Guest editorial. Deep neural networks for graphs: theory, models, algorithms, and applications

Guest Editorial: Deep Neural Networks for Graphs: Theory, Models, Algorithms and Applications

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I. Introduction

Deep neural networks for graphs (DNNGs) represent an emerging field that studies how the deep learning method can be generalized to graph-structured data. Since graphs are a powerful and flexible tool to represent complex information in form of patterns and their relationships, ranging from molecules to protein-to-protein interaction networks, to social or transportation networks, or up to knowledge graphs, potentially modelling systems at very different scales, these methods have been exploited for many application domains.

Since the pioneering works on trees, namely Recursive Neural Networks [1], [2], and directed acyclic graphs [3], [4], up to methods extended to general graphs, both by recursive approaches (namely Graph Neural Networks (GNNs) [5], [6]), or Graph Convolutional Network approaches (namely NN4Gs [7], GCNs, etc.), a plethora of neural models for graphs have been proposed [8], [9]. Moreover, beyond the pure neural networks paradigm, the term Deep Graph Networks (DGNs) has been introduced to include also the class of Bayesian-based and generative graph networks [9]. In particular, after 2015 a broader class of models have been introduced and in their various incarnations, DNNGs and DGNs have become a topic of intense research by the remarkable ability of graph representations in learning tasks such as node classification, graph classification, graph generation and link prediction. To witness the interest in the field, numerous surveys have appeared, e.g. [8], [9], and the survey paper [8] has received the 2024 IEEE TNNLS Outstanding Paper Award.

However, this area of research and applications is still highly vibrant and constantly growing [10]. Indeed, the increasing number of works in DNNGs and related areas indicates that both academic and industrial communities have still a considerable demand for developing more advanced technology and algorithms, consider also the inclusion of trustworthy concepts in the model design, theoretical foundations, tools and platforms for real-world applications, including practical scenarios, such as large-scale, dynamic, ambiguous graphs, etc.

This special issue would contribute to collecting advancements in the field, focusing on new challenges for fully exploiting the potential of DGN approaches. The special issue received over 140 submissions, out of which 40 were chosen for publication. These selected papers are categorically divided into three groups: (a) theoretical research, (b) innovative methodologies, including models and algorithms that enhance deep neural networks for graphs, GNNs, Graph Representation Learning, and similar fields, and (c) a diverse range of applications in areas like computer vision, recommendation systems, community detection, molecular generation, multivariate time series forecasting, etc.

A. Theoretical Studies

Salim and Sumitra [11] revisited the state-of-the-art filter designs for spectral GCNs (SGCNs) in the context of regularization theory, and based on this principle, they explored various optimization strategies for SGCNs, design challenges, and recent developments in the field. Pasa et al. [12] reexamined graph spectral filtering theory, conducting a theoretical analysis of straightforward graph convolution operators with varying complexity, based on linear transformations or controlled nonlinearities, suitable for implementation in single-layer GCNs. Li et al. [13] advanced geometric deep learning on spheres by introducing CNNs for spherical signal processing, utilizing area-regular spherical Haar tight framelets. Fan et al. [14] theoretically demonstrated that selection bias in DNNGs inevitably leads to a biased correlation between the aggregation mode and class label, which drastically hinders the model's generalization ability.

B. Models and Algorithms

Cui et al. [15] introduced a series of aligned vertex convolutional network models designed to learn multiscale features from local-level vertices, specifically for the purpose of graph classification. He et al. [16] proposed an unsupervised heterogeneous graph contrastive learning approach, HGCA, specifically designed for analyzing heterogeneous information networks with missing attributes. He et al. [17] introduced a novel end-to-end parallely adaptive graph convolutional clustering model, which replaces the fixed, pre-trained graph in GCNs with an adaptive graph learned directly from the data through two pathway networks. Wang et al. [18] introduced

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a new framework to mitigate the over-smoothing problem encountered in DNNGs. Their model involves selectively dropping edges based on their 'edge strength', defined by the frequency with which an edge serves as a bridge on the shortest path between pairs of nodes. To address the channel mixing issue and lower the over-fitting risk inherent in traditional GCN models, Zhang et al. [19] developed the scale graph convolution technique, which leverages channel-wise scale transformation for extracting node features. Fan et al. [14] demonstrated how selection bias significantly impedes the generalization capabilities of DNNGs and proposed a novel debiased GCN with a differentiated decorrelation regularizer to mitigate this bias in GCN estimation. Wang et al. [20] proposed a parallel graph deep learning approach using the Alternating Direction Method of Multipliers (pdADMM-G), which enables simultaneous parameter updates across each layer of GA-MLP models, facilitating model parallelism. Sun et al. [21] proposed a new graph embedding model, i.e., attribute force-based graph (AGForce), which effectively preserves structural information while adaptively integrating attribute data into node features. In [22], the authors introduced a graph navigated dual attention network for zero-shot learning, designed to learn discriminative visual embeddings that facilitate accurate visual-semantic interactions, thus enabling efficient knowledge transfer from seen to unseen classes. Peng et al. [23] introduced a reverse graph learning framework for GCNs, capable of generating high-quality graphs for enhanced feature learning, and featuring a novel out-of-sample extension method that enables both supervised and semi-supervised learning applications. Eliasof et al. [24] developed an efficient compression technique for GCNs that combines the use of compressed Haar wavelets with quantization methods. Yang et al. [25] proposed a revised mutual information maximization framework, termed Channel Capacity Maximization (CapMax), designed to learn informative representations for dynamic networks characterized by time-varying topology and evolving node attributes. Zheng et al. [26] addressed the challenges of encoding nodes' transition structures by introducing transition propagation GCNs that include a transition propagation module and a bilevel graph convolution module, enabling the adaptive and dynamic generation of temporal node embeddings through diverse interactions. Lin et al. [27] developed a status-aware graph neural network tailored for directed signed graphs, incorporating a loss function derived from status theory, i.e., a social-psychological approach specifically formulated for these types of graphs. Ai et al. [28] introduced a two-level DNNG framework designed to concurrently capture microscopic (small scale) and macroscopic (large scale) structural information, thereby enhancing the overall representation of a graph. Lin et al. [29] introduced a framework of structure-aware prototypical neural process for few-shot graph classification (FSGC), marking, to our knowledge, the first attempt to approach FSGC through the lens of neural process. Zhao et al. [30] uncovered that contrastive learning essentially functions as a type of learning to rank, and from this viewpoint, they introduced a coarse-to-fine contrastive Learning framework on graphs, incorporating a self-ranking paradigm to ensure the preservation of discriminative information across different nodes and to reduce the impact of perturbations of various magnitudes. Cui et al. [31] introduced DyGCN, an efficient dynamic embedding framework for GCN-based methods, designed to update node embeddings in dynamic graphs efficiently while maintaining performance. Spinelli et al. [32] developed an algorithm within a meta-learning framework to enhance the explainability of a GNN during its training phase. Joshi et al. [33] explored GNN representation distillation with a focus on maintaining global topology, introducing the first contrastive distillation technique for DNNGs. Their method, known as graph contrastive representation distillation, trains student networks to implicitly retain the global topology found in the teacher's node embedding space. In recent years, graph drawing techniques aimed at creating aesthetically pleasing node-link layouts have been developed. Tiezzi et al. [34] introduced a new framework for creating Graph Neural Drawers (GNDs), which are machines utilizing neural computation to construct efficient and complex maps. GNDs are a type of DNNG that can be trained using various loss functions, including those typically used in graph drawing.

C. Applications

As DNNGs and graph representation learning rapidly evolve, community detection emerges as a research field of growing practical importance. For those interested in further exploration, we recommend the survey paper [35]. In [36], Android entities and their behavioral relationships are represented as a heterogeneous information network, utilizing its complex semantic meta-structures to define implicit high-order relationships. Ding et al. [37] proposed a causal incremental graph convolution approach for the problem solving of GCN model retraining for the recommendation. Seo et al. [38] introduced an innovative GCN-aided recommender system that optimally utilizes user-item interaction data following the construction and partitioning of a signed graph. Liu et al. [39] developed a new adversarial defense mechanism tailored for DNNG-based multivariate time series forecasting, capable of effectively counteracting adversarial attacks while maintaining local information. In [40], the authors developed a discrete hashing method for cross-modal retrieval using a graph convolutional network. This method includes a GCN-based unified classifier module that explores label-implicit information to improve feature representation for cross-modal hashing. In the context of online multi-agent forecasting, the authors in [41] introduced a new collaborative prediction unit, designed to combine predictions from various collaborative predictors based on a collaborative graph. For skeleton-based action recognition, Qin et al. [42] introduced a novel framework that combines GCNs with angular encoding of high-order features, aiming to robustly discern the interconnections between joints and body segments. Du et al. [43] developed a novel method for 3D point cloud semantic segmentation, using a local-global graph convolutional approach that constructs local graphs and applies a self-attention mechanism to generate adjacency matrices with short-range dependencies. Huang et al. [44] introduced a dual-graph attention convolution network for 3D point cloud classification, designed to simultaneously learn both low-level extrinsic and

high-level intrinsic graph features within point clouds. In [45], the authors developed a mutually supervised graph attention network tailored for few-shot segmentation, aimed at optimizing the use of a limited quantity of annotated samples. Wang et al. [46] presented a graph-based contrastive learning approach for the description and detection of local features, a technique that significantly enhances the accuracy of correspondence establishment in sequential images, a critical aspect in various computer vision tasks. For the task of molecular generation, Li et al. [47] proposed an effective geometric embedding approach, encompassing the spatial structure representations of drug molecules by transforming their 3-D coordinates into images, and the geometric graph representations of protein targets by modeling the protein surface as a mesh. In the context of functional connectivity prediction, Etemadyrad et al. [48] developed a deep learning approach for graph transformation, incorporating additional meta-features through a newly developed graph neural network-based generative model. Ling et al. [49] created a GCN-based model for survival analysis that not only generates survival predictions but also identifies local neighborhoods. This is achieved by employing multiple sparse geometric graphs constructed directly from high-dimensional features. The authors in [50] introduced an innovative framework that effectively combines the structural patterns and individual node representations in retweeting trees for the purpose of detecting rumors.

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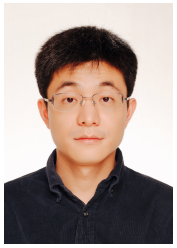

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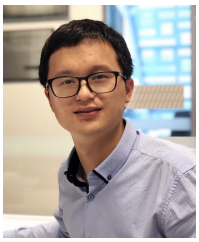

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