Exploiting Edge Features in Graph Neural Networks

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Abstract

Edge features contain important information about graphs. However, current state-of-the-art neural network models designed for graph learning, e.g. graph convolutional networks (GCN) and graph attention networks (GAT), adequately utilize edge features, especially multi-dimensional edge features. In this paper, we build a new framework for a family of new graph neural network models that can more sufficiently exploit edge features, including those of undirected or multi-dimensional edges. The proposed framework can consolidate current graph neural network models; e.g. graph convolutional networks (GCN) and graph attention networks (GAT). The proposed framework and new models have the following novelties: First, we propose to use doubly stochastic normalization of graph edge features instead of the commonly used row or symmetric normalization approches used in current graph neural networks. Second, we construct new formulas for the operations in each individual layer so that they can handle multi-dimensional edge features. Third, for the proposed new framework, edge features are adaptive across network layers. As a result, our proposed new framework and new models can exploit a rich source of graph information. We apply our new models to graph node classification on several citation networks, whole graph classification, and regression on several molecular datasets. Compared with the current state-of-the-art methods, i.e. GCNs and GAT, our models obtain better performance, which testify to the importance of exploiting edge features in graph neural networks.

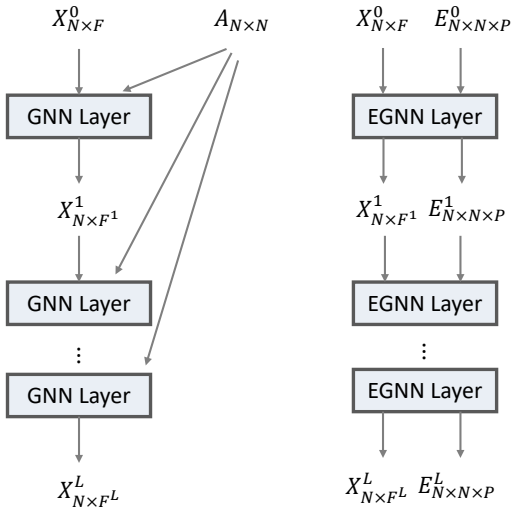


Figure 1: Schematic illustration of the proposed edge enhanced graph neural network (EGNN) architecture (right), compared with the original graph neural network (GNN) architecture (left). An GNN layer could be a GCN layer, or a GAT layer, while a EGNN layer is an edge enhanced counterpart of it. EGNN differs from GNN structurally in two folds. Firstly, the adjacency matrix A in GNN is either a binary matrix that indicates merely the neighborhood of each node and is used in GAT layers, or a positive-valued matrix that has one dimensional edge features and is used in GCN layers; in contrast, EGNN uses it with the multi-dimensional positive-valued edge features represented as a tensor E which may exploit multiple attributes associated with each edge. Secondly, in GNN the same original adjacency matrix A is fed to every layer; in contrast, the edge features in EGNN are adapted at each layer before being fed to next layer.

1. Introduction

Deep neural networks have become one of the most successful machine learning techniques in recent years. In many important problems, they achieve state-of-the-art performance, e.g., covolutional neural networks (CNN) [19] in image recognition, recurrent neural networks (RNN)[12] and Long Short Term Memory (LSTM) [14] in natural language processing, etc. In real world, many problems can be naturally modeled with graphs rather than conventional tables, grid type images or time sequences. Generally, a graph contains nodes and edges, where nodes represent entities in real world, and edges represent interactions or relation-

ships between entities. For example, a social network naturally models users as nodes and friendship relationships as edges. For each node, there is often an asscociated feature vector describing it, e.g. a user's profile in a socail network. Similarly, each edge is also often associated with features depicting relationship strengths or other properties. Due to their complex structures, a challenge in machine learning on graphs is to find effective ways to incorporate different sources of information contained in graphs into models such as neural networks.

Recently, several neural network models have been developed for graph learning, which obtain better performance than traditional techniques. Inspired by graph Fourier transform, Defferrard et al. [11] propose a graph covolution operation as an analogue to standard convolutions used in CNN. Just like the convolution operation in image spatial domain is equivalent to multiplication in the frequency domain, covolution operators defined by polynomials of graph Laplacian is equivalent to filtering in graph spectral domain. Particularly, by applying Chebyshev polynomials to graph Laplacian, spatially localized filtering is obtained. Kipf et al. [18] approximate the polynomials using a re-normalized first-order adjacency matrix to obtain comparable results on graph node classification. Those graph covolutional networks (GCNs) [11][18] combine graph node features and graph topological structural information to make predictions. Velickovic et al. [27] adopt attention mechanism into graph learning, and propose a graph attention network (GAT). Unlike GCNs, which use a fixed or learnable polynomial of Laplacian or adjacency matrix to aggregate (filter) node information, GAT aggregates node information by using an attention mechanism on graph neighborhoods. The essential difference between GAT and GCNs is stark: In GCNs the weights for aggregating (filtering) neighbor nodes are defined by the graph topological strcuture, which is independent on node contents; in contrast, weights in GAT are a function of node contents due to the attention mechanism. Results on graph node classification show that the adaptiveness of GAT makes it more effective to fuse information from node features and graph topological structures.

One major problem in the current GNN models such as GAT and GCNs is that edge features are not fully incorporated. In GAT, graph topological information is injected into the model by forcing the attention coefficient between two nodes to zero if they are not connected. Therefore, the edge information used in GAT is only the indication about whether there is an edge or not, i.e. connectivities. However, graph edges are often in possession of rich information like strengths, types, etc. Instead of being a binary indicator variable, edge features could be continous, e.g. strengths, or multi-dimensional. GCNs can utilize one-dimensional real value edge features, *e.g.* edge weights, but the edge features are restricted to be one-diemansional. Properly addressing this problem is likely to benefit many graph learning problems. Another problem of GAT and GCNs is that each GAT or GCN layer filters node features based on the original adjacency matrix that is given as an input. The original adjacency matrix is likely to be noisy and not optimal, which will limit the effectiveness of the filtering operation.

In this paper, we address the above problems by proposing new GNN models to more adequately exploit edge information, which naturally enhance current GCNs and GAT models. Our models construct different formulas from those of GCNs and GAT, so that they are capable of exploiting multi-dimensional edge features. Also our new models can exploit one-dimensional edge features more effectively by making them adaptive across network layers. Moreover, our models leverage doubly stochastic normalization to augment the GCNs and GAT models that use ordinary row or symmetric edge normalization. Doubly stochastic matrices have nice properties that can facilitate the use of edges.

We conduct experiments on several citation network datasets and molecular datasets. For citation networks, we encode directed edges as three dimensional edge feature vectors. For molecular datasets, different atom bond types are naturally encoded as multi-dimensional edge attributes. By leveraging those multi-dimensional edge features our methods outperform current state-of-the-art approches. The results confirm that edge features are important for graph learning, and our proposed EGAT model effectively incorporates edge features.

As a summary, the novelties of our proposed EGAT model include the following:

- A new framework for adequately exploiting multi-dimensional edge features. Our new framework is able to incorporate multi-dimensional positive-valued edge features. It eliminates the limitation of GAT which can handle only binary edge indicators and the limitation of GCNs which can handle only one dimensional edge features.

- Doubly stocahstic edge normalization. We propose to normalize edge feature matrices into doubly stochastic matrices which show improved performance in denoising [29].

- Attention based edge adaptiveness across neural network layers. We design a new graph network architecture which can not only filter node features but also adapt edge features across layers. Leveraging this new architecture, in our model the edge features are adaptive to both local contents and the global layers when passing through the layers of the network.

- Multi-dimensional edge features for directed edges. We propose a method to encode edge directions

as multi-dimensional edge features. Therefore, our EGAT can effectively learn on directed graph data.

The rest of this paper is organized as follows: Section 2 briefly reviews the related works. Details of the proposed EGNN architecture and two types of proposed EGNN layers are described in Section 3. Section 4 presents the experimental results, and Section 5 concludes the paper.

2. Related works

A critical challenge in graph learning is the complex non-Euclidean structure of graph data. To address this challenge, traditional machine learning approaches extract graph statistics (e.g. degrees) [5], kernel functions [28][24] or other hand-crafted features which measure local neighborhood structures. Those methods lack flexibility in that designing sensible hand-crafted features is time consuming and extensive experiments are needed to generalize to different tasks or settings. Instead of extracting structural information or using hand-engineered statistics as features of the graph, graph representation learning attempts to embed graphs or graph nodes in a low-dimensional vector space using a data-driven approach. One kind of embedding approaches are based on matrix-factorization, e.g. Laplacian Eigenmap (LE) [4], Graph Factorization (GF) algorithm [2], GraRep [7], and HOPE [21]. Another class of approaches focus on employing a flexible, stochastic measure of node similarity based on random walks, e.g. DeepWalk [22], node2vec [2], LINE [26], HARP [9], etc. There are several limitations in matrix factorization-based and random walk-based graph learning approaches. First, the embedding function which maps to low-dimensional vector space is linear or overly simple so that complex pattern cannot be captured; Second, they typically do not incorporate node features; Finally, they are inherently transductive, for the whole graph structure is required in the training phase.

Recently these limitations in graph learning have been addressed by adopting new advances in deep learning. Deep learning with neural networks can represent complex mapping functions and be efficiently optimized by gradient-descent methods. To embed graph nodes to a Euclidean space, deep autoencoders are adopted to extract connectivity patterns from the node similarity matrix or adjacency matrix, e.g. Deep Neural Graph Representations (DNGR) [8] and Structural Deep Network Embeddings (SDNE) [30]. Although autoencoder based approaches are able to capture more complex patterns than matrix factorization based and random walk based methods, they are still unable to leverage node features.

With celebrated successes of CNN in image recognition, recently, there has been an increase interest in adapting convolutions to graph learning. In [6], the convolution operation is defined in the Fourier domain, that is, the spectral space, of the graph Laplacian. The method is afflicted by two major problems: First, the eigen decomposition is computationally intensive; second, filtering in the Fourier domain may result in non-spatially localized effects. In [13], a parameterization of the Fourier filter with smooth coefficients is introduced to make the filter spatially localized. [11] proposes to approximate the filters by using a Chebyshev expansion of the graph Laplacian, which produces spatially localized filters, and also avoids computing the eigenvectors of the Laplacian.

Attention mechanisms have been widely employed in many sequence-based tasks [3][33][16]. Compared with convolution operators, attention machanisms enjoy two benefits: Firstly, they are able to aggregate any variable sized neighborhood or sequence; further, the weights for aggregation are functions of the contents of a neighborhood or sequence. Therefore, they are adaptive to the contents. [27] adapts an attention mechanism to graph learning and proposes a graph attention network (GAT), achieving current state-of-the-art performance on several graph node classification problems.

3. Edge feature enhanced graph neural networks

3.1. Architecture overview

Given a graph with N nodes, Let X be an $N \times F$ matrix representation of the node features of the whole graph. We denote an element of a matrix or tensor by indices in the subscript. Specifically, the subscript $\cdot$ is used to select the whole range (slice) of a dimension. Therefore, X_{ij} will represent the value of the j^{th} feature of the i^{th} node. $X_{i\cdot} \in \mathbb{R}^F, i = 1, 2, \ldots, N$ represents the F dimensional feature vector of the i^{th} node. Similarly, let E be an $N \times N \times P$ tensor representing the edge feautres of the graph. Then $E_{ij\cdot} \in \mathbb{R}^P, i = 1, 2, \ldots, N; j = 1, 2, \ldots, N$ represents the P-dimensional feature vector of the edge connecting the i^{th} and j^{th} nodes, and E_{ijp} denotes the p^{th} channel of the edge feature in $E_{ij\cdot}$. Without loss of generality, we set $E_{ij\cdot} = \mathbf{0}$ to mean that there is no edge between the i^{th} and j^{th} nodes. Let $\mathcal{N}_i, i = 1, 2, \ldots, N$ be the set of neighboring nodes of node i.

Our proposed network has a multi-layer feedforward architecture. We use superscript l to denote the output of the l^{th} layer. Then the inputs to the network are X^0 and E^0. After passing through the first EGAT layer, X^0 is filtered to produce an $N \times F^1$ new node feature matrix X^1. In the mean time, edge features are adapted to E^1 that preserves the dimensionality of E^0. The adapted E^1 is fed to the next layer as edge features. This procedure is repeated for every subsequent layer. Within each hidden layer, nonlinear activations can be applied to the filtered node features X^l. The node features X^L can be considered as an embe-

ding of the graph nodes in an F^L-dimensional space. For a node classification problem, a softmax operator will be applied to each node embedding vector $X^L_{i\cdot}$ along the last dimension. For a whole-graph prediction (classification or regression) problem, a pooling layer is applied to the first dimension of X^L so that the feature matrix is reduced to a single vector embedding for the whole graph. Then a fully connected layer is applied to the vector, whose output could be used as predictions for regression, or logits for classification. The weights of the network will be trained with supervision from ground truth labels. Figure 1 gives a schematic illustration of the EGNN architecture with a comparison to the existing GNN architecture. Note that the input edge features in E^0 are already pre-normalized. The normalization method will be described in the next subsection. Two types of EGNN layers, attention based EGNN (EGNN(A)) layer and convolution based EGNN (EGNN(C)) layer will also be presented in the following subsections.

3.2. Doubly stocahstic normalization of edges

In graph convolution operations, the edge feature matrices will be used as filters to multiply the node feature matrix. To avoid increasing the scale of output features by multiplication, the edge features need to be normalized. Let $\hat{E}$ be the raw edge features, our normalized features E is produced as follows:

$$\tilde{E}_{ijp} = \frac{\hat{E}_{ijp}}{\sum_{k=1}^{N} \hat{E}_{ikp}} \tag{1}$$

$$E_{ijp} = \sum_{k=1}^{N} \frac{\tilde{E}_{ikp}\tilde{E}_{jkp}}{\sum_{v=1}^{N} \tilde{E}_{vkp}} \tag{2}$$

Note that all elements in $\hat{E}$ are positive. It can be easily verified that such kind of normalized edge feature tensor E satisfys the following properties:

$$E_{ijp} \geq 0, \tag{3}$$

$$\sum_{i=1}^{N} E_{ijp} = \sum_{j=1}^{N} E_{ijp} = 1. \tag{4}$$

In other words, the edge feature matrices $E_{\cdot\cdot p}$ for $p = 1, 2, \cdots, P$ are square nonnegative real matrices with rows and columns sum to 1. Thus, they are doubly stochastic matrices, *i.e*. they are both left stochastic and right stochastic. Mathematically, a stationary finite Markov chain with a doubly stochastic transition matrix will have a uniform stationary distribution. Since in a multi-layer graph neural network, the edge feature matrices will be repeatedly multiplied across layers, doubly stocahstic normalization could help stablize the process, compared with the previously used row normalization as in GAT [27]:

$$E_{ijp} = \frac{\hat{E}_{ijp}}{\sum_{j=1}^{N} \hat{E}_{ijp}} \tag{5}$$

or symmetric normalization as in GCN [18]:

$$E_{ijp} = \frac{\hat{E}_{ijp}}{\sqrt{\sum_{i=1}^{N} \hat{E}_{ijp}}\sqrt{\sum_{j=1}^{N} \hat{E}_{ijp}}} \tag{6}$$

The effectiveness of doubly stochastic matrix has been recently demostrated for graph edges denoising [29].

3.3. EGNN(A): Attention based EGNN layer

We describe the attention based EGNN layer. The original GAT model [27] is only able to handle one dimensional binary edge features, *i.e*., the attention mechanism is defined on the node features of the neighborhood, which does not take the real valued edge features, *e.g*. weights, into account. To address the problem of multi-dimensional positive real-valued edge features, we propose a new attention mechanism. In our new attention mechanism, feature vector $X^l_{i\cdot}$ will be aggregated from the feature vectors of the neighboring nodes of the i^{th} node, i.e. $\{X_j, j \in \mathcal{N}_i\}$, by simultaneously incorporating the corresponding edge features, where $\mathcal{N}_i$ is the indices of neighbors of the i^{th} node. Utilizing the matrix and tensor notations and the fact that zero valued edge features mean no edge connections, the aggregation operation is defined as follows:

$$X^l = \sigma\left[\Big\|_{p=1}^{P}\left(\alpha^l_{\cdot\cdot p}(X^{l-1}, E^{l-1}_{\cdot\cdot p})g^l(X^{l-1})\right)\right]. \tag{7}$$

Here σ is a non-linear activation; α is a function which produces an $N \times N \times P$ tensor and $\alpha_{\cdot\cdot p}$ is its p channel matrix slice; g is a transformation which maps the node features from the input space to the output space, and usually a linear mapping is used:

$$g^l(X^{l-1}) = W^l X^{l-1}, \tag{8}$$

where W^l is an $F^l \times F^{l-1}$ parameter matrix.

In Eq. (7), α^l is the so-called attention coefficients, whose specific entry α^l_{ijp} is a function of $X^{l-1}_{i\cdot}$, $X^{l-1}_{j\cdot}$ and E_{ijp}, the p^{th} feature channel of the edge connecting the two nodes. In existing attention mechanisms [27], the attention coefficient depends on the two points $X_{i\cdot}$ and $X_{j\cdot}$ only. Here we let the attention operation be guided by edge features of the edge connecting the two nodes, so α depends on edge features as well. For multiple dimensional edge features, we consider them as multi-channel signals, and each channel will guide a separate attention operation. The results from different channels are combined by the concatenation operation. For a specific channel of edge features,

our attention function is chosen to be the following:

$$\alpha^l_{\cdot\cdot p} = \mathrm{DS}(\hat{\alpha}^l_{\cdot\cdot p}), \tag{9}$$

$$\hat{\alpha}^l_{ijp} = f^l(X^{l-1}_{i\cdot}, X^{l-1}_{j\cdot})E^{l-1}_{ijp}, \tag{10}$$

where DS is the doubly stochastic normalization operator defined in Eqs. (1) and (2). f^l could be any ordinary attention function which produces a scalar value from two input vectors. In this paper, we use a linear function as the attention function for simplicity:

$$f^l(X^{l-1}_{i\cdot}, X^{l-1}_{j\cdot}) = \exp\left\{\mathrm{L}\left(a^T[WX^{l-1}_{i\cdot} \| WX^{l-1}_{j\cdot}]\right)\right\}, \tag{11}$$

where L is the LeakyReLU activation function; W is the same mapping as in (8); $\|$ is the concatenation operation.

The attention coefficients will be used as new edge features for the next layer, *i.e.*,

$$E^l = \alpha^l. \tag{12}$$

By doing so, EGNN adapts the edge features across the network layers, which helps capture essential edge features as determined by our new attention mechanism.

3.4. EGNN(C): Convolution based EGNN layer

Following the fact that graph convolution operation is a special case of graph attention operation, we derive our EGNN(C) layer from the formula of EGNN(A) layer. Indeed, the essential difference between GCN[18] and GAT[27] is whether we use the attention coefficients (*i.e.* matrix α) or adjacency matrix to aggregate node features. Therefore, we derive EGNN(C) by replacing the attention coefficient matricies $\alpha_{\cdot\cdot p}$ with corresponding edge feature matrices $E_{\cdot\cdot p}$. The resulting formula for EGNN(C) is expressed as follows:

$$X^l = \sigma\left[\Big\|_{p=1}^{P}\left(E_{\cdot\cdot p}X^{l-1}W^l\right)\right], \tag{13}$$

where the notations have the same meaning as in Section 3.3.

3.5. Edge features for directed graph

In real world, many graphs are directed, i.e. each edge has a direction associated with it. Often times, edge direction contains important information about the graph. For example, in a citation network, machine learning papers sometimes cite mathematics papers or other theoretical papers. However, mathematics papers may seldom cite machine learning papers. In many previous studies including GCNs and GAT, edge directions are not considered. In their experiments, directed graphs such as citation networks are treated as undirected graphs. In this paper, we show in the experiment part that discarding edge directions will lose important information. By viewing directions of edges as a kind of edge features, we encode a directed edge channel E_{ijp} to be

$$\begin{bmatrix} E_{ijp} & E_{jip} & E_{ijp} + E_{jip} \end{bmatrix}.$$

Therefore, each directed channel is augmented to three channels. Note that the three channels define three types of neighborhoods: forward, backward and undirected. As a result, EGNN will aggregate node information from these three different types of neighborhoods, which contains the direction information. Taking the citation network for instance, EGNN will apply the attention mechanism or convolution operation on the papers that a specific paper cited, the papers cited this paper, and the union of the former two. With this kind of edge features, different patterns in different types of neighborhoods can be effectively captured.

4. Experimental results

For all the experiments, We implement the algorithms in Python within the Tensorflow framework [1]. Because the edge and node features in some datasets are highly sparse, we further utilize the sparse tensor functionality of Tensorflow to reduce the memory requirement and computational complexity. Thanks to the sparse implementation, all the datasets can be efficiently handled by a Nvidia Tesla K40 graphics card with 12 Gigabyte graphics memory.

4.1. Citation networks

To benchmark the effectiveness of our proposed model, we apply it to the network node classification problem. Three datasets are tested: Cora [23], Citeseer [23], and Pubmed [20]. Some basic statistics about these datasets are listed in Table 1. All the three datasets are directed graphs,

Table 1: Summary of citation network datasets

	Cora	Citeseer	Pubmed
# Nodes	2708	3327	19717
# Edges	5429	4732	44338
# Node Features	1433	1433	3703
# Classes	7	6	3

where edge directions represent the directions of citations. For Cora and Citeseer, node features contains binary indicators representing the occurrences of predefined keywords in a paper. For Pubmed, term frequency-inverse document frequency (TF-IDF) features are employed to describe the network nodes (*i.e.* papers).

The three citation network datasets are also used in [32] [18] [27]. However, they all use a pre-processed version

Table 2: Classification accuracies on citation networks. Mehods with suffix "-D" mean no doubly stochastic normalization, thus using row normalization in EGNN(A) and using symmetric normalization in EGNN(C). Similarly, "-M" means ignoring multi-dimensional edge features (*i.e.*, using undirected one-dimensional edge features); "-A" means no adaptiveness across layers; "*" means the model is trained using weighted loss which takes the class-imbalance of training sets into account.

Dataset	Cora		CiteSeer		Pubmed	
Splitting	Sparse	Dense	Sparse	Dense	Sparse	Dense
GCN	$72.9 \pm 0.8\%$	$72.0 \pm 1.2\%$	$69.2 \pm 0.7\%$	$75.3 \pm 0.4\%$	$83.3 \pm 0.4\%$	$83.4 \pm 0.2\%$
GAT	$75.5 \pm 1.1\%$	$79.0 \pm 1.0\%$	$69.5 \pm 0.5\%$	$74.9 \pm 0.5\%$	$83.4 \pm 0.1\%$	$83.4 \pm 0.2\%$
GCN*	$82.7 \pm 0.6\%$	$87.6 \pm 0.6\%$	$69.3 \pm 0.6\%$	$76.0 \pm 0.5\%$	$84.5 \pm 0.2\%$	$84.3 \pm 0.4\%$
GAT*	$82.7 \pm 0.6\%$	$86.6 \pm 0.6\%$	$69.4 \pm 0.5\%$	$74.9 \pm 0.8\%$	$83.1 \pm 0.2\%$	$82.7 \pm 0.2\%$
EGNN(C)-M	$81.8 \pm 0.5\%$	$85.1 \pm 0.5\%$	$\mathbf{70.6} \pm 0.3\%$	$75.0 \pm 0.3\%$	$84.3 \pm 0.1\%$	$84.1 \pm 0.1\%$
EGNN(C)-D	$80.2 \pm 0.4\%$	$86.1 \pm 0.5\%$	$69.4 \pm 0.3\%$	$76.8 \pm 0.4\%$	$\mathbf{86.2} \pm 0.2\%$	$\mathbf{86.7} \pm 0.1\%$
EGNN(C)	$83.0 \pm 0.3\%$	$\mathbf{88.8} \pm 0.3\%$	$69.5 \pm 0.3\%$	$76.7 \pm 0.4\%$	$86.0 \pm 0.1\%$	$86.0 \pm 0.1\%$
EGNN(A)-D-M	$76.0 \pm 1.0\%$	$79.1 \pm 1.0\%$	$69.5 \pm 0.4\%$	$74.6 \pm 0.3\%$	$83.4 \pm 0.1\%$	$83.6 \pm 0.2\%$
EGNN(A)-A-M	$80.1 \pm 1.0\%$	$85.4 \pm 0.5\%$	$70.1 \pm 0.4\%$	$74.7 \pm 0.4\%$	$84.3 \pm 0.2\%$	$84.2 \pm 0.1\%$
EGNN(A)-A-D	$81.7 \pm 0.4\%$	$87.9 \pm 0.4\%$	$69.4 \pm 0.3\%$	$75.7 \pm 0.3\%$	$85.5 \pm 0.1\%$	$86.0 \pm 0.1\%$
EGNN(A)	$82.5 \pm 0.3\%$	$88.4 \pm 0.3\%$	$69.4 \pm 0.4\%$	$76.5 \pm 0.3\%$	$85.7 \pm 0.1\%$	$\mathbf{86.7} \pm 0.1\%$
EGNN(C)-M*	$83.2 \pm 0.3\%$	$87.4 \pm 0.4\%$	$70.3 \pm 0.3\%$	$75.4 \pm 0.5\%$	$84.1 \pm 0.1\%$	$84.1 \pm 0.1\%$
EGNN(C)-D*	$82.3 \pm 0.4\%$	$87.2 \pm 0.4\%$	$69.4 \pm 0.3\%$	$\mathbf{77.1} \pm 0.4\%$	$\mathbf{86.2} \pm 0.1\%$	$86.4 \pm 0.3\%$
EGNN(C)*	$\mathbf{83.4} \pm 0.3\%$	$88.5 \pm 0.4\%$	$69.5 \pm 0.3\%$	$76.6 \pm 0.4\%$	$85.8 \pm 0.1\%$	$85.6 \pm 0.2\%$
EGNN(A)-D-M*	$82.6 \pm 0.6\%$	$86.3 \pm 0.9\%$	$69.4 \pm 0.4\%$	$74.9 \pm 0.4\%$	$83.7 \pm 0.2\%$	$82.8 \pm 0.3\%$
EGNN(A)-A-M*	$82.7 \pm 0.4\%$	$87.2 \pm 0.5\%$	$69.5 \pm 0.3\%$	$74.5 \pm 0.5\%$	$83.9 \pm 0.2\%$	$83.3 \pm 0.2\%$
EGNN(A)-A-D*	$82.8 \pm 0.3\%$	$87.0 \pm 0.6\%$	$69.1 \pm 0.3\%$	$76.3 \pm 0.5\%$	$85.2 \pm 0.2\%$	$85.3 \pm 0.3\%$
EGNN(A)*	$83.1 \pm 0.4\%$	$88.4 \pm 0.3\%$	$69.3 \pm 0.3\%$	$76.3 \pm 0.5\%$	$85.6 \pm 0.2\%$	$85.7 \pm 0.2\%$

which discards the edge directions. Since our EGNN models require the edge directions to construct edge features, we use the original version from [23] and [20]. For each of the three datasets, we split nodes into 3 subsets for training, validation and testing. Two splittings were tested. One splitting has 5%, 15% and 80% sized subsets for training, validation and test, respectively. Since it has a small training set, we call it "sparse" splitting. Another splitting has 60%, 20% and 20% sized subsets, which is called "dense" splitting.

Following the experiment settings of [18][27], we use two layers of EGNN in all of our experiments for fair comparison. Throughout the experiments, we use the Adam optimizer [17] with learning rate 0.005. An early stopping strategy with window size of 100 is adopted for the three citation networks; i.e. we stop training if the validation loss does not decrease for 100 consecutive epochs. We fix the output dimension of the linear mapping W to 64 for all hidden layers. Futhermore, we apply dropout [25] with drop rate 0.6 to both input features and normalized attention coefficients. L_2 regularization with weight decay 0.0005 is applied to weights of the model (i.e. W and a). Moreover, exponential linear unit (ELU) [10] is employed as nonlinear activations for hidden layers.

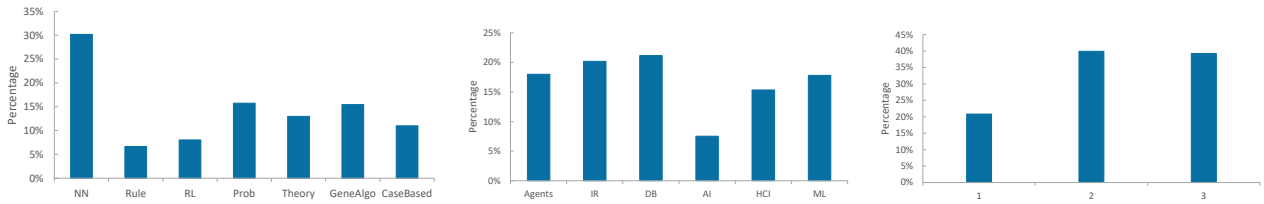
We notice that the class distributions of the training subsets of the three datasets are not balanced. To test the effects of dataset imbalanceness, we train each algorithm with two different loss functions, *i.e.* unweighted and weighted losses, then test performances of both. The weight of a node belonging to class k is calculated as

$$\frac{\sum_{k=1}^{K} n_k}{K n_k}, \tag{14}$$

where K and n_k are the numbers of classes and nodes belonging to the k^{th} class in the training subset, respectively. Basically, nodes in a minority class are given larger weights than a majority class, and thus are penalized more in the loss.

The baseline methods we used are GCN [18] and GAT [27]. To further investigate the effectivenesses of each components, *i.e.* doubly stochastic normalization, multi-dimensional edge features and edge adaptiveness, we also test different versions of EGNN(A) and EGNN(C) that keep only one component and discard the others. The performances are recorded for abalation study. Totally, 9 models are tested:

- GCN: baseline as described in [18].



(a) Cora (b) Citeseer (c) Pubmed

Figure 2: Node class distribution of the training subsets of the three citation networks. The Cora dataset is more imbalanced than the other two.

- GAT: baseline as described in [27].
- EGNN(C)-M: EGNN(C) variant which ignores multi-dimensional edge features, *i.e.*, it treats directed edges as undirected ones. Note that the doubly stocahstic normalization component is kept.
- EGNN(C)-D: EGNN(C) variant without doubly stochastic normalization.
- EGNN(C): Full EGNN(C) with doubly stochastic normalization and multi-dimensional edge features.
- EGNN(A)-D-M: EGNN(A) variant without doubly stochastic normalization as well as without multi-dimensional edge features.
- EGNN(A)-A-M: EGNN(A) variant without edge adaptiveness across layers as well as multi-dimensional edge features.
- EGNN(A)-A-D: EGNN(A) variant without edge adaptiveness across layers as well as doubly stochastic normalization.
- EGNN(A): Full EGNN(A) with all functionalities.

Note that each algorithm has both a weighted loss version and unweighted loss version.

We run each version of the algorithms 20 times, and record the mean and standard deviation of the classification accuracies, which are listed in Table 2. From the table, we can observe serval interesting phenomena which warrant further investigations:

- Overall, almost all EGNN variants outperform their corresponding baselines, which indicates that all the three components incorporate useful information for classification. Particularly, multi-dimensional edge features and doubly stochastic normalization improve more than edge adaptiveness.
- The two baselines fail on both the sparse and dense splittings of the Cora dataset. This is caused by the class imbalance of the Cora dataset. We illustrate the class distributions of the three datasets in Figure 2. From the distributions, we can see that Cora is more imbalanced than Citeseer and Pubmed.
- On the Cora dataset, the baselines with weighted loss perform normal. Again, this indicates that their failures are caused by the class imbalance.
- Our proposed methods are highly resistant to class imbalance. Without weighted training, our framework obtain high accuracies on the Cora dataset.
- Weighted training does not always improve performance, especially on less imbalanced datasets, e.g. Pubmed. This indicates that simply weighting the nodes is not sufficient to fully solve the class imbalance problem. Therefore, more sophisticated methods need to be designed to address this problem.
- Performances on dense splittings are consistently higher than on sparse splitting. It is not unexpected because more training data gives an algorithm more information to tune parameters.
- Either EGNN(C)-M* or EGNN(C)-D* is close to or a little bit worse than GCN* on the dense splitting of the Cora dataset. However, EGNN(C)* is considerably better than GCN*. This interesting phenomena indicates doubly stochastic normalization and multi-dimensional edge feature may not work well individually on some datasets, but can improve performance considerably if combined.

4.2. Molecular analysis

One promising application of graph learning is molecular analysis. A molecular can be represented as a graph, where each atom is a node, and chemical bonds are edges. Unlike citation network analysis in Section 4.1, the problem here is whole-graph prediction, either classification or regression. For example, given a graph representation of a molecular, the goal might be to classify it as toxic or not, or to predict the soluability (regression). In other words, we need to predict one value for the whole graph, rather

Table 3: Performance on molecular datasets

Dataset	Tox21 (AUC)		Lipo (RMSE)		Freesolv (RMSE)	
	Validation	Test	Validation	Test	Validation	Test
RF	0.78 ± 0.01	0.75 ± 0.03	0.87 ± 0.02	0.86 ± 0.04	1.98 ± 0.07	1.62 ± 0.14
Weave	0.79 ± 0.02	0.80 ± 0.02	0.88 ± 0.06	0.89 ± 0.04	1.35 ± 0.22	1.37 ± 0.14
EGNN(C)	$\mathbf{0.82} \pm 0.01$	$\mathbf{0.82} \pm 0.01$	0.80 ± 0.02	$\mathbf{0.75} \pm 0.01$	$\mathbf{1.07} \pm 0.08$	1.09 ± 0.08
EGNN(A)	$\mathbf{0.82} \pm 0.01$	0.81 ± 0.01	$\mathbf{0.79} \pm 0.02$	$\mathbf{0.75} \pm 0.01$	1.09 ± 0.12	$\mathbf{1.01} \pm 0.12$

than one value for a graph node. Usually, for each chemical bond, there are several attributes associated with it, *e.g.*, Atom Pair Type, Bond Order, Ring Status, etc. Therefore, the graphs intrinsically contain multi-dimensional edge features.

Three datasets (Tox21, Lipophilicity and Freesolv) are used to test our algorithms. Tox21 contains 7831 enviromental compounds and drugs. Each compound is associated with 12 labels, *e.g.* androgen receptor, estrogen receptor, and mitochondrial membrane potential, which defines a multi-label classification problem. Lipophilicity contains 4200 compounds. The goal is to predict compound soluability, which is a regression task. Freesolv includes a set of 642 neutral molecules, which similarly defines a regression task. For all the three datasets, compounds are converted to graphs. For all the three datasets, nodes are described by 25-d feature vectors. The dimensionality of edge feature vectors are 42, 21 and 25 for Tox21, Lipo, and Freesolv, respectively.

For both EGNN(A) and EGNN(C), we implement a network containing 2 graph processing layers, a global max-pooling layer, and a fully connected layer. For each graph processing layer, the output dimensions of the linear mapping g are fixed to be 16. For Tox21, sigmoid cross entropy losses are applied to the output logits of the fully connected layer. For Lipo and Freesolv, mean squared error losses are employed. The networks are trained by Adam optimizer [17] with learning rate 0.0005. An early stopping strategy with window size of 200 is adopted. L_2 regularization with weight decay 0.0001 is applied to parameters of the models except bias parameters. Moreover, exponential linear unit (ELU) [10] is employed as nonlinear activations for hidden layers.

Our methods are compared with two baseline models which are shown in MoleculeNet [31]: Random Forest and Weave. Random Forest is a traditional learning algorithm which is widely applied to various problems. Weave model [15] is similar to graph convolution but specifically designed for molecular analysis.

All the three datasets are split into training, validation and test subsets sized 80%, 10% and 10%, respectively. We run our models 5 times, and record the means and standard deviations of performance scores. For classification task (*i.e.*, Tox21), Area Under Curve (AUC) scores of the receiver operating characteristic (ROC) curve is recorded. Since it is a multi-label classification problem, we record the AUCs of each class and take the average value as the final score. For regression (*i.e.*, Lipo and Freesolv), root mean square error (RMSE) are recorded. We list the scores in Table 3. The results show that our EGNN(C) and EGNN(A) outperform the two baselines with considerable margins. On the Tox21 dataset, the AUC scores are improved by more than 0.2 compared with the Weave model. For the two regression tasks, RMSEs are improved by about 0.1 and 0.3 on the Lipo and Freesolv datasets, respectively. On the other hand, the scores of EGNN(C) and EGNN(A) are very close on the three datasets.

5. Conclusions

In this paper, we propose a new framework to address the existing problems in the current state-of-the-art graph neural network models. Specifically, we propose a new attention mechanism by generalizing the current graph attention mechansim used in GAT to incorporate multi-dimensional real-valued edge features. Then, based on the proposed new attention mechanism, we propose a new graph neural network architecture that adapts edge features across neural network layers. Our framework admits a formula that allows for extending convolutions to handle multi-dimensional edge features. Moreover, we propose to use doubly stochastic normalization, as opposed to the ordinary row normalization or symmetric normalization used in the existing graph neural network models. Finally, we propose a method to design multi-dimensional edge features for directed edges so that our model is able to effectively handle directed graphs. Extensive experiments are conducted on three citation network datasets for graph node classification evaluation, and on three molecular datasets to test the performance on whole graph classification and regression tasks. Experimental results show that our new framework outperforms current state-of-the-art models such as GCN and GAT consistently and significantly on all the datasets. Detailed abalation study also show the effectiveness of each

individual component in our model.

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