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Quantum-based Subgraph Convolutional Neural Networks

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Abstract

This paper proposes a new graph convolutional neural network architecture based on a depth-based representation of graph structure deriving from quantum walks, which we refer to as the *quantum-based subgraph convolutional neural network* (QS-CNNs). This new architecture captures both the global topological structure and the local connectivity structure within a graph. Specifically, we commence by establishing a family of K-layer expansion subgraphs for each vertex of a graph by quantum walks, which captures the global topological arrangement information for substructures contained within a graph. We then design a set of fixed-size convolution filters over the subgraphs, which helps to characterise multi-scale patterns residing in the data. The idea is to apply convolution filters sliding over the entire set of subgraphs rooted at a vertex to extract the local features analogous to the standard convolution operation on grid data. Experiments on eight graph-structured datasets demonstrate that QS-CNNs architecture is capable of outperforming fourteen state-of-the-art methods for the tasks of node classification and graph classification.

Keywords: Graph convolutional neural networks, spatial construction, quantum walks, subgraph.

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1. Introduction

Numerous problems (social networks, transport networks, protein-interaction networks, knowledge graphs, ...) involve data lying on irregular or non-Euclidean space that can be efficiently described with graph data structures, which are universal representations of heterogeneous pairwise relationships [1]. Graphs can encode complex geometric structures and can be studied using efficient machine learning techniques. Recently, numerous results have proven that deep learning methods provide an effective architecture for analyzing the large-scale and high-dimensional regular or Euclidean data. In particular, Convolutional Neural Networks (CNNs) [2] allow us to extract meaningful statistical patterns from large sets of data and this property allows them to gain significant improvement in image, sound and video recognition tasks [3], where the underlying data representation has a regular grid structure. When confronted by graph data-streams, on the other hand, one is confronted with irregular structures. Because such data is ubiquitous, there has been significant interest in the generalization of CNNs to graph data [1]. Unfortunately, this is not a straightforward problem since the basic operations of convolution, pooling and weight-sharing are only designed for regular grids. These three points make the application of CNNs to graph data streams both theoretically and implementally challenging.

There are two main strategies adopted in extending CNNs to non-lattice graphical structures, namely a) spectral and b) spatial methods. Spectral approaches draw on the properties of convolution operators in the graph Fourier domain and are related to the Laplacian matrix of the graph [4, 5, 6]. By transforming graphs into the spectral domain using the eigenvectors derived from the eigendecomposition of the graph Laplacian, graphs can be multiplied by an array of filter coefficients to perform a filtering operation. However, spectral approaches require each of the graphs samples in a particular problem to have the same number of nodes. Thus they are not directly transferable to different graphs of different size and having a different Fourier basis.

Spatial approaches, on the other hand, generalize the convolution using the

spatial structure of a graph by sliding a filter over the spatially neighboring vertices in a manner analogous to the convolution performed on images in standard CNNs [7, 8, 4, 9, 10]. This approaches however present two challenges, namely (1) the definition of a receptive field/neighborhood, because spatial convolutions are usually position dependent and lack a meaningful global interpretation and (2) how to implement weight sharing in a spatial structure with a variable number of adjacent neighbors adjacent and where the ordering of neighborhoods is not well defined.

To solve these problems, in this paper, we adopt a graph decomposition strategy based on quantum walks. When compared to their classical counterparts, quantum walks capture different aspects of the patterns of node connectivity in a graph via constructive and destructive interference. Here we use them to determine the nodes belonging of each receptive field used for convolution in a CNN. This can lead to the convolution operations being performed both more effectively and more efficiently. We commence by decomposing a graph into a family of K-layer m-ary expansion trees, each rooted at a unique vertex. We then scan a subgraph based window defined over an m-ary tree in a manner similar to the standard convolution operation on grid data (depicted in Figure 1). This allows us to extract structural features reflecting the local connectivity, and this in turn helps in capturing multi-scale patterns in the data. In particular, the convolution operation not only captures local structural information within the graph, but also exhibits weight sharing among the subgraphs. This results in a significant parameter reduction. The weight sharing is induced by a pooling operation that acts directly on the output of the preceding network layer, and without resorting to a preprocessing scheme (e.g., clustering or other techniques). Finally, we can learn a better representation for the purposes of prediction by simultaneously considering both the node features and graph structure information delivered by our subgraph convolution operation.

The remainder of this paper is organized as follows. In Section 2, we present related work and discuss the relationship between our proposed model QS-CNNs and alternative methods. In Section 3, we introduce some preliminary concepts

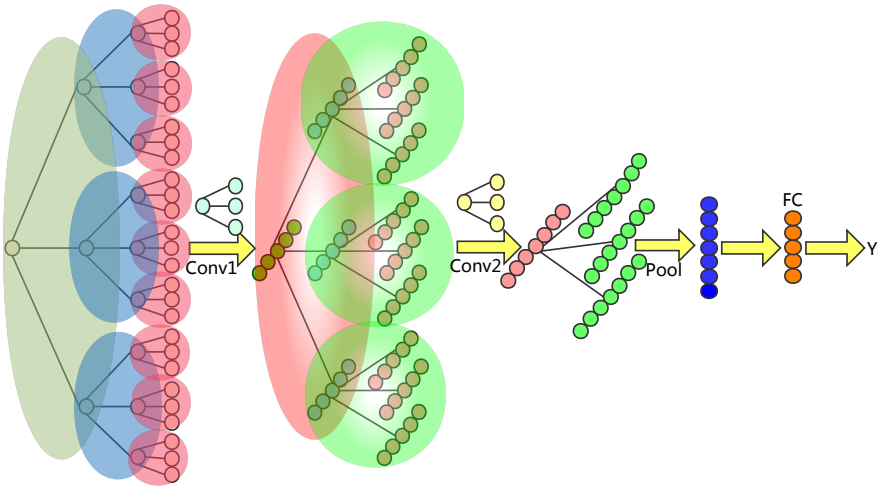

Figure 1: An illustrative example of our QS-CNNs with $K = 4$ and $m = 3$. The 'Conv' arrow depicts the convolution operation. The subgraph above the 'Conv' arrow represents a convolution kernel, extracting structural features along the tree. Then the extracted features are summarized by pooling operation.

that will be used for developing the work presented in this paper. In Section 4, we present a formal definition of the model, including descriptions of graph depth-based representation and graph learning procedures (i.e. subgraph convolution and pooling operations). This is followed by an experimental evaluation in Section 5 which explores the performance of QS-CNNs at node and graph classification tasks. Finally, conclusions and directions for future work are presented in Section 6.

2. Related Work

Most of the recent work on extending CNNs to non-lattice graphical structures fall into two broad categories a) spectral and b) spatial approaches.

2.1. Spectral Methods

Spectral approaches provide a well-defined localization operator on graphical data via convolutions in the spectral domain. Spectral graph theory defines

convolutions in terms of an array of filter coefficients multiplied by the graph signals, after transforming the graph signal to a spectral domain representation. Several authors propose graph CNN models that are based on this method of filtering [4, 6, 5]. For instance, Bruna et al. [4] and Henaff et al. [6] used a generalization of graph convolutions via the graph Fourier transform. Unfortunately, this involves the computationally expensive multiplication of node features with the eigenvector matrix of the graph Laplacian. Furthermore, computing the required eigenvector matrix is cubic in the number of vertices. To circumvent this problem, Defferrard et al. [11] have proposed an efficient filtering scheme which operates in the spectral domain by using Chebyshev polynomials, and which does not require explicit computation of the Laplacian eigenvectors. Instead, it uses the k^{th} order Chebyshev polynomials of Laplacian eigenvalues as the parameters of filters that act on k-hop neighbourhoods of the graph. This model was later simplified by Kipf and Welling [12] to use first order polynomials only for the task of semi-supervised nodes classification.

The major drawback of most spectral methods is that they are based on a spectral formulation of the convolution which uses the spectrum of graph Laplacian [13]. It is thus restricted to a fixed and regular graph structure, i.e. the graphs must have the same number of nodes and the nodes must have a fixed degree. This precludes applications on heterogeneous graph datasets, whose structure (number of nodes and nodes degrees) varies from sample to sample. Examples of such heterogeneous data include biochemical datasets.

To overcome these limitations of spectral methods, and considering the restrictions imposed by complexity, we formulate our approach in the spatial domain by using a depth-based representation of a graph. The main challenge here is to define a receptive field over the neighbourhoods and to specify how weights are shared between different local neighbourhoods [4]. Recently, quantum walks have provided a powerful way to solve this challenge. By analogy with a particle propagating on a graph structure, a quantum walk allows different paths interfere with each other in both constructive and destructive manner. This property exponentially speeds up the computation compared to other spectral

algorithms [14, 15]. As a consequence, quantum walkers can reach a vertex through multiple paths, thus the probability of visiting nodes in the neighbourhoods increases. This leads to the probability of identifying local neighbour structure more effectively and efficiently [16, 17].

2.2. Spatial Methods

As mentioned above, spatial approaches have the advantage over spectral approaches in that they can operate on problems where the graph structure varies in the dataset. However, they generally require sophisticated data transformations to enable effective learning. Bruna et al. [4] used a spatial method based on multi-scale clustering. Here the required convolutions are defined per cluster, without any weight sharing among neighbourhoods. Duvenaud et al. [9] on the other hand, have proposed a convolution-like propagation rule on graphs. This induces weight sharing among edges. Local filters are applied over neighbouring nodes. Another interesting example of a weight-sharing strategy has recently been suggested by Atwood and Towsley [10]. They perform a random walk on the graph in order to select spatially close neighbouring nodes. These nodes are used for the purposes of convolution. Weight sharing is controlled by the number of hops between two nodes. However, the convolution operations underpinning this method are related to the power series of the full transition matrix. Computing this series is computationally expensive, and thus limits its range of applications. In related work, Niepert et al. [7] use a node ordering step which converts graphs locally to a regular 1D grid so that a conventional 1D Euclidean CNN can be used. The main drawback of this method is that the 1D sequences extracted from the graphs discard large amounts of structural information about the detailed arrangement of the nodes. Thus, it does not replicate the standard convolution on regular grids. Moreover, this method [7] is limited since it is only designed for graph classification and does not admit any pooling operations.

In contrast to the previous research, we suggest a novel method which is implemented using subgraph convolution and pooling operators that capture both

the global topological and local connectivity structures within the graph. This allows the method to capture multi-scale patterns in the data. We implement the method by applying convolution filters that slide over the entire subgraphs of a vertex. In this way extract local features in a manner similar to the standard convolution operation on grid data. As a result, it induces weight sharing property. Moreover, our method can be applied to the tasks of both node and graphs classification, where pooling operations can be used.

3. Preliminary Concepts

In this section, we introduce some preliminary concepts that will be used for developing the work presented in this paper. To this end, we commence by introducing the background on convolutional neural networks. We then introduce the related basics of graph theory and quantum walks.

3.1. Convolutional Neural Networks

Convolutional neural networks (CNNs) introduce hidden convolution and pooling layers to identify localized features which are independent of spatial location via a set of rectangular filters. The convolution operator scans a set of 'square' kernel filters across a grid-structure as input, returning feature maps that represent the response to the filters. Given a multi-channel input, a feature map is the summation of the convolutions with separate kernels for each input channel. In the CNN architecture, the pooling operator is utilized to compress the spatial resolution of each feature map, leaving the number of feature maps unchanged. Applying a pooling operator across a feature map enables the algorithm to handle a large number of feature maps and, moreover, it generalizes the feature maps by resolution reduction. Common pooling operations are those of taking the average and the maximum of the receptive cells over the input map [18].

In order to extract input feature effectively for the convolution operation, we need to assume that there exists some locality structure for the spatial arrangement of the input. This means that the input signal should be highly correlated

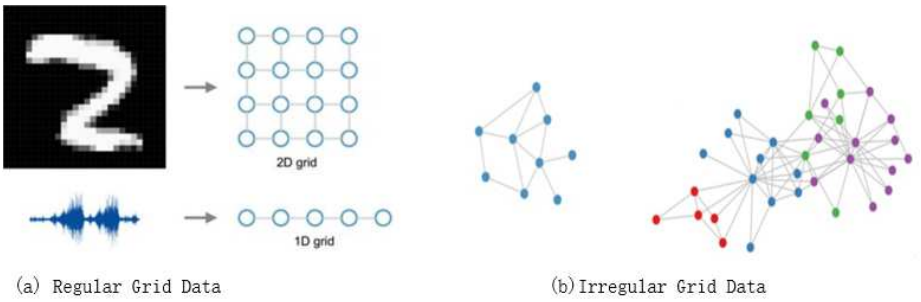

Figure 2: Example of regular grid data and irregular grid data.

over local regions and mostly uncorrelated at a global scale. This works well for data on a regular low-dimensional grid, for instance, images and sound are modeled as 2-D grids and 1-D sequences respectively (see Figure 2(a)). However, in many real world problems, the data reside on irregular grids or more generally in non-Euclidean domains. Examples are furnished by social networks, chemical compounds, protein and knowledge graphs, all of which are better structured as a graph (see Figure 2(b)). When confronted by graph data-streams, on the other hand, one is confronted with irregular structures, the basic operations of convolution, pooling and weight-sharing in CNNs, which are only designed for regular grids, are no longer applicable. Therefore, it is necessary to reformulate the convolution operator on graph structured data. Moreover, to explicitly capture such structures in the data, it may be important and beneficial to integrate priors that capture the structure of the mammalian visual cortex into the network architecture [19].

3.2. Graphs

A graph G is a pair of sets (V, E), where $V = \{v_1, ..., v_n\}$ is the set of vertices and $E \subseteq V \times V$ is the set of edges, formed by pairs of vertices. Each graph can be represented by an adjacency matrix A of size $n \times n$, where n is the number of vertices in G. In particular, $A_{i,j} = 1$ if there is an edge between vertex v_i and vertex v_j, i.e. v_i and v_j are adjacent, and $A_{i,j} = 0$ otherwise. A walk is a

sequence of edges and vertices, where the endpoint of each edge are adjacent. A path is a walk in which all vertices are distinct (except possibly the first and last).We denote $d(v_i, v_j)$ as the length of the shortest path between vertex v_i and vertex v_j, and denote k-hop(v_i) as the k-neighborhoods of vertex v_i, i.e. $d(v_i, v_j) = k$ for any vertices v_j of k-hop(v_i).

3.3. Quantum Walks

Quantum walks have recently emerged as a tool for designing novel algorithms on graph structures. They have important properties not exhibited by their classical counterparts [16, 14, 17]. A quantum walk is defined as a dynamical process over the vertices of the graph. Moreover, because it is determined by the complex solutions of the Schrödinger equation, the continuous time quantum walk allows different paths of the walk to interfere with each other in both a constructive and a destructive manner via a complex amplitude. This produces non-classical behavior of quantum walks [20]. While classical walks are ergodic and irreversible, their quantum counterparts are non-ergodic and reversible. As a result, a quantum walk does not approach a steady state with time.

The Dirac notation represents the complex amplitudes corresponding to the different states of quantum system using bras and kets. A ket $|m\rangle$ can be interpreted as a column vector, while a bra with the same state label $\langle m|$ is its conjugate transpose (which is a row vector). We use the Dirac notation to represent the basis state corresponding to the walk being at vertex $u \in V$ as $|u\rangle$. The ket $|\psi_t\rangle$ is a vector representing the state of the walk at time t , such that its u-th entry determines the probability of the walk being at vertex u at time t. A general state of the walk is a complex linear combination of the basis states, which is defined as

$$|\psi_t\rangle = \sum_{u \in V} \alpha_u(t)|u\rangle \tag{1}$$

where both $\alpha_u(t)$ and $|\psi_t\rangle$ are complex numbers, and $\alpha_u(t)\alpha_u^\star(t)$ gives the probability of finding the walk at the vertex u at time t. Thus $\sum_{u \in V} \alpha_u(t)\alpha_u^\star(t) = 1$ and $\alpha_u(t)\alpha_u^\star(t) \in [0, 1]$ for all $u \in V$ and $t \in \mathbb{R}$.

The evolution of the walk is then given by the Schrödinger equation, where we denote the time independent Hamiltonian as $\mathcal{H}$

$$\frac{\partial}{\partial t}|\psi_t\rangle = -i\mathcal{H}|\psi_t\rangle \tag{2}$$

Given an initial state $|\psi_0\rangle$, the solution for Eq(2) is

$$|\psi_t\rangle = e^{-i\mathcal{H}t}|\psi_0\rangle \tag{3}$$

The Hamiltonian operator governs the time evolution of the continuous time quantum walk. It is characterized by a unitary matrix, which renders the walk reversible. In the case where the Hamiltonian is identical to the graph Laplacian matrix [21, 22], i.e., $\mathcal{H} = L$, then the structural information residing in the graph is encoded by the Hamiltonian. In the Hilbert space formulation of Quantum Mechanics, the state of a quantum mechanical system associated to the n-dimensional Hilbert space $H \cong C^n$ is identified with an $n \times n$ positive semidefinite, trace-one, Hermitian matrix, called a density matrix. The Laplacian of a graph is symmetric and positive semidefinite. The Laplacian of a graph G, scaled by the degree-sum of G, has trace one and it thus has the requested properties of a density matrix.

4. Proposed QS-CNNs Model

In this section we combine the idea of subgraph convolution with that of using a depth-based representation to develop a novel subgraph convolution architecture for a graph. Our idea is to decompose a graph into substructures (i.e., subgraphs) spanned from a root vertex to the remaining vertices with a K-layer expansion. More specifically, for each vertex, a neighborhood subgraph consisting of exactly m vertices is extracted by quantum walks and normalized as a m-ary tree by leveraging graph grafting and graph pruning procedures. The leaf nodes of the m-ary tree are further replaced by their own neighbourhood m-ary trees. This process is performed recursively until a K-level m-ary tree is constructed for each vertex. We then construct a set of subgraph feature

detectors, which can be viewed as convolution with a set of finite support kernels. These are computed by sliding the kernels over the K-level m-ary tree to extract local features, in a manner analogous to that used in the standard convolution operation. After one layer of convolution computations over different positions of the subgraph along the tree structure, structural features are extracted, and a new tree is generated. The new tree has a reduced number of levels when compared with the original input tree. Each parent node and its child nodes in the input layer become a single new node in the next layer. The extracted local features produced by the convolution layer are forwarded to the pooling layer. Thereafter they are packed into one or more fixed-size vectors by taking the max/mean value in each dimension. After the pooling layer, the fixed-size feature vector is subsequently presented to the fully-connected layers (FC) to compute the predicted probability over the class labels. One merit of such an architecture is that each vertex has K-layer expansion subgraphs. Hence both the a) global topological arrangement information and b) local connectivity structural information contained within a graph can be learned effectively and efficiently by subgraph convolution. This allows our method to capture multi-scale patterns in the data.

4.1. The Depth-Based Representation for a Graph

In order to exploit topological information concerning the arrangement of vertices and edges in a graph, we develop a K-layer depth-based representation for a graph. Concretely, the representation comprises two steps: (1) Performing quantum walks on graph for node ranking; (2) Mapping graph to tree: we construct a m-ary tree for each vertex in the original graph by leveraging graph grafting and graph pruning procedures. The leaf nodes of the i-level m-ary tree are replaced by their neighborhood m-ary trees and thus a K-level m-ary tree is recursively constructed for each vertex.

4.1.1. Quantum Walks on Graph

The fundamental challenge in generalizing CNNs to graph-structured data is to determine the nodes belonging of each receptive field used for convolution while maintaining the shared weights. Recall that the standard convolution operator selects the neighboring pixels of a given pixel and computes the inner product of the weights and these neighbors. We propose a spatial convolution that performs a quantum walk on the graph in order to select the top m closest neighbors for every node, as shown in Figure 1. The intuition underpinning the use of a quantum walk is that it can capture the global topological arrangement information for substructures contained within a graph. Quantum walks capture different patterns of node connection. Moreover, a quantum walk allows the complex amplitudes corresponding to different paths between two nodes on a graph interfere with each other in both a constructive and a destructive manner. Although the classical concepts of hitting and commute time, allow the averaging of path length over the different paths [23] in the case of a quantum walk the effects are more subtle because of the complex nature of the associated amplitude [14]. For instance, if the walk is suitably initialised, then symmetric structure results in a zero amplitude and the amplitude capture long-range as well as local connectivity information [14]. In fact for certain types of symmetrically structured graphs, quantum walks have exponentially faster hitting times than their classical counterparts [24]. This has obvious benefits in terms of problems involving search on a graph or network.

As a consequence, quantum walkers can reach a vertex simultaneously through multiple paths, and thus at a given time the probability of visiting nodes in the neighbourhoods increases with respect to the classical counterpart. This means that a quantum walker can potentially identify the salient connectivity or neighbourhood structure more effectively and efficiently than its classical counterpart.

Given the adjacency matrix A of a graph, the spectral decomposition of the adjacency matrix is $A = \Phi\Lambda\Phi^T$, where $\Phi = (|\psi_1\rangle, |\psi_2\rangle, \cdots, |\psi_n\rangle)$ is the $n \times n$ matrix and Λ is the ordered eigenvalue matrix $\Lambda = diag(\lambda_1, \lambda_2, \cdots, \lambda_n)$. According to Eq.(3), we set the initial state Φ_0 as Φ and the evolution of the

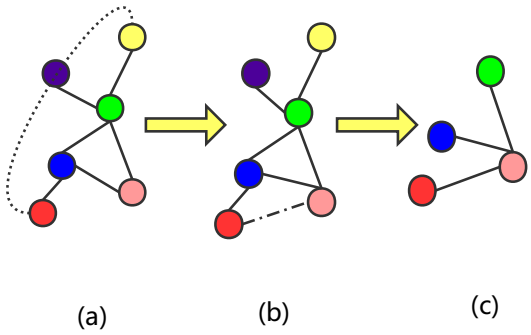

Figure 3: An illustrative example of graph grafting. Vertices connected in dotted line are the pink vertex's 2-hop, the red vertex has a higher QW score than other vertices of pink vertex's 2-hop.

quantum walk on the graph at time t is given by

$$\Phi_t = e^{-iLt}\Phi_0 \tag{4}$$

After the above measurement, the $n \times n$ state matrix A_t in quantum walks at time t becomes

$$A_t = \Phi_t \Lambda \Phi_t^T \tag{5}$$

For every node u, we define the quantum walks score (referring to as QW) for the node as

$$QW(u) = \sum_{v \in n} (A_t)_{uv} \tag{6}$$

We then sort all the nodes according to their QW scores in descending order.

4.1.2. Mapping Graph to Tree

For each vertex, a receptive field of the same size should be constructed. However, the size of the 1-hops for different nodes are different. To overcome

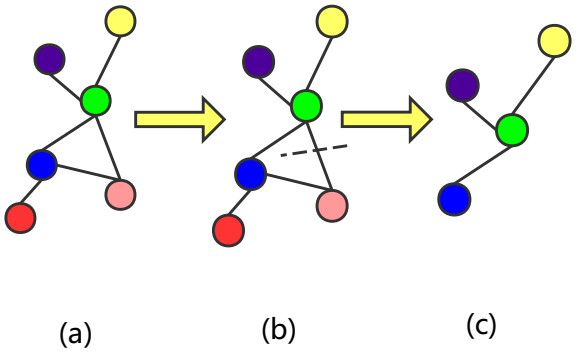

Figure 4: An illustrative example of graph pruning. The pink vertex has a smaller QW score than other vertices of green vertex's 1-hop.

this problem, we use graph grafting and graph pruning to standardise the neighborhood subgraph for each node to be an m-ary tree.

Graph Grafting For node v whose 1-hop size is less than m, we use graph grafting to choose nodes from node k-hop(v) (k >=2) to fill node 1-hop(v). As shown in Figure 3, besides the vertex coloured pink itself, we still need to incorporate $m = 1$ vertex into the receptive field from node k-hop(v) (k >=2). We commence by selecting nodes from node 2-hop(v). However, if the nodes in the 2-hop are insufficient in number, then we select nodes from the 3-hop and so on. If there exist more nodes than we need, we select nodes with higher QW scores. In this way, the neighborhood subgraph consisting of exactly m vertices is extracted and standardised as an m-ary tree. We then rank the leaf nodes of the m-ary tree according to their QW scores.

Graph Pruning For node v whose 1-hop size is greater than m, we use graph pruning to select nodes from node 1-hop(v). As shown in Figure 4, besides the vertex coloured green, we need to cut one node so that only $m = 3$ vertices are reserved. We cut nodes with smaller QW scores. In this way,

the neighborhood subgraph consisting of exactly m vertices is extracted and standardised as an m-ary tree. We then rank the leaf nodes of the m-ary tree according to their QW scores.

Using graph grafting and graph pruning, we normalized the subgraph of each node's as an m-ary tree. The leaf nodes of each m-ary tree are further replaced by their own m-ary neighborhood trees. In this way, a K-level m-ary tree is recursively constructed for each vertex. Algorithm 1 gives the steps of the Mapping Graph to Tree algorithm.

Algorithm 1: Mapping Graph to Tree

Input: state matrix A_t, receptive field size $m+1$, the depth K

Output: normalized neighborhood graph (K-level m-ary tree) for each vertex

initialization;
compute the QW score for each vertex according to Eq.6;
construct a m-ary tree with each vertex by the graph grafting and graph pruning algorithm;
for $i = 2, i \leq K-1$ **do**
    The leaf nodes of the i-level m-ary tree are further replaced by their own neighborhood m-ary trees;
end
return K-level m-ary tree for each vertex;

4.2. Depth-based Subgraph Convolution Operator

In this section, we first list the notation used in the paper, in Table 1. We then present our depth-based subgraph convolution operator for the K-level m-ary tree. Figure 1 shows an example of the complete process with $K = 4$ and $m = 3$. In a manner similar to CNNs on images, our QS-CNNs also involves convolution and pooling operations. Our depth-based subgraph convolution operation extracts structural features on the tree. The extracted features are

then summarized by a depth-based subgraph pooling operation. In this way, our QS-CNNs allows effective structural feature learning.

Table 1: Important notations used in this paper and their descriptions.

Symbol	Definition
$node(s,t)$	the t-th node in level s
$X^{l,p}$	the p-th feature channel in layer l
$X_{s,t}^{l,p}$	the node $(s,t)'$ p-th feature channel in layer l
$H_{s,t}^{l,p}$	$H_{s,t}^{l,p} = \{X_{s,t}^{l,p}, X_{s+1,(t-1)m+1}^{l,p}, ..., X_{s+1,tm}^{l,p}\}$ i.e. the p-th feature channel of node $(s,t)'$ receptive field in layer $l+1$
$W^{l,k,p}$	the filter mapping from the p-th feature channel in layer l to the k-th feature channel
f	the activation function
f_{l-1}	the number of filters in layer $l-1$
$b^{l,k}$	the bias of the k-th filter in layer l
$\odot$	element-wise multiplication

When CNNs are applied to images, a square grid is moved over each image with a particular step size to extract structural features as the output of the convolution. More precisely, a receptive field in the preceding layer becomes a neuron in the next layer after a convolution operation. In this way, the local structural features of images are well captured by the convolution operation. By generalizing CNNs to the K-level m-ary tree obtained in previous steps of graph grafting and graph pruning, we scan a subgraph-based window along the tree to extract structural features as the output of our convolution.

The convolutional activation $X_{s,t}^{l,k}$ for node (s,t), feature k and layer l is given by

$$X_{s,t}^{l,k} = f(\sum_{p=1}^{f_{l-1}}(\sum_{j=1}^{m+1} W_j^{l,k,p} H_{s,t,j}^{l-1,p}) + b^{l,k}) \qquad s \leq K-l+1$$

The activation $X^{l,k}$ for k-th feature channel in layer l can be expressed more concisely using tensor notation as

$$X^{l,k} = f(\sum_{p=1}^{f_{l-1}}(W^{l,k,p} \odot H^{l-1,p}) + b^{l,k})$$

4.3. Depth-based Subgraph Pooling Operator

Another important operation proposed by CNNs is pooling. Reducing the dimensionality of the input data allows the convolution filters to have a large receptive field and at the same time decrease the number of parameters. One of the most common methods for pooling graphs is by performing multi-scale clustering of the grid and then performing a pooling operation over each extracted cluster. Instead, our pooling operation acts directly on the output of the preceding layer without any kind of preprocessing scheme. The pooling activation $X_{s,t}^{l+1,k}$ for node (s,t), feature k and layer $l+1$ is given by

$$X_{s,t}^{l+1,k} = f(W^{l+1,k} \cdot pool(H_{s,t}^{l,k}) + b^{l+1,k})$$

A maximum pooling function $pool_{max}$ can be found by taking the maximum value over a region and an average pooling function $pool_{ave}$ can be obtained by taking the mean value over a region, thus

$$pool_{max}(R_k) = max_{i \in R_k} a_i$$

$$pool_{avg}(R_k) = \frac{1}{|R_k|} \sum_{i \in R_k} a_i$$

4.4. Applying QS-CNNs to Node Classification

For the purpose of node classification, each node can be represented by a K-level m-ary tree constructed through Algorithm 1. After multiple layers of applying the depth-based subgraph convolution and pooling operations, multiple features which carry different structural information constitute the final representation X_N of the input node. Then, the final node representation X_N is passed to a fully connected layer and outputs a conditional probability distribution $\mathbb{P}(Y|X)$, which can be obtained by applying the softmax function. This process can be formulated as below:

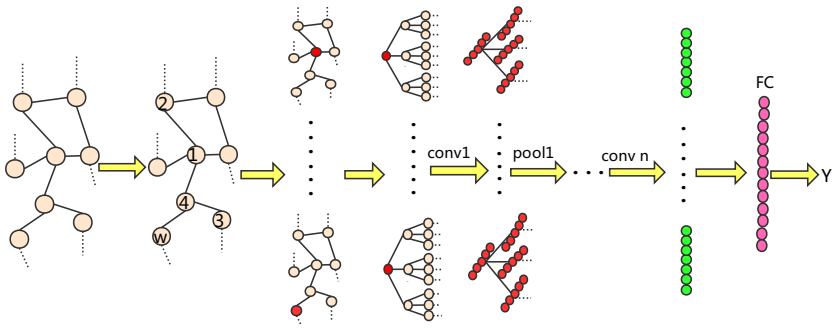

Figure 5: Illustration of the proposed QS-CNNs model for graph classification.

$$\mathbb{P}(Y|X) = \text{softmax}(f(W^d \odot X_N))$$

4.5. Applying QS-CNNs to Graph Classification

For the graph classification task, we encapsulate a graph by the information conveyed by a set of selected nodes. This potentially allows us to make predictions concerning the features of these nodes. We use a node sequence selection algorithm to select a sequence (V) of important nodes. Algorithm 2 illustrates the Node Sequence Selection steps. First, we sort the nodes of the input graph into descending order according to their QW scores. Second, we select the first W nodes to represent the graph and create a null entry for the node sequence if the number of nodes is smaller than W.

The resulting node sequence is traversed and each visited node is represented by a K-level m-ary tree constructed through the algorithm above if the node value is not 0. Otherwise, we represent the node with a K-level m-ary tree, with all node values set to zero. After multiple depth-based subgraph convolution and pooling operations simultaneously have acted on these K-level m-ary trees, we obtain the feature map X_G of the graph. The architecture is completed by a dense layer that connects X_G to predict Y. A conditional probability

Algorithm 2: Node Sequence Selection

Input: QW scores for all nodes, width W

Output: selected node sequence V

initialization;

sort (descend) the nodes of the input graph using the given QW scores to get V_{sort};

if $|V_{sort}| >= W$ **then**

  V = the first W elements of V_{sort}

else

  $V = V_{sort}$ and $W - |V_{sort}|$ dummy nodes

end

return selected node sequence V;

distribution $\mathbb{P}(Y|X)$ can be obtained by applying the softmax function:

$$\mathbb{P}(Y|X) = \text{softmax}(f(W^d \odot X_G))$$

A generic illustration of the proposed QS-CNNs architecture for graph classification is shown in Figure. 5. It is important to note that our depth-based convolutional representation for the graph is invariant with respect to the permutation of node index (rather than the node position). This means that the activations of two isomorphic input graphs will be the same. We prove it as follows.

Theorem 1. *The depth-based convolutional activations of two isomorphic input graphs will be the same.*

Proof. We prove this theorem by contradiction.

Assume two graphs G_1 and G_2 are isomorphic but their depth-based convolutional activations are different. At least a pair of nodes u, w, where u, v belongs to the resulting node sequence of graph G_1 and G_2 respectively and will have the same position in the resulting node sequence. The activations of u and v in layer l are different. The depth-based convolutional activations of two nodes

can be written as

$$X_u^{l,k} = f(\sum_{p=1}^{f_{l-1}} (W_u^{l,k,p} \odot H_u^{l-1,p}) + b_u^{l,k})$$

$$X_v^{l,k} = f(\sum_{p=1}^{f_{l-1}} (W_v^{l,k,p} \odot H_v^{l-1,p}) + b_v^{l,k})$$

Note that

$$W_u^{l,k,p} = W_v^{l,k,p} = W^{l,k,p}$$

$$b_u^{l,k} = b_v^{l,k} = b^{l,k}$$

Graphs that are isomorphic (the same except for vertex labels) become identical after canonical graph labeling, so

$$H_u^{l-1,p} = H_v^{l-1,p} = H^{l-1,p}$$

by isomorphism, allowing us to rewrite the activation as

$$X_u^{l,k} = f(\sum_{p=1}^{f_{l-1}} (W^{l,k,p} \odot H^{l-1,p}) + b^{l,k})$$

$$X_v^{l,k} = f(\sum_{p=1}^{f_{l-1}} (W^{l,k,p} \odot H^{l-1,p}) + b^{l,k})$$

Which implies that $X_u^{l,k} = X_v^{l,k}$ and presents a contradiction and completes the proof. □

4.6. Learning Filters

We assume that each convolution layer l is followed by a pooling layer $l+1$. According to the back propagation algorithm, in order to compute the sensitivity for a unit at layer l, we should first sum over the sensitivities of the next layer corresponding to units that are connected to the node of interest in the current layer l. We multiply each of these connections by the associated weights defined at layer $l+1$. We then multiply this quantity by the derivative of the activation function evaluated at the pre-activation inputs of the current layer Z. In the case of a convolutional layer followed by a pooling layer, we can upsample the pooling

layers sensitivity map $\delta^{l+1,k}$ to make it the same size as the convolutional layer map. Then we perform elementwise multiplication of the upsampled sensitivity map from layer $l+1$ with the activation derivative map at layer l. The 'weights' defined at a pooling layer map are all equal to $W^{l,k}$, snd so we simply scale the previous step result by $W^{l,k}$ to complete the computation of $\delta^{l,k}$. So we can get:

$$\delta^{l,k} \triangleq \frac{\partial E}{\partial Z^{l,k}}$$
$$\delta^{l,k} = \frac{\partial E}{\partial Z^{l+1,k}} \cdot \frac{\partial Z^{l+1,k}}{\partial X^{1,k}} \cdot \frac{\partial X^{l,k}}{\partial Z^{1,k}}$$
$$\delta^{l,k} = f'(Z^l) \odot (\text{up}(W^{l+1,k}\delta^{l+1,k}))$$
$$\delta^{l,k} = W^{l+1,k}(f'(Z^l) \odot \text{up}(\delta^{l+1,k}))$$

where up is the Upsampling function and E is the loss energy. Finally, the gradients for the kernel weights are computed using back propagation:

$$\frac{\partial E}{\partial W^{l,k,p}} = \sum_{i,j} (\delta^{l,k})_{i,j} (P^{l-1,p})_{i,j}$$

where $(P^{l-1,p})_{i,j}$ is the patch in $X^{l-1,p}$ that was multiplied element-wise by $W^{l,k,p}$ during convolution. we can compute the bias gradient by simply summing over all the entries in $\delta^{l,k}$:

$$\frac{\partial E}{\partial b^{l,k}} = \sum_{i,j} (\delta^{l,k})_{i,j}$$

5. Experiments and Comparisons

In this section, we experimentally investigate the merits and limitations of the proposed QS-CNNs model, including its computational complexity and parameter determination. A comprehensive experimental study on a variety of data sets is conducted in order to compare our proposed model QS-CNNs with several state-of-art methods for node classification and graph classification tasks. In this section, we denote a graph convolution layer with k feature maps by C_k and a fully connected layer with k hidden units by FC_k. In addition, lr stands for the learning rate, L2 denotes the L2 regularization parameter and dropout denotes the drop out rate.

5.1. Node Classification

To demonstrate the effectiveness of the proposed approach on the node classification task, we conduct experiments on two citation network datasets and one data set arising from e-mail communications in a social network. These are respectively the Cora, Pubmed datasets [25] and the Email-Eu dataset [26]. Each citation dataset consists of scientific papers (represented by nodes), citation links (represented by edges), and topics or subjects (represented by labels). Table. 2 summarizes the coverage and properties of the three data sets. For node classification, six alternative algorithms are selected as baseline comparators. We briefly describe these methods in turn.

Table 2: Dataset statistics of node classification task.

Dataset	Type	Nodes	Edges	Classes	Features
Cora	Citation network	2,708	5,429	7	1433
Pubmed	Citation network	19,717	44,338	3	500
Email-Eu	Communication network	1005	25,571	42	-

Datasets The Cora dataset [25] contains 2,708 machine learning articles categorized into seven possible machine learning subject or topic classes. Each article is represented by a binary 0/1-valued word vector where each feature corresponds to the presence or absence of a term drawn from a dictionary. The dictionary contains 1,433 unique entries. This graph contains 5,429 citation edges. We treat the citation links as undirected edges and construct a binary, symmetric adjacency matrix.

The Pubmed dataset [25] consists of 19,717 scientific papers from the Pubmed database on the subject of diabetes. Each paper is classified into one of three classes. This citation network that links the papers consists of 44,338 links. Each paper is represented by a Term Frequency Inverse Document Frequency (TFIDF) vector drawn from a dictionary with 500 terms. As with the CORA corpus, we construct an adjacency-based QS-CNNs that treats the citation net-

work as an undirected graph.

The Email-Eu dataset [26] was generated using email data from a large European research institution. There is an edge (u, v) in the network if person u sent person v at least one email. The e-mails only represent communication between institution members. The dataset also contains "ground-truth" community memberships of the nodes. Each individual belongs to exactly one of 42 departments at the research institute. Note that the vertices of the Email-Eu-Core have no vertex information, so we only take the structural information of the vertices as the input.

Baseline Methods We compare our proposed method QS-CNNs with six state-of-the-art methods for node classification. The methods used for comparisons are (1) $\ell 1$-regularized logistic regression (l1logistic), (2) $\ell 2$-regularized logistic regression (l2logistic), (3) exponential diffusion kernels-on-graphs (KED) [25], (4) Laplacian exponential diffusion kernels-on-graphs (KlED) [25], (5) diffusion convolutional neural networks (DCNNs) [10], (6) GraphSAGE [27]. For the 'l1logistic' and 'l2logistic' methods, we use node features alone as the input for logistic regression. This means that graph structure information is not considered, and the regularization parameter is fine tuned by the validation set. For 'KED' and 'KlED' , we take the graph structure as input, which means that node feature information is not considered. Similar to previous work [10], we chose parameters for various baseline methods as follows: a) the penalty for l1logistic and l2logistic is chosen from the set $\{10^{-4}, 10^{-3}, ..., 10^{3}, 10^{4}\}$, b) the parameter α for 'KED' and 'KlED' is chosen from the set $\{10^{-6}, 10^{-5}, ..., 10^{2}\}$, c) the parameter $H = 2$ is used for DCNNs because it results in the best classification accuracy, d) GraphSAGE provides a variety of alternative approaches for aggregating features within a sampled neighborhood, and we choose GraphSAGE-mean because it almost always results in the best accuracy. For each baseline method, we report the results for the parameters which give the best classification accuracy.

Table 3: The details of some parameters for node classification.

Dataset	Layer2	Layer3	FC layer	lr	L_2	dropout
Cora	C_{32}	C_{32}	FC_{64}	10^{-6}	10^{-2}	0.3
Pubmed	C_{32}	C_{64}	FC_{32}	10^{-6}	10^{-2}	0.8
Email-Eu	C_{32}	C_{32}	FC_{64}	10^{-4}	10^{-2}	0.8

Experimental Set-up For all datasets, we standardize each node as a 3 level 3-ary tree. We train a five-layer QS-CNNs, where the first layer is the input layer, the second and third layers are the convolutional layer, the fourth layer is the fully-connected layer, and the final layer is the output layer. We use the Adam optimization algorithm [28] for gradient descent. All weights are randomly initialized from a normal distribution with mean zero and variance 0.01. We choose ReLU as the activation function. This model was implemented in Python using tensorflow [29]. A 10-fold cross-validation strategy is employed to evaluate the classification performance. Specifically, the entire sample is randomly partitioned into 10 subsets and then we choose one subset for test and use the remaining 9 for training, and this procedure is repeated 10 times. The final accuracy is computed by averaging the accuracies from each of the random subsets.

Network Configuration For node classification, our QS-CNNs has 3 parametric layers. Its configuration for different datasets are as follows: a) for Cora: $C_{32}-C_{32}-FC_{64}$, 10^{-6} (learning rate), 10^{-2} (L2 regularization) and 0.3 (dropout rate); b) for Pubmed: $C_{32}-C_{64}-FC_{32}$, 10^{-6} (learning rate), 10^{-2} (L2 regularization) and 0.8 (dropout rate); and c) for Email-Eu: $C_{32}-C_{32}-FC_{64}$, 10^{-4} (learning rate), 10^{-2} (L2 regularization) and 0.8 (dropout rate). These properties can be found in Table 3.

Results Discussion Table. 4 reports the average classification accuracy of the different algorithms on node classification. The boldfaced values are the best result in each row. Our proposed five-layer QS-CNNs outperforms each of the

Table 4: Study of node classification: classification accuracy (in MEAN ± STD). A comparison of the performance between six baseline methods and our proposed QS-CNNs on three node classification datasets. The QS-CNNs offers the best performance. - means the model is not suitable for the data set.

Model	Cora	Pubmed	Email-Eu
l1logistic	71.63 ± 0.71	87.68 ± 0.89	-
l2logistic	71.81 ± 0.69	86.54 ± 0.93	-
KED	81.92 ± 0.91	83.15 ± 0.64	70.28 ± 0.87
KlED	83.27 ± 0.76	84.11 ± 0.77	71.54 ± 0.81
DCNN	82.52 ± 2.11	88.57 ± 1.34	-
GraphSAGE	82.68 ± 1.83	88.41 ± 1.25	73.59 ± 1.72
DS-CNNs	84.72 ± 2.28	89.63 ±1.67	76.61 ± 2.33
QS-CNNs	**85.95 ± 1.58**	**89.63 ±1.67**	**77.63 ±1.94**

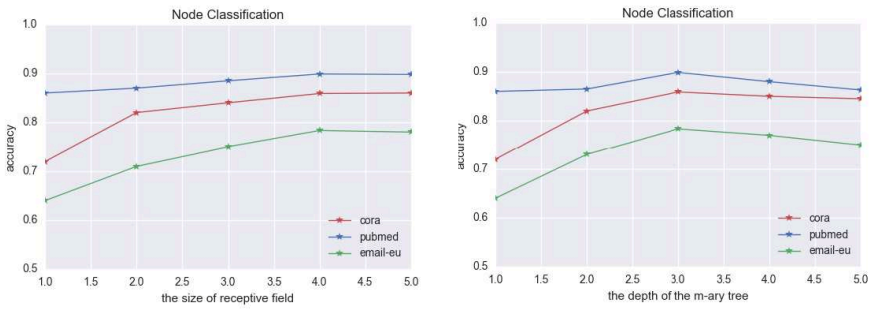

Figure 6: Impact of the receptive field size and the depth of the m-ary tree on performance for node classification

competing methods for all datasets studied and the improvement is in the range from 2.68% to 14.32% on the Cora dataset, from 1.06% to 6.48% on the Pubmed dataset and from 4.04% to 7.35% on the Email-Eu dataset respectively. On the Cora dataset, l1logistic and l2logistic give the worst performance. This may be explained by the fact that the logistic regression models only take the node features as input and neglect graph structure information. KED and KLED both take graph structure as input (e.g. node features are not used) and show inferior performance to our QS-CNNs. This indicates that our QS-CNNs is able to extract graph structure features. On the Pubmed dataset, we observed that those methods which incorporate node features outperform those methods that do not, i.e., l1logistic and l2logistic are superior to both KED and KLED in terms of accuracy. Furthermore, our QS-CNNs still maintains the best classification accuracy. Our QS-CNNs outperforms GraphSAGE-mean (taking the elementwise mean value of feature vectors) suggesting that assigning different weights to different nodes within a subgraph while dealing with differently sized neighbourhoods may be beneficial. Based on these results, it is demonstrated that our proposed method QS-CNNs integrates the merits of using both the global topological and local connectivity structures within a graph. Thus, it performs better than the traditional methods.

To investigate the effect of different receptive field size of $m+1$ and the depth K of the m-ary tree on the node classification performance of our proposed method QS-CNNs, we test several values of $m+1$ and K. We report the results in Figure 6, in which we plot the classification accuracies of our QS-CNNs method versus $m+1$ and K respectively. The different coloured lines represent the results on the different datasets. The classification accuracies tend to increase with increasing values of $m+1$ and K. This is because the greater the values of $m+1$ and K, the more global topological and local connectivity information can be captured using our QS-CNNs method.

5.2. Graph Classification

To demonstrate the effectiveness of the proposed approach on graph classification, we conduct experiments on five benchmark data sets abstracted from bioinformatics databases, i.e., a) MUTAG [30], b) PTC [31], c) NCI1 [32], d) D&D [33], and e) PROTEINS [34]. Information concerning the properties of these datasets is listed below and summarized in Table. 5. For graph classification, eight alternative algorithms are selected as baselines. We will briefly detail these methods in turn.

Table 5: Dataset statistics for graph classification task.

Dataset	Size	Classes	Avg.nodes	Labels
NCI1	4110	2	29.8	37
MUTAG	188	2	17.9	7
PTC	344	2	25.5	19
D&D	1178	2	284.32	89
PROTEINS	1113	2	39.1	3

Datasets The NCI1 [32] dataset made publicly available by the National Cancer Institute (NCI) is a subset of balanced datasets of chemical compounds screened for the ability to suppress or inhibit the growth of tumours. It consists of 4100 graphs that represent chemical compounds and each node is assigned one of 37 possible labels. MUTAG [30] is a data set of 188 nitro compounds where the class label is as either aromatic or heteroaromatic with seven node features. PTC [31] comprises 344 compounds where the class label indicates whether they are carcinogenic or not in rats with 19 node features. D&D is a data set of 1178 protein structures obtained from [33], classified into enzymes and non-enzymes. Each protein is represented as a graph whose nodes correspond to amino acids and two nodes are linked by an edge if they are less than 6 Ångstroms apart. PROTEINS is a dataset obtained from [34] where these nodes are secondary structure elements and there is an edge between two nodes if they are neigh-

bours in the amino-acid sequence or in 3D space. It has 3 discrete labels, which represent helix, sheet or turn.

Baseline Methods We compare our proposed method QS-CNNs with eight state-of-the-art methods for graph classification. These methods are used for comparisons are (1) the Weisfeiler-Lehman subtree kernel (WL) [35], (2) the random walk kernel (RW) [36], (3) the shortest-path kernel (SP) [37], (4) the graphlet count kernel (GK) [38], (5) the PATCHY-SAN method which combining receptive fields for nodes and edges using a merge layer $k = 10^E$ (PSCN-10^E) [7], (6) p-step random-walk kernel (p-RW) [39], (7) Ramon-Gärtner kernels (RG) [40], (8) FGSD[41]. In accordance with established [42], the decay factor for random-walk is chosen from $\{10^{-6}, 10^{-5}, \ldots, 10^{-1}\}$, the p value in the p-step random-walk kernel is chosen from $\{1, 2, \ldots, 10\}$, the height parameter in Ramon-Gärtner subtree kernel is chosen from $\{1, 2, 3\}$. For each kernel, we report the results for the parameters which give the best classification accuracy. For Weisfeiler-Lehman subtree kernel, we set the height parameter $h = 2$ for it could increase the feature space exponentially. For the graphlet kernel, we set the size of the graphlets k to 7 since it could exhibit the sparsity problem. We set the parameter $k = 10^E$ for PSCN becasue a receptive size of 10 results in the best classification accuracy and the result is quoted from [7]. For FGSD, the parameters are set the same as [41].

Experimental Set-up For the NCI1 dataset, we set width W=25 (W represents the number of selected nodes from each graph), and standardize each vertex as a 3 level 9-ary tree. We train a six-layer QS-CNNs, where the first layer is the input layer, the second, third and fourth layers are the convolutional layer, the fifth layer is the fully-connected layer, and the final layer is the output layer. For the remaining datasets, we set the width W=15, and again standardize each vertex as a 3 level 9-ary tree, but instead, we train a five-layer QS-CNNs, where the second and third layers are the convolutional layer, the fourth layer is the fully-connected layer. We again use the Adam optimization

Table 6: The details of some parameters for graph classification.

Dataset	Layer2	Layer3	Layer4	FC	lr	L_2	dropout
NCI1	C_{32}	C_{32}	C_{64}	FC_{32}	$5 \cdot 10^{-3}$	10^{-2}	0.8
MUTAG	C_{32}	C_{32}	-	FC_{64}	10^{-2}	10^{-2}	1
PTC	C_{32}	C_{32}	-	FC_{64}	10^{-2}	10^{-2}	1
D&D	C_{32}	C_{32}	-	FC_{64}	10^{-2}	10^{-2}	1
PORTEINS	C_{32}	C_{32}	-	FC_{64}	10^{-2}	10^{-2}	1

Table 7: Study of graph classification: classification accuracy (in MEAN ± STD). A comparison of the performance between eight baseline methods and our proposed QS-CNNs on five graph classification datasets. The last column shows the averaged classification accuracy of all the algorithms over the five datasets. The QS-CNNs offers the best performance.

Algorithm	NCI1	MUTAG	PTC	PROTEIN	D&D	AVG
WL	80.22 ± 0.51	80.71 ± 0.31	56.77 ± 2.11	72.92 ± 0.56	77.95 ± 0.7	73.71 ± 0.84
RW	>72h	83.73 ± 1.51	57.85 ± 1.30	74.22 ± 0.42	>72h	-
SP	73.00± 0.24	85.22 ± 2.43	58.24 ± 2.44	75.07 ± 0.54	>72h	-
GK	62.28 ± 0.29	81.66 ± 2.11	57.26 ± 1.41	71.67 ± 0.55	78.45 ± 0.26	70.26 ± 0.92
p-RW	>72h	80.05 ± 1.64	59.38 ± 1.66	71.16 ± 0.35	>72h	-
RG	56.61 ± 0.53	84.88 ± 1.86	59.47 ± 1.66	70.73 ± 0.35	>72h	-
PSCN-10^E	78.59 ± 1.89	92.63 ± 4.21	60.00 ± 4.82	75.89 ± 2.76	77.12 ± 2.41	76.85 ± 3.22
FGSD	79.80 ± 2.36	92.12 ± 3.98	62.80 ± 4.07	73.42 ± 3.42	77.10 ± 2.78	76.46 ± 3.25
DS-CNNs	80.12 ± 2.87	92.87 ± 4.81	64.67 ± 5.00	78.35 ± 4.00	79.22 ± 4.06	79.05 ± 4.15
QS-CNNs	**81.43 ± 2.56**	**93.13 ± 4.67**	**65.99 ± 4.43**	**78.80 ± 4.63**	**81.41 ± 3.46**	**80.15 ± 3.95**

algorithm [28] for gradient descent. The initial values of weights, the type of activation function and the implementation environment are set in the same manner as for node classification. We again adopt a 10-fold cross-validation strategy as described above.

Network Configuration For graph classification, we used the following sets of hyperparameters a) for MUTAG, PTC, D&D and PORTEINS: $C_{32}-C_{32}-FC_{64}$, 10^{-2} (learning rate), 10^{-2} (L2 regularization) and 1 (dropout rate); b) for NCI1: $C_{32} - C_{32} - C_{64} - FC_{32}$, $5 \cdot 10^{-3}$ (learning rate), 10^{-2} (L2 regularization) and 0.8 (dropout rate). These properties can be found in Table 6.

Discussion of Results The classification accuracies obtained with the different

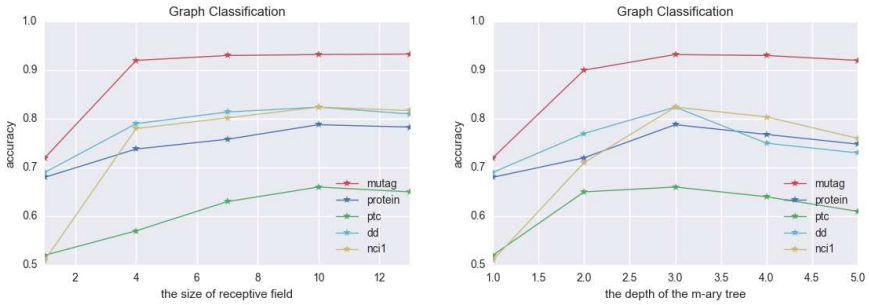

Figure 7: Impact of the receptive field size and the depth of the m-ary tree on the performance for graph classification

methods are shown in Table 7, in which the boldfaced values again indicate the best result in each row. Again, we observe that our proposed method QS-CNNs outperforms the alternative for all five datasets. The last column of Table. 7 shows the averaged classification accuracy over all the algorithms tested for the five datasets. Note that, some kernels cannot complete the kernel matrix computation on some of the datasets. For these kernels, we perform the statistical analysis on those datasets on which the computation can be completed. Our method has improved the classification accuracy by 6.44% (WL), 9.89% (GK), 3.3% (PSCN-10^E) and 3.69% (FGSD) respectively, compared to the averaged classification of all competing methods over the five datasets. Moreover, our QS-CNNs performs better than the PSCN-10^E algorithm, although they are both have a CNN architecture. The main reason is that the PSCN-10^E [7] uses node ordering step which converts graphs locally to a regular 1D grid hence discarding a large amount of the structural information residing in the graphs. Our proposed QS-CNNs is fundamentally different from most existing graph CNNs framework, where each vertex has K-layer expansion subgraphs, and hence structural information can be learned effectively and efficiently by subgraph convolution. Thus, it is capable of revealing both the global topological and local connectivity structures for a graph. The relatively high standard deviations can be explained by the small size of the benchmark datasets and the

fact that we normalize each node neighbourhood as the same 3 level 9-ary tree for different datasets. Finally, as with node classification, we evaluate how the graph classification accuracies vary with increasing receptive field size of $m+1$ and the depth K of the m-ary tree. Figure 7 gives the classification results. The results show that with increasing $m+1$ and K, the classification accuracy first increases to a maximum value (i.e., at $m+1=4$ and $K=3$) and then decreases slightly, finally reaching a steady state. This observation further verifies the effectiveness of our proposed method QS-CNNs which integrates both global topological arrangement information and local connectivity properties within a graph to conduct graph convolution.

5.3. The Effect of Quantum Walks

Finally, in order to study the contribution of quantum walks in terms of its impact on final classification accuracy, we ran experiments by replacing quantum walks with random walk (referred to as DS-CNNs) and keep the pruning and grafting trick. The results are shown in Table. 4 and Table. 7. As can be observed, QS-CNNs is superior to DS-CNNs in terms of accuracy values for all datasets studied. Meanwhile, QS-CNNs gives a lower standard deviation and hence more stable than the DS-CNNs. It is demonstrated that quantum walks can identify local neighbor structure of nodes more effectively and efficiently.

6. Conclusions and Future Work

In this paper, we have shown how to construct quantum-based subgraph convolution network for a graph. The convolution process makes use of both the global topological arrangement information and local connectivity structures within a graph. Experimental results on node classification and graph classification show our QS-CNNs is superior to a number of baseline methods.

Our future plans are to extend the work in a number of ways. First, in prior work, we have developed methods for characterizing graphs using the commute time [23] and the heat kernel [43]. For an undirected graph, both of these

methods encapsulate the path length distribution between vertices. It would be interesting to use the commute time or heat kernel as a means of node ordering. Second, the current formulations of graph convolution are restricted to use vertex information and do not make use of edge labels. It would be interesting to design convolution operation which simultaneously learns properties from both graph vertices and edges. Finally, in [44], Brabandere et al. proposed dynamic filter networks, to define a subnetwork, taking the preceding feature maps as input and generating data-adaptive convolutional filters that can be applied to the preceding feature maps. It would be interesting to use such a subnetwork to determine the local filters dynamically for each specific input subgraph. This may provide a more meaningful interpretation concerning the graph structure by the means of filter generating networks.

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