Abstract

Graph Convolutional Network (GCN) has shown strong effectiveness in graph learning tasks. However, GCN faces challenges in flexibility due to the fact of requiring the full graph Laplacian available in the training phase. Moreover, with the depth of layers increases, the computational and memory cost of GCN grows explosively on account of the recursive neighborhood expansion, which leads to a limitation in processing large graphs. To tackle these issues, we take advantage of image processing in agility and present Node2Img, a flexible architecture for large-scale graph learning. Node2Img maps the nodes to "images" (i.e. grid-like data in Euclidean space) which can be the inputs of Convolutional Neural Network (CNN). Instead of leveraging the fixed whole network as a batch to train the model, Node2Img supports a more efficacious framework in practice, where the batch size can be set elastically and the data in the same batch can be calculated parallelly. Specifically, by ranking each node’s influence through degree, Node2Img selects the most influential first-order as well as second-order neighbors with central node fusion information to construct the grid-like data. For further improving the efficiency of downstream tasks, a simple CNN-based neural network is employed to capture the significant information from the Euclidean grids. Additionally, the attention mechanism is implemented, which enables implicitly specifying the different weights for neighboring nodes with different influences. Extensive experiments on real graphs’ transductive and inductive learning tasks demonstrate the superiority of the proposed Node2Img model against the state-of-the-art GCN-based approaches.

1 Introduction

Graph Convolutional Network [1] has achieved a great success in graph learning tasks, including node classification [2, 3], link prediction [4, 5] and community detection [6, 7]. By applying convolutional operations to gather the embeddings of neighbors layer by layer, GCN significantly gains embeddings for the given nodes. For instance, when processing node classification tasks, GCN utilizes the node features and adjacency relations as inputs to predict the labels for testing nodes by the convolutional operations which enable aggregating the characters of neighbors.

However, GCN is inherently a full-batch based framework [8], which leads to the challenges in practice. Specifically, GCN requires the features and adjacency relations of nodes from the full graph are visible, including the nodes for testing. And the matrix manipulations are operated over the whole graph. On one hand, with the layers increase, the receptive field size of GCN grows exponentially because of the recursive information aggregation from neighbors [9], which leads to the greatly expensive requirements of computation and memory when processing large-scale graphs. On the other hand, GCN tends to leverage the fixed entire graph as a full-batch to train the model. However, for numerous cases, the graph is expanding dynamically rather than in a fixed state, which requires an inductive framework [10] capable of generalizing well to any augmentation graph by a significant model utilizing only training set for learning [11].

Instead of taking the full-batch as inputs like GCN, the mini-batch strategy [12] achieves better performance in flexibility when processing large-scale data and inductive learning tasks. Specifically, mini-batch training updates the learnable parameters only based on the training nodes in a mini-batch, which reduces the size of input data in each iteration to outperform in efficiency and memory requirement [8]. Inspired by these advantages, there are various studies attempting to address the limitation of GCN by virtue of mini-batch strategy. GraphSAGE [13] proposes an inductive learning architecture and utilizes a fixed number of neighbors to aggregate feature information. Similar to GraphSAGE, GAT [14] trains a global model for the unseen testing nodes, introducing the attention mechanism to learn the weights for different neighbors. FastGCN [11] samples a fixed number of nodes for each graph layer based on the node importance. LGCN [15] builds the sub-graphs for the training nodes by adjacent information, which reduces the batch size for the training progress. Recently, Cluster-GCN [8] obtains a great performance in large-scale inductive learning problems, sampling a block of nodes from the dense graph through the clustering algorithms. Even though the aforementioned approaches enable enhancing GCN to some extent, they share a drawback in adopting...
with, the central node is mapped to the Euclidean structured grid with size of $k \times 1 \times 3$. Then a convolutional layer will be further used to extract the information from the grid-like data. In the next step, the proposed model employs an attention filters to learn the weight of each "pixel" (i.e. grid). Finally, the fully-connected layers are applied to gain an output for node classification.

more complex computations to make up the distortion between the mini-batch graph and the raw entire graph, such as increasing the depth of neural networks or introducing the complex pre-processings.

Referring to mini-batch strategy, image processing tasks [16, 17] achieve good flexibility by setting the batch size elastically. When analyzing images, Convolutional Neural Networks [18] plays an important role to extract the meaningful information, whose local receptive field and sharing weights greatly reduce the number of parameters which raises the learning efficiency. For taking advantage of image processing, numerous studies transform graph learning problems to "image" processing problems. Mathias Niepert et al. [19] propose to choose the sequence of fixed size nodes and build the significant neighborhood, using the CNN to extract the information. LGCN [15] constructs the grid-like data for nodes and applies CNN to learn the meaningful characters. DGCNN [20] utilizes traditional neural networks to process graph data after sorting graph vertices in a consistent order. Graph U-Nets [21] adopts the graph pooling approach to build an encoder-decoder model on graphs. hGANet [22] introduces the hard graph attention and channel-wise attention to overcome the limitation of consuming excessive computational resources. Yet such methods tend to aggregate information of neighbors by means of GCN, which results in the limitation of flexibility.

To take full advantage of mini-batch based image processing, we present Node2Img, a flexible architecture for large-scale graph learning. The framework of our proposed model consists of two parts: (1) mapping the nodes (graph data) to "images" (Euclidean structured data), and (2) employing a simple three-layer neural network based on CNN to capture the characters from the grid-like data in Euclidean space.

The strategy about mapping aims to create Euclidean structured data consistent to the original graph, which is a handy pre-processing progress. To be specific, Node2Img ranks each node’s influence by degree [23] which reflects the network topology naturally [24], selecting a fixed number of most influential first-order as well as second-order neighbors to construct the grid-like data. For fully expressing the raw graph, Node2Img represents the information of central nodes globally by the approach of fusing their characters with neighbors’ during the mapping step. Moreover, instead of employing the large receptive field method like GCN [1], we apply CNN [18] and fully-connected network in the three-layer network, which speeds up the training progress. By adopting partial nodes from the training set as a mini-batch to train the model, the proposed architecture is capable of predicting unseen nodes in the testing data (i.e. enables conducting inductive learning tasks). The batch size can be set elastically and the data in the same batch can be computed parallelly, which reduce the computational and memory requirements. In brief, the proposed Node2Img not only adapts to transductive learning tasks but also have a strong ability to process large-scale graph and inductive learning tasks efficaciously.

## 2 Related Work

Our model is related to previous graph learning techniques including Graph Convolutional Network, some recent developments in large-scale graph and inductive learning, and CNN-based frameworks.

**Graph Convolutional Network.** The process of discrete convolution is essentially operations of weighted sum [26]. Based on the spectral domain [27], GCN [1] introduces the convolutional operations on topological graph and reaches state-of-the-art performance on some datasets. Specifically, for a given graph, GCN gains a node representation by aggregating its neighbors’ layer by layer. At each layer, the operations can be described as linear transformations and non-linear activation functions. However, the receptive field size of GCN grows exponentially as the layers increase, which causes a great limitation in efficiency and memory usage for large-scale graph learning. And the strategy of utilizing the fixed whole graph as a full-batch results in that original GCN is inapplicable for inductive learning tasks.

**Large-scale graph and inductive learning.** Hamilton et al. [13] propose the concept of inductive learning on large graph, where the nodes from testing set is unavailable during the training progress. In order to process inductive learning problems, GraphSAGE [13] train the model through a fixed number of neighbors for each given node, where the representations are aggregated from the local neighborhood. At infer-
enhances the original GCN [1] in flexibility through the sub-

Figure 2: An example of the proposed mapping algorithm with $k = 8$. The input graph has 6 nodes with 3 features (i.e. $f = 3$), and the brown node 3 is the given central node. To begin with, Node2Img selects the first-order neighbors $N_1 = \{0, 1, 2, 4\}$ and second-order neighbors $N_2 = \{5\}$. Then the $N_1$ and $N_2$ are ranked respectively according to the node degree. In grid-like data, each feature of the nodes represents a channel. For each channel, the proposed algorithm fills the feature of the nodes in $N_1$ and $N_2$ into the grids respectively to create the Euclidean structured data ($N_1$ have the higher priority than $N_2$ when padding). Note that if $k > |N_1| + |N_2|$, the default value of an unfilled grid is zero. In the last step, after creating an "image" with the size of $8 \times 1 \times 3$, Node2Img conducts information fusion (with $\theta_{bias} = 0.5$) between the central node and its neighbors, i.e. the features of the central nodes are introduced to update the grid-like data.

- Figure 3: An example of real-word graph and grid-like data. The graph data is constructed by connected nodes. And the grid-like data consists of the regular grids.

gence time, GraphSAGE employs the trained model to generate embeddings for entirely invisible testing nodes. While GraphSAGE still suffers from the high requirements of memory due to the exponential neighborhood growing problem. Graph Attention Network (GAT) [14] applies the attention mechanism to learn the attentions between central node and its neighbors. By gathering the features of neighbors layer by layer, GAT has an ability to specify the different weights for different neighboring nodes without costly matrix operations. However, just as GCN, the size of GAT’s receptive field is upper-bounded by the network depth.

**CNN-based graph learning.** Convolutional Neural Network [18] is effective and efficient in analyzing Euclidean structured data. In order to introduce CNN to graph learning tasks, it is crucial to transform graph data to grid-like data. Mathias et al. [19] propose a framework to apply CNN on arbitrary graphs. They present a general method to transform graphs to locally connected regions. This framework applies the measures of centrality to labeling and ranking procedures, determining a strategy for mapping the graph data to vector representations by neighborhood assembly and graph normalization. But optimal graph normalization is a NP-hard problem which leads to the limitation in efficiency. LGCN [15] enhances the original GCN [1] in flexibility through the sub-

3.1 Grid-like Data Generating

Instead of the complex pre-processing, our proposed Node2Img model adopts a handy mapping approach to aggregate the characters of neighbors. Moreover, for taking advantage of CNN, we apply CNN-based network to extract the meaningful information from grid-like data, in which the batch size is set elastically rather than the full-batch method requiring nodes from the whole graph as inputs. These strategies make the graph processing tasks efficient and flexible, achieving great performances in both transductive and inductive learning problems.

3 Proposed Method

3.1 Grid-like Data Generating

For applying conventional operations to graph learning tasks, some challenges arise due to the gaps between graph data and grid-like data. In the general graph, the number of neighbors of a node is not constant, but CNN requires that the size of the spatial neighborhood remains unchanged. In addition, since there is no naturally recognized node ordering rule, the neighbors in the graph cannot be sorted directly, rather than the neighbors in grid-like data. In this section, we explain the details of the mapping method, which transforms graphic data into grid-like data. The algorithm of mapping can be categorized into three strategies, i.e. node selection, neighborhood expansion and information fusion. Notably, the mapping processing can be conducted in parallel.

**Node selection.** We propose a degree-based mapping method that can convert graphic data into structured Euclidean data. Nodes with higher degree tend to have a greater
level of influence. In addition, node degree is a common feature in graph data, which makes the proposed model adapt to various graph data.

**Neighborhood selection.** As graphs are naturally sparse in the real world, we consider that the information contained in the first-order neighbors is limited, which is insufficient to present the character of a given node. Therefore, we introduce second-order neighbors to extend the neighbors of a given central node. Specifically, a second-order neighbor is a node that can be reached from a given node through two hops, not included in the first-order neighbor and the central node. In this case, we consider the secondary transmission of node characters to enrich the expression, which achieves obtaining the more expressive Euclidean grid.

**Information fusion.** This model uses the characteristics of the central node and its neighborhood to construct grid-like data. Compared with the information carried by neighboring nodes, it is more important to consider the expression of a given central node. There should be two keys to fully represent a given node. First, in the mapped Euclidean structure data, the proportion of the features of the central node should be larger than the proportion of the adjacent nodes. Second, the expression of the central node needs to be included in the global grid data, not in the local locations. Therefore, we introduce the method of information fusion to globally disperse the features of the central node into the Euclidean grid. In Section 4.5, we will demonstrate the effectiveness of information fusion through experiments.

The proposed model builds a channel of grids for each feature. Supposing the given central node with $f$ features utilizes $k$ neighbors to construct the Euclidean structured grid, we set the dimension of the grid-like data to $k \times 1 \times f$, where $f$ is the number of node features and $k \times 1$ is the grid size in each channel. Mapping methods is illustrated in Figure 2. For a given central node, we use the first-order neighbors $N_1$ and second-order neighbors $N_2$ for padding by selecting the top $k$ neighbors ranking by their degree value. Searching second-order neighbors increases the time consuming, Node2Img can control whether to bring in second-order neighbors or not by adjusting the setup of $k$ according to the connectivity about network. Notably, if $k > |N_1| + |N_2|$, the default value of an unfilled grid is set to zero.

At the last step, the proposed Node2Img conducts information fusion. To illustrate the importance of the given node around the grid-like data, we fuse current grids’ features with the corresponding given node’s. Concretely,

$$G = \theta_{bias} * G_c + (1 - \theta_{bias}) * G_n,$$  \hspace{1cm} (1)

where $G_n \in \mathbb{R}^{k \times 1 \times f}$ is the grid-like data built by only selected neighbors. We obtain $G_c \in \mathbb{R}^{k \times 1 \times f}$ extended from the central node, in which the grids of each channel are filled with the corresponding features of the central node. And $\theta_{bias}$ is the bias coefficient of information fusion, which enables modifying the proportion of central node character.

### 3.2 Grid-like Data Processing

As an effective Euclidean structured data processing method, we applies ordinary convolutional neural network (CNN) to perform downstream tasks instead of GCN. We use grid-like data as “images” in the training phrase, and apply a 1-D convolution kernel to extract important information from the grid-like data. For performing node classification tasks, Node2Img implements a simple but flexible three-layer neural network. In addition, we use the attention mechanism to learn the weight of each grid in grid-like data around all channels.

**Attention Mechanism.** For general Euclidean structured data such as images, “pixels” in different grids play different roles in expressing the “image” [25]. Similarly, different neighbors have different influences to the central node [14]. Thus, it’s significant to learn the attentions on the neighbors with different level influences. We propose a learning attention filter to specify the weights in grid like data. It is worth noting that all channels of grid like data share the same filter parameters, which greatly reduces the parameters, since it needs to focus on neighborhood rather than the features.

Hadamard product implements a convenient attention mechanism on Node2Img’s structured grid data, which is different from the previous framework’s massive attention operations on all adjacent nodes.

**CNN-based network architecture.** After mapping, we use the general convolution kernel to extract the high-level information from the mapped Euclidean structure data. Compared with the previous work of neighborhood feature aggregation using GCN, a simple three-layer network structure based on CNN is adopted to deal with grid data, which boots the training progress, saves memory and improves flexibility. Specifically, we apply a convolutional layer and two fully connected layers in our architecture. It is worth noting that the second fully connected layer is used as a classifier. And the layer-wise propagation rule of Node2Img is formulated as:

$$x_l = \text{Conv}(G),$$

$$x'_l = x_l + \frac{1}{h} \sum_{t=1}^{h} F_{att} \circ x_t,$$ \hspace{1cm} (2)

$$\tilde{x}_l = g(x'_l),$$

where $G \in \mathbb{R}^{k \times 1 \times f}$ is the mapped Euclidean structured data, in which $k \times 1$ represents the grid size in each channel and $f$ represents the number of channels. In this case, $G$ contains the fusion characters between the central node and its neighbors. $\text{Conv}(\cdot)$ is a regular 1-D CNN that extracts the significant information for grid-like data, in which the kernel size is $n_{ker}$ and the stride is set to 1, without any padding strategy. Besides, Node2Img employs the Hadamard product $\circ$ to realize attention mechanism. Note that the multi-head attention mechanism is applied, the $F_{att} \in \mathbb{R}^{(k-n_{ker}+1) \times 1 \times f}$ is a single attention filter, where the number of learnable parameters is $(k-n_{ker}+1) \times 1$ (i.e. all channels of grid-like data share the same filters’ parameters). In addition, $g(\cdot)$ is the function of fully-connected layers and $\tilde{x}_l$ is the output of the three-layer network.

### 3.3 Modified Loss Function

For making the general L2 loss function adapted to the proposed model, we modify it by multi-value $l_2$-regularization.
The modified loss function of Node2Img is defined as:

\[ L_{total} = L(y, \bar{y}) + \lambda \sum w^2 + \lambda_{att} \sum w^2_{att}, \]  

where \( y \) and \( \bar{y} \) are predicted labels and real labels of nodes respectively, \( w \) and \( w_{att} \) are the learnable parameters in neural networks and attention filters respectively. In addition, \( \lambda \) and \( \lambda_{att} \) are \( l_2 \)-regularization coefficients for neural networks and attention filters respectively. \( L(y, \bar{y}) + \lambda \sum w^2 \) is the general loss function with \( l_2 \)-regularization. And \( \lambda_{att} \sum w^2_{att} \) is the formula of \( l_2 \)-regularization for attention filters to prevent over-fitting. Notably, \( \lambda_{att} > \lambda_{l_2} \), which allows a stronger constraints to the parameters updating for attention filters.

4 Experiments

In this section, we describe the proposed Node2Img in two classes of node classification tasks, i.e. transductive and inductive learning problems. We describe the datasets applied for node classification tasks and the setups of our model. In addition to demonstrate the effectiveness against the state-of-the-art GCN-based approaches, we also verify the high efficiency of the proposed model by comparing with leading approaches. Moreover, we discuss the effect of hyper-parameters as well as the effectiveness of attention mechanism.

4.1 Datasets

We conduct the experiments on both transductive and inductive learning datasets. The statistics of the datasets are summarized in Table 1.

| Dataset | #Nodes | #Features | #Classes | #Training Nodes | #Validation Nodes | #Test Nodes | Task          |
|---------|--------|-----------|----------|----------------|------------------|-------------|---------------|
| Cora    | 2708   | 1433      | 7        | 140            | 500              | 1000        | Transductive  |
| Citeseer| 3327   | 3703      | 6        | 120            | 500              | 1000        | Transductive  |
| Pubmed  | 19717  | 500       | 3        | 60             | 500              | 1000        | Transductive  |
| PPI     | 56944  | 50        | 121      | 44906          | 6514             | 5524        | Inductive     |

Table 1: Summary of the datasets used in the experiments.

The training progress, which requires the model to trains a global function to obtain embeddings for testing or validation nodes. To this problem, we conduct the experiments on protein-protein interaction (PPI) dataset [29] which contains graphs corresponding to different human tissues. The dataset consists of 20 training graphs, 2 validation graphs and 2 testing graphs. The average number of nodes are 2372 in each graph. There are 50 features for each nodes, including positional sets, motif genes sets and signatures. And there are multiple labels from 121 classes for each node. Notably, the validation graphs and testing graphs are unseen during the training progress.

4.2 Experimental Setup

In this section, we describe the experimental setup in the proposed model in both transductive and inductive learning tasks.

Transductive learning task. For general graph convolutional approaches, transductive learning task is based on semi-supervised learning theory requiring nodes from the full graph are available when training, including the testing nodes whose labels is invisible. In comparison, the proposed model modifies the full-batch based strategy, only leveraging partial nodes from the training set with batch size elastically set. For Cora, Citeseer and Pubmed datasets, the batch sizes are 15, 30 and 8 respectively. We apply RMSprop optimizer [30] to train the model, with the learning rate as 0.008 and weight decay as 0.0005. The dropout strategy [31] is applied in the first fully-connected layer, with the rate of 0.5. Note that the attention mechanism is introduced, there are 50 attention heads with the \( \lambda_{att} \) set to 0.0008, 0.025 and 0.07 for Cora, Citeseer and Pubmed datasets respectively.

Inductive learning task. We conduct the inductive learning experiments on protein-protein interaction (PPI) dataset which is a large-scale graph. The batch size is set to 2000 in each iteration. The Nadam optimizer [32] is employed, in which the learning rate is set to 0.001 and the value of coefficient A is set to 5 \( \times 10^{-7} \) for \( l_2 \) regularization. In addition, The dropout [31] rate is set to 0.5 in both convolutional layer and the first fully-connected layer. And there are also 50 attention heads applied with \( \lambda_{att} = 1 \times 10^{-6} \) for \( l_2 \) regularization.

4.3 Comparison of Effectiveness

In the experiments, the proposed Node2Img is compared with the prior state-of-art approaches in both inductive and transductive learning tasks. We demonstrate the comparative evaluations of the proposed Node2Img model on Cora, Citesser, Pubmed and PPI datasets.
For node classification tasks, the proposed Node2Img model significantly exceeds the prior leading frameworks in and LGCN, by margins of 0.477 and 0.205 respectively. GCN-based mini-batch approaches. (i.e., GraphSAGE-GCN especially gaining a great progress over the representative set over 10 runs. From Table 3, it can be observed that the score (with standard deviation) of the nodes in unseen testing.

results for both transductive and inductive learning tasks. The superior performance of Node2Img demonstrates the great effectiveness in two aspects. Firstly, the mapping strategy can efficaciously reflect the raw graph, paving the way for downstream missions. In addition, the three-layer neural network structure does well in extracting meaningful characters from the grid-like data.

### 4.4 Comparison of Computational Efficiency

In this part, we verify the high efficiency of the proposed model by comparison with previous GCN-based approaches. We conduct experiments on the three benchmark datasets (i.e., Cora, Citeseer and Pubmed datasets) as well as the simulation graphs, on the configuration of i7-7820X CPU and GTX 1080 Ti. Notably, there are two factors having impacts on the time cost, which are (1) time spending for each epoch, (2) the convergence speed. To this end, we report the average time by the training progress from startup to obtain a valid testing model over 30 runs. For the sake of fairness, we take into account the time of generating the grid-like data in Node2Img, and these three models do calculations on both training set (for training the model) and validation set (just for validation) in each iteration.

The results of comparison on real-world networks are summarized in Table 4, where the LGCN sub is LGCN model with the sub-graph generating algorithm to speedup the training progress. From the results shown in Table 4, GCN achieves better efficiency on Cora and Citeseer datasets due to the parallel computations in small graphs. However, for Pubmed dataset, it’s harder to process a large number of nodes for GCN, with efficiency greatly reduced. As for LGCN sub, it spends more time because of sampling a relatively large subgraph for validation set which need to be processed by GCN.

The performance demonstrates the significant efficiency and effectiveness of the proposed Node2Img model, especially in Pubmed which is a large graph with 19717 nodes.

In order to further evaluate the scalability of Node2Img, we conduct experiments on large simulation networks. We generate nodes with labels based on the planted-l-partition model [35], where the feature distributions are assigned on the basis of Madelon benchmark networks [36]. Specially, we refer to Pubmed dataset to set average node degree and class number to 6 and 3 respectively. Additionally, each node belongs to a single class with 500 features. Two magnitudes of networks

| Method                  | PPI       |
|-------------------------|-----------|
| GraphSAGE-GCN [13]      | 0.500     |
| GraphSAGE-LSTM [13]     | 0.612     |
| LGCN [15]               | 0.772     |
| GAT [14]                | 0.973     |
| Node2Img without Attention | 0.971 ± 0.003 |
| Node2Img (Ours)         | 0.977 ± 0.002 |

**Baseline methods.** DeepWalk [33] is a representative network embedding method, using the random walk to sample some nodes and obtains the embedding for the given node by these sampled nodes. Chebyshev [34] and GCN [1] is the leading approaches for graph learning in spectral domain. Based on GCN, hGANet [22] is the state-of-the-art model by introducing modified attention mechanism. GraphSAGE [13], GAT [14] and LGCN [15] is the minibatch based strategies, which can conduct the inductive learning tasks on large-scale graph. Notably, GraphSAGE-GCN [13] is an framework extending GCN to inductive learning tasks. And GraphSAGE-LSTM [13] is the GraphSAGE-based model employing LSTM as aggregators.

**Transductive learning task.** In transductive learning problem, the results are reported by mean classification accuracy with the standard deviation over 100 runs as [1]. From the results summarized in Table 2, the proposed Node2Img outperforms the current leading GCN-based models, especially achieving a great improvement over the original GCN by margins of 2.2%, 2.9% and 0.8% on the datasets of Cora, Citeseer and Pubmed respectively.

**Inductive learning task.** In inductive learning problem, we follow the study of [13] to report the micro-averaged F1 score (with standard deviation) of the nodes in unseen testing set over 10 runs. From Table 3, it can be observed that the proposed Node2Img performs better than previous methods, especially gaining a great progress over the representative GCN-based mini-batch approaches. (i.e., GraphSAGE-GCN and LGCN, by margins of 0.477 and 0.205 respectively).

For node classification tasks, the proposed Node2Img model significantly exceeds the prior leading frameworks in

| Method                  | Cora       | Citeseer   | Pubmed    |
|-------------------------|------------|------------|-----------|
| DeepWalk [33]           | 67.2%      | 43.2%      | 65.3%     |
| Chebyshev [34]          | 75.7%      | 64.7%      | 77.2%     |
| GCN [1]                 | 81.5%      | 70.3%      | 79.0%     |
| GAT [14]                | 83.0%      | 72.5%      | 79.0%     |
| LGCN [15]               | 83.3%      | 73.0%      | 79.5%     |
| hGANet [22]             | 83.5%      | 72.7%      | 79.2%     |
| Node2Img without Attention | 83.1 ± 0.2% | 72.4 ± 0.5% | 76.3 ± 0.7% |
| Node2Img (Ours)         | 83.7 ± 0.2% | 73.2 ± 0.4% | 79.8 ± 0.5% |

**Table 2:** The Summary of results for transductive learning experiments in terms of average node classification accuracy, on the dataset of Cora, Citeseer and Pubmed.

| Method                  | Cora       | Citeseer   | Pubmed    |
|-------------------------|------------|------------|-----------|
| Node2Img without Attention | 83.1 ± 0.2% | 72.4 ± 0.5% | 76.3 ± 0.7% |
| Node2Img (Ours)         | 83.7 ± 0.2% | 73.2 ± 0.4% | 79.8 ± 0.5% |

**Table 3:** The summary of results in terms of average micro-averaged F1 score for inductive learning tasks, on the dataset of PPI.
Table 4: Results of comparison in time cost and node classification accuracy with GCN and LGCN (using the sub-graph strategy for LGCN, i.e LGCN$_{sub}$), on the datasets of Cora, Citeseer and Pubmed. The time cost is averaged from the start to the end of the training over 30 runs. Notably, the time cost consists of both mapping and training progress in the proposed Node2Img model.

|                | Cora          | Citeseer      | Pubmed        |
|----------------|---------------|---------------|---------------|
| **GCN**        |               |               |               |
| Batch size     | 2708          | 3327          | 19717         |
| Time           | 2.8s          | 4.6s          | 20.9s         |
| Accuracy       | 81.5%         | 70.3%         | 79.0%         |
| **LGCN$_{sub}$** |               |               |               |
| Batch size     | 644           | 442           | 354           |
| Time           | 53.2s         | 27.6s         | 57.6s         |
| Accuracy       | 83.3%         | 73.0%         | 79.5%         |
| **Node2Img (Ours)** |           |               |               |
| Batch size     | 15            | 30            | 8             |
| Time           | 5.3s          | 5.9s          | 7.3s          |
| Accuracy       | 83.7 ± 0.2%   | 73.2 ± 0.4%   | 79.8 ± 0.5%   |

Figure 4: The results of experiments on large simulation networks, where N represents the size of dataset (i.e. the number of nodes in a network). The average node classification accuracy and time cost over 30 runs are reported in these experiments. In addition, the memory usages are reported on 0.1M and 1M graphs, with 500 and 5000 training nodes on these two graphs respectively.

4.5 The Study of Central-Fusion and Grid Size

In this section, we explore the influence of hyper-parameter $k$ and $\theta_{bias}$ on the datasets of Cora, Citeseer and Pubmed respectively. The Node2Img utilized central node fusion (Central-Fusion) to make sure that the character of the given central node can be expressed over the grid-like data globally, in which the $\theta_{bias}$ represents the level of central node fusion. (i.e. the greater $\theta_{bias}$, the more partition of central node character in the Euclidean grid). We select $k$ neighbors based on the value of degree and construct $k$-D grid-like data in each channel for the given node. Intuitively, the hyper-parameter $k$ represents the level of introducing neighbors’ information. We report node classification accuracy to evaluate the effect of $k$ and $\theta_{bias}$. The results are summarized in Figure 5.

For the effect of Central-Fusion, it can be obviously discovered that this strategy achieves positive influence by comparing the situation of $\theta_{bias} = 0$ to a significant value of $\theta_{bias}$. From Figure 5, the model performs best on these three datasets when $\theta_{bias} = 0.4$. Particularly, Node2Img performs worse when the $\theta_{bias}$ is greater or less than the applicable value, which indicates that it exists a reasonable proportion for central node fusion. In other words, deficiency or redundant of the central node character will result in the deviation of expressing the raw graph. As for inductive learning tasks on PPI dataset, there also exist an applicable setup for $\theta_{bias}$ with a value of 0.55.

On Cora, Citeseer and Pubmed datasets, these three networks are sparse with the average node degrees of 4, 5 and 6 respectively. It can be seen from the Figure 5 that $k$ is set appropriately with values of 16, 12 and 12 for Cora, Citeseer and Pubmed respectively. Notably, these best setups for $k$ introduce proper second-neighboring characters to enrich the grid-like data. At a word, the proposed Node2Img model requires a reasonable grid size (i.e. $k$) to build the grid-like data. When $k$ is too small, it’s difficult for the inadequate neighbors to reflect the origin graph. While $k$ is too large, there are two aspects of decreasing the performance for Node2Img: on
Figure 5: The results of exploring the influence of $\theta_{bias}$ and $k$ on the datasets of Cora, Citeseer and Pubmed respectively. The setups described in Section 4.2 are used. The node classification accuracy is reported in these experiments. The x-coordinate and y-coordinate represent $k$ and mean accuracy respectively. And the different colored lines represent the different occasions for $\theta_{bias}$.

Figure 6: An example of the average convergent attention filters, where the $1 \times 1$ convolutional kernel and 8-D grid-level attention filters are applied, with $\theta_{bias}$ set to zero. We select the top 8 neighbors to build candidate sets which are ranked by node degree. The order we put the neighbors into grids is from the top to bottom. In (a) and (b), the nodes from candidate sets are putted to the grids in order and in reverse order respectively. The case of (c) is that the given central node features are put into the first 3 grids from the top to bottom and the other grids are filled with neighbors in order from the candidate set.

On one hand, the large $k$ means selecting various of second-order neighbors for mapping, resulting in bringing in the redundant second-order information which causes a negative impact on expression of the closer first-order neighbors; On the other hand, the model pads too much zero in the grid-like data, which compromises the performance of subsequent extraction task. Moreover, we also conduct the experiments to explore the setting of $k$ for PPI dataset. Note that the best setup for $k$ is 16 in PPI graphs which is smaller than its average node degree (with a value of 31), indicating that the Euclidean grid can be built without introducing the second-order neighbors if the network is not sparse.

4.6 The Study of Attention Mechanism

During the progress of grid-like data processing, we employ the grid-level attention mechanism to learn the weights of grids in the grid-like data. As shown in Table 2, Node2Img with attention mechanism gains better performances by margins of 0.6%, 0.8% and 3.5% on Cora, Citeseer and Pubmed datasets respectively against the model without attention mechanism. As for inductive learning tasks on PPI dataset, Node2Img applying attention mechanism also outperforms by a margin of 0.006 in Table 3.

In addition, we further analyze the “attentions” of the grid-level attention filters. For the constructed Euclidean grid, the different grids in a channel should have different status. Due to the factor that the node degree represents the influences of nodes, we suspect the grids filled with more influential neighbors have greater weights intuitively. In Figure 6, we present the average convergent attention filters of Cora dataset in the form of heat map, where the grids with greater value are drawn darker. Specially, the $1 \times 1$ convolutional kernel and $\theta_{bias} = 0$ are applied to avoid the fusion of extra nodes. It can be observed from Figure 6(a)(b) that the grids with greater node degree have the darker color regardless of placing the sorted nodes in order or inversion. Besides, from Figure 6(c), it can be discovered that the grids filled with central nodes have almost the same darkest color. Through the aforementioned phenomenons, we demonstrate that the attention mechanism enables specifying the weights for neighbors with different level influences implicitly. Furthermore, from the results that the more influential neighbors tend to gain more attentions, we can prove that the effectiveness of degree-based selection strategy indirectly.

5 Conclusion

In this paper, we present a flexible framework which demonstrates the great superiority in processing large-scale graph. Compared with the full-batch approach as original GCN, Node2Img achieves the flexibility by elastic mini-batch strategy, mapping the graph data to Euclidean grid which can be processed by CNN-based approaches. Through extensive experiments, we show that Node2Img enjoys significantly lower cost in both time and memory against the original GCN, meanwhile gains the great effectiveness on both transductive and inductive learning tasks against state-of-the-art models, which indicates that Node2Img is more applicable than GCN-based methods in practice. Moreover, we explore the availability of the strategies applied in Node2Img during the experiments. As a novel approach for processing graph data, we believe that it is well worth further study on account of its remarkable adaptability. In the future, it’s meaningful to extent this flexible architecture to various graph learning tasks.
References

[1] Thomas N. Kipf, Max Welling. 2017. Semi-supervised classification with graph convolutional networks. In International Conference on Learning Representations (ICLR).

[2] Abu-El-Haija, Sami and Kapoor, Amol and Perozzi, Bryan and Lee, Jooneok. 2018. N-gcn: Multi-scale graph convolution for semi-supervised node classification. arXiv preprint arXiv:1802.08888.

[3] Wenting Zhao, Zhen Cui, Chunyan Xu, Chengzheng Li, Tong Zhang, Jian Yang. 2019. Hashing Graph Convolution for Node Classification. In Proceedings of the 28th ACM International Conference on Information and Knowledge Management. 519-528

[4] Muhan Zhang, Yixin Chen. 2018. Link prediction based on graph neural networks. 2018. In Advances in Neural Information Processing Systems (NIPS). 5165-5175.

[5] Lei Kai, Meng Qin, Bo Bai, Gong Zhang, Min Yang. 2019. GCN-GAN: A non-linear temporal link prediction model for weighted dynamic networks. In IEEE INFOCOM 2019-IEEE Conference on Computer Communications. 388-396.

[6] Di Jin, Ziyang Liu, Weihao Li, Dongxiao He, Weixiong Zhang. 2019. Graph convolutional networks meet Markov random fields: Semi-supervised community detection in attribute networks. In Proceedings of the AAAI Conference on Artificial Intelligence. 33: 152-159.

[7] Fanghua Ye, Chuan Chen, Zibin Zheng, Rong-Hua Li, Jeffrey Xu Yu. Discrete Overlapping Community Detection with Pseudo Supervision. 2019. 2019 IEEE International Conference on Data Mining (ICDM). 708-717.

[8] Wei-Lin Chang, Xuanqing Liu, Si Si, Yang Li, Samy Bengio, Cho-Jui Hsieh. 2019. Cluster-gcn: An efficient algorithm for training deep and large graph convolutional networks, In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD). 257-266.

[9] Jianfei Chen, Jun Zhu, Le Song. Stochastic training of graph convolutional networks with variance reduction. 2018. In International Conference on Machine Learning. 941–949.

[10] Michalski, Ryszard S. 1983. A theory and methodology of inductive learning. Machine learning. Springer. 83-134.

[11] Jie Chen, Tengfei Ma, Cao Xiao. 2018. Fastgcn: fast learning with graph convolutional networks via importance sampling. In International Conference on Learning Representations (ICLR).

[12] Hinton Geoffrey, Nitish Srivastava, Kevin Swersky. 2012. Overview of mini-batch gradient descent. In Neural Networks for Machine Learning. 575.

[13] Will Hamilton, Rex Ying, Jure Leskovec. 2017. Inductive representation learning on large graphs. In Advances in neural information processing systems. 1024-1034.

[14] Petar Velickovic, Guillem Cucurull, Arantxa Casanova, Pietro Lio, Yoshua Bengio. 2018. Graph attention networks. In International Conference on Learning Representations (ICLR).

[15] Hongyang Gao, Zhengyang Wang, and Shuiwang Ji. 2018. Large-scale learnable graph convolutional networks. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD). 1416-1424.

[16] Jiang Wang, Yi Yang, Junhua Mao, Zhiheng Huang, Chang Huang, Wei Xu. 2016. CNN-RNN: A Unified Framework for Multi-Label Image Classification. In The IEEE Conference on Computer Vision and Pattern Recognition (CVPR). 2285-2294

[17] Thibaut Durand, Taylor Mordan, Nicolas Thome, Matthieu Cord. 2017. WILDCAT: Weakly Supervised Learning of Deep ConvNets for Image Classification, Pointwise Localization and Segmentation. In The IEEE Conference on Computer Vision and Pattern Recognition (CVPR). 642-651

[18] Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton. 2012. Imagenet classification with deep convolutional neural networks. In Advances in neural information processing systems (NIPS). 1097-1105.

[19] Mathias Niepert, Mohamed Ahmed, and Konstantin Kutzkov. 2016. Learning convolutional neural networks for graphs. In International Conference on Machine Learning (ICML). 2014–2023

[20] Muhan Zhang, Zhicheng Cui, Marion Neumann, and Yixin Chen. 2018. An end-to-end deep learning architecture for graph classification. In Proceedings of AAAI Conference on Artificial Intelligence.

[21] Hongyang Gao, Shuiwang Ji. Graph u-net. 2019. In Proceedings of the 36th International Conference on Machine Learning (ICML).

[22] Hongyang Gao, Shuiwang Ji. Graph representation learning via hard and channel-wise attention networks. 2019. In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD). 741-749.

[23] Xiaohui Zhao, Fangai Liu, Jinlong Wang and Tianlai Li. 2017. Evaluating influential nodes in social networks by local centrality with a coefficient. In ISPRS International Journal of Geo-Information. 6(2):35.

[24] Hong-suda Tangmunarunki, Ramesh Govinda, Sugih Jami, Scott Shenke, Walter Willinge. 2002. Network topology generators: Degree-based vs. structural. In ACM SIGCOMM Computer Communication Review. 32(4): 147-159.

[25] Jim Adams, Ken Parulski, and Kevin Spaulding. 1998. Color processing in digital cameras. In IEEE micro. 18(6): 20-30.
[26] Shuangbiao Liu, Qian Wang, Geng Liu. 2000. A versatile method of discrete convolution and FFT (DC-FFT) for contact analyses. Wear. 243(1-2): 101-111.

[27] Hongyun Cai, Vincent W. Zheng, and Kevin Chen-Chuan Chang. 2018. A comprehensive survey of graph embedding: Problems, techniques, and applications. In IEEE Transactions on Knowledge and Data Engineering. 30(9): 1616-1637.

[28] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Gallagher, and Tina Eliassi-Rad. 2008. Collective classification in network data. AI magazine. 29(3): 93-93.

[29] Marinka Zitnik and Jure Leskovec. 2017. Predicting multicellular function through multi-layer tissue networks. Bioinformatics. 33(14): i190–i198.

[30] Tijmen Tieleman and Geoffrey Hinton. 2012. Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude. In Coursera: Neural Networks for Machine Learning.

[31] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. 2014. Dropout: A simple way to prevent neural networks from overfitting. In Journal of Machine Learning Research. 15(1): 1929–1958

[32] Timothy Dozat. Incorporating Nesterov Momentum into Adam. 2016. In ICLR Workshop. (1):2013–2016.

[33] Bryan Perozzi, Rami Al-Rfou, Steven Skiena. 2014. Deepwalk: Online learning of social representations. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining (KDD). 701-710.

[34] Michäel Defferrard, Xavier Bresson, Pierre Vandergheynst. 2016. Convolutional neural networks on graphs with fast localized spectral filtering. In Advances in neural information processing systems (NIPS). 3844-3852.

[35] Santo Fortunato. 2010. Community detection in graphs. Physics reports. 486(3-5): 75-174.

[36] Guyon, Isabelle. 2003. Design of experiments for the NIPS 2003 variable selection benchmark.