and node classification. The authors highlight the fact that commonly adopted methods for graph-level representations may overlook the role of nodes or substructures in the graph composition process. To address this, the paper proposes a new pooling operator called RecPool which probabilistically models the feature distribution of a coarsened graph, constructs feature distributions for each cluster, and resamples features back into original nodes based on a soft assignment matrix. The reconstructed graph is optimised by clustering nodes that play similar roles in the composition process. Experimental results on four benchmark datasets showcase RecPool's performance, offering a promising alternative for graph representation learning.

The paper *Edgeless-GNN: Unsupervised Representation Learning for Edgeless Nodes* by Shin et al. addresses the

Digital Object Identifier 10.1109/TETC.2024.3374581

challenge of embedding edgeless nodes, such as new users entering a network, using graph neural networks (GNNs). Traditional GNNs struggle with edgeless nodes, as these nodes lack connections for message passing. The proposed Edgeless-GNN introduces an inductive framework for unsupervised learning, allowing GNNs to generate node embeddings for edgeless nodes. The approach involves constructing a proxy graph based on node attribute similarity, which serves as the GNN's computation graph. Model parameters are trained using the known network structure, and a topology-aware loss function guides the learning process by encoding positive, negative, and second-order relations between nodes. Inductive inference for edgeless nodes involves expanding the computation graph. Empirical evaluations demonstrate Edgeless-GNN's superiority over state-of-the-art inductive network embedding methods, effectiveness of the topology-aware loss function, robustness to incomplete node attributes, and linear scaling with graph size.

GNNs for Drug Repurposing and Network Biology. In the broad field of bioinformatics, GNNs can be applied to many different tasks. Specifically, three contributions to this special section dealt with the tasks of drug repurposing and network biology. Drug repurposing, also referred to as drug repositioning or drug reprofiling, is the process of uncovering new indications of approved or failed/abandoned compounds for use in a different disease, while network biology seeks to understand the structure and function of the interactions between macromolecules within complex biological systems by using the graph formalism.

In the paper titled *Fusing Higher and Lower-order Biological Information for Drug Repositioning via Graph Representation Learning*, Zhao et al. propose FuHLDR, a graph representation learning model able to exploit higher-order connectivity patterns within biological heterogeneous information networks (HINs). FuHLDR integrates both higher and lower-order biological information. Using a HIN, FuHLDR initially learns representations of drugs and diseases at a lower-order level, considering biological attributes and drug-disease associations through a graph convolutional network model. A meta-path-based strategy is then employed to derive higher-order representations involving associations among drugs, proteins, and diseases. The integrated representations fuse both higher- and lower-order information. Finally, FuHLDR uses a random vector functional link network to identify novel drug-disease associations. Experimental results on benchmark datasets demonstrate FuHLDR's superiority over several state-of-the-art drug repositioning models. Case studies of Alzheimer's disease and breast neoplasms showcase the ability of the model to leverage rich, higher-order biological information for improved accuracy in drug repositioning.

In a similar vein, *Deep Graph Networks for Drug Repurposing with Multi-Protein Targets* by Bacciu et al. analyses the problem drug repurposing during the early stages of the COVID-19 pandemic. The proposed GNN architecture combines structural and biological information to suggest a refined set of drugs with potential efficacy against unknown diseases. The main contribution lies in the repurposing of drugs against multiple proteins, deviating from the common single-drug/single-protein paradigm. The method employs graph embeddings to encode information about relevant proteins and drugs based on gene ontology data and structural similarities. The research provides a unified data repository for graph-based analysis, particularly for COVID-19 and drug repurposing studies. Empirical validation in a general drug repurposing setting demonstrates the method's superior generalization compared to single protein repurposing schemes.

In contrast, the work titled *Graph embedding techniques to predict missing links in biological networks: An Empirical Evaluation* by Teji et al. addresses the problem of modelling complex relationships among macromolecules within biological systems through Network Biology and graph formalism. Due to the expensive nature of wet lab experiments, potential links among macromolecules are typically predicted via computational tools. Conventional link prediction techniques, which rely on local network topology, often fail to adequately incorporate global structure. The paper explores graph representation learning, with the aim of describing entire graph properties through optimized, structure-preserving encoding of nodes or (sub)graphs into lower-dimensional vectors. The study evaluates the performance of ten state-of-the-art graph embedding techniques in predicting missing links, emphasizing both homogeneous and heterogeneous biological networks. Leveraging latent representations, the research reconstructs the network using various similarity and kernel functions, evaluating nine similarity functions in combination with embedding techniques. Comparative analysis against five traditional link prediction techniques demonstrates the superior predictive quality of embedding-based methods.

Action Segmentation and Computer Vision. This category collects two contributions which apply GNN architectures to Computer Vision (CV)-related tasks. Specifically, *Skeleton-Based Action Segmentation with Multi-Stage Spatial-Temporal Graph Convolutional Neural Networks* by Filtjens et al. focuses on the task of identifying and temporally segmenting fine-grained actions in motion capture sequences for applications in human movement analysis. Traditional motion capture systems encode human movement as a time series of joint locations and orientations. Existing state-of-the-art action segmentation approaches rely on multiple stages of temporal convolutions, generating initial predictions and refining them through subsequent stages. According to the authors, these approaches often neglect the spatial hierarchy among human joints. To this end, the paper introduces Multi-Stage Spatial-Temporal Graph Convolutional Neural Networks (MS-GCN) to replace the initial temporal convolutions with spatial graph convolutions and dilated temporal convolutions to better capture the spatial configuration of joints and their long-term temporal dynamics. Comparative experiments with four baselines on five tasks demonstrate that MS-GCN serves as a robust baseline for skeleton-based action segmentation.

Another CV-related task which is gaining increasing popularity is related to suggesting complementary clothing items to compose an outfit. In the work titled *Transformer-based Graph Neural Networks for Outfit Generation*, Becattini et al. explore such task by merging outfit recommendation and generation. Unlike previous works that focused on scoring visual appeal or pairwise compatibility, this research introduces a novel approach by leveraging a graph-based representation of clothing items. The proposed transformer-based architecture, named TGNN, employs multiheaded self-attention to capture relations between clothing items within a graph, utilizing Convolutional Graph Neural Networks for message passing. Starting with a seed garment or garments, the model iteratively generates outfits by selecting the most compatible items. Experiments conducted

on two datasets showcase the model's ability for seeded outfit generation and achieving state-of-the-art results in compatibility estimation tasks.

Other Applications. This group collects three separate papers demonstrating that GNNs and other graph-based computational tools can be effective when applied to tasks in extremely different scenarios. Álvarez-Ayllón et al. in the work titled *PresQ: Discovery of Multidimensional Equally-Distributed Dependencies via Quasi-Cliques on Hypergraphs*, address the challenge of cross-matching data from separate files, particularly in the scientific domain where the relationship between attributes may not be evident. Drawing inspiration from techniques used for discovering foreign keys in relational databases, the paper introduces Equally-Distributed Dependencies (EDD), akin to Inclusion Dependencies in the relational domain. To bridge existing concepts, the authors propose PresQ, a novel algorithm based on searching for maximal quasi-cliques on hypergraphs. This algorithm aims to enhance robustness in handling uncertain numerical data. Tested on three public datasets, PresQ exhibits promising results in efficiently identifying multidimensional equally-distributed attribute sets, showcasing its potential for practical applications.

The paper *Coupled Attention Networks for Multivariate Time Series Anomaly Detection* by Xia et al. introduces a Coupled Attention Network (CAN), designed for effective Multivariate Time Series Anomaly Detection (MTAD). Addressing challenges arising from changing dependencies among sensors and variables over time, CAN combines adaptive graph learning techniques with graph attention. This enables the creation of a global-local graph that captures both global and dynamic local correlations among sensors. To model intersensor relationships and temporal dependencies, a coupled attention module integrates a convolutional neural network based on the global-local graph with a temporal self-attention module. The proposed multi-level encoder-decoder architecture accommodates both reconstruction and prediction tasks, enhancing the characterization of multivariate time series data. Extensive experiments on real-world datasets demonstrate that CAN outperforms state-of-the-art baselines, highlighting its effectiveness in addressing the complexities of MTAD.

Lastly, the work *MFDS-STGCN: Predicting the Behaviors of College Students with Fine-Grained Spatial-Temporal Activities Data* by Zhou et al. introduces MFDS-STGCN, a novel predictive model for college students' behaviors utilizing fine-grained campus spatial-temporal activities data. Traditional methods often employ shallow learning algorithms, lacking the ability to capture long-term spatial-temporal dependencies and semantic correlations. MFDS-STGCN addresses this limitation by leveraging a multiple fragment dynamic semantic spatial-temporal graph convolution network, built upon a spatial-temporal graph convolutional network (STGCN). The proposed model shows superior performance in predicting general and abnormal behavior of college students compared to multiple baseline methods.

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ACKNOWLEDGMENT

The authors thank the authors and reviewers for their valuable work in helping us assemble this special issue. The authors express our gratitude to Prof. D. Conte for his contribution the Special Section management, and to Prof. G. Grossi and Dr. V. Cuculo for their efforts to promote the Special Section. The authors extend our thanks to the Editor-in-Chief, Prof. Paolo Montuschi, for providing this opportunity and guidance throughout the process, as well as to Prof. Ronald DeMara, and the editorial staff for their continued support and professionalism.

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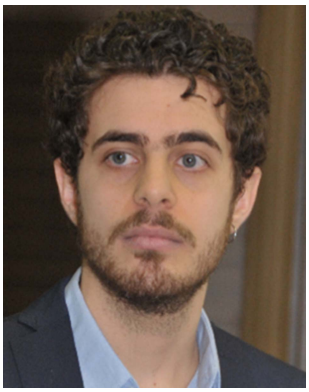

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