GRAPH SELF-ATTENTION FOR LEARNING GRAPH REPRESENTATION WITH TRANSFORMER

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ABSTRACT

We propose a novel Graph Self-Attention module to enable Transformer models to learn graph representation. We aim to incorporate graph information on the attention map and hidden representations of Transformer. To this end, we propose context-aware attention which considers the interactions between query, key and graph information. Moreover, we propose graph-embedded value to encode the graph information on the hidden representation. Our extensive experiments and ablation studies validate that our method successfully encodes graph representation on Transformer architecture. Finally, our method achieves state-of-the-art performance on multiple benchmarks of graph representation learning, such as graph classification on images and graph regression on quantum chemistry.

1 INTRODUCTION

A graph is a data structure that consists of nodes and edges, which can represent many forms of data from various domains, e.g., molecule for drug development (Wu et al., 2018; Hu et al., 2020), social network analysis (Vashishth et al., 2019; Ali et al., 2021), or image classification with a graph of superpixels (Dwivedi et al., 2020). Due to its distinctive structure, specialized neural networks, such as graph convolutional networks (GCN), are proposed (Kipf & Welling, 2016; Veličković et al., 2017; Gilmer et al., 2017; Xu et al., 2018; Corso et al., 2020).

In the meantime in other domains, such as natural language processing (Devlin et al., 2018; Brown et al., 2020) or image processing (Dosovitskiy et al., 2020; Touvron et al., 2021; Liu et al., 2021), Transformer (Vaswani et al., 2017) is adopted as a de-facto standard architecture instead of specialized neural networks. However, learning a graph representation with a Transformer model is particularly challenging due to the structural flexibility of a graph, because the Transformer was devised for sequential data, not for a graph. Recently, several algorithms have been proposed to leverage Transformers for learning graph representation (Dwivedi & Bresson, 2020; Kreuzer et al., 2021; Ying et al., 2021).

Those methods incorporate graph information on the Transformer in two perspectives: (1) how to encode graph information on the attention map of the self-attention module? (2) how to encode graph information on the hidden representations of Transformer?. For instance, Ying et al. (2021) encodes graph information on the attention map by adding bias terms and encodes graph information on the input with centrality encoding. Meanwhile, Dwivedi & Bresson (2020); Kreuzer et al. (2021) replace positional encoding into graph Laplacian (Belkin & Niyogi, 2003). We examine possible improvements from previous methods and propose our novel self-attention module for learning graph representation on Transformer.

Our design choices are based on resolving the issues in the two perspectives. For encoding graph information on the attention map, we introduce context-aware attention which considers the interactions between query, key, graph structure, and edges. For the hidden representations of Transformer, we devise graph-embedded value which encode graph information directly on the value. Putting all these improvements together, we propose Graph Self-Attention (GSA) module for learning graph representation on Transformer. In our experiments, we achieve state-of-the-art performance on var-

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Figure 1: Our proposed Graph Self-Attention module (GSA). GSA is a variant of self-attention module of Transformer (Vaswani et al., 2017) to learn graph representation. GSA learns graph representation by encoding graph structure on both the attention map and the hidden representation.

ious graph benchmarks from graph classification to graph regression with Transformer models built with GSA, showing the efficacy of our proposed method.

2 Transformer for Graph

There are many attempts of leveraging transformer into the graph domain. Existing methods (Velickovic et al., 2017; Kreuzer et al., 2021; Dwivedi & Bresson, 2020; Zhang et al., 2020; Ying et al., 2021) have improved the transformer architecture to fit the graph input by improving the attention map or replacing the positional embedding to fit the graph, or both, which are more related to our GSA. Methods like Graph Attention Networks (GAT) (Velickovic et al., 2017) and Graph Transformer (GT) (Dwivedi & Bresson, 2020) constrain the self-attention mechanism to neighboring nodes. GT (Dwivedi & Bresson, 2020) suggests that the attention mechanism in transformers on graph data should only aggregate the information from the neighborhood by using the adjacent matrix as an attention mask to ensure graph sparsity with Laplacian eigenvector positional encoding. They surpass GNN baseline methods on the graph representation task. Spectral Attention Network (SAN) (Kreuzer et al., 2021) employs a learned positional encoding (LPE) of Laplacian spectrum to learn the position of nodes in a graph. Graph-BERT (Zhang et al., 2020) uses several types of relative positional encodings to embed the information about the edges within a subgraph. Graphormer (Ying et al., 2021) proposes centrality and spatial encoding to capture node importance and structural relations by modifying attention map and node encodings. Graphormer integrates edges in the graph as a bias added to the attention map.

Some methods (Rong et al., 2020) have proposed a method that mixes GNN and transformers. GROVER (Rong et al., 2020) modifies several parts of the transformer by employing an additional graph neural network to produce inputs of transformers, long-range residual connection, and two branches of fully-connected layers.

3 Background

Notation. We denote a set of nodes on the graph \( \{n_i\}_{i=1}^N \) and a set of edges on the graph \( \{e_{ij}\}_{i=1}^N \subseteq \mathcal{N}_i \) where \( N \) is the number of nodes and \( \mathcal{N}_i \) is a set neighbors of a node \( n_i \). Both \( n_i \) and \( e_{ij} \) are positive integer numbers to index the type of nodes or edges, e.g., atom numbers or bond types of a molecule. \( \psi(i, j) \) denote a function encodes structural relationship between the node \( n_i \) and \( n_j \). For the remaining section, \( \psi \) is a structural relationship encoder that outputs the shortest path distance between node \( n_i \) and \( n_j \). \( \cdot \) denotes the inner product between two vectors.

3.1 Transformer

The Transformer encoder are built by stacking multiple self-attention layers. Self-attention (Vaswani et al., 2017) is a major module of the Transformer. It maps a query and a set of key pairs to compute an attention map. A value is aggregated with the attention map to output the hidden feature for the following layer.
Specifically, \( x_i \in \mathbb{R}^{d_x} \) denotes the input feature of the node \( n_i \), and \( z_i \in \mathbb{R}^{d_z} \) denotes the output feature of the self-attention module. The self-attention module computes query \( q \), key \( k \), and value \( v \) with independent linear transformations: \( W^{\text{query}} \in \mathbb{R}^{d_x \times d_z} \), \( W^{\text{key}} \in \mathbb{R}^{d_x \times d_z} \), and \( W^{\text{value}} \in \mathbb{R}^{d_x \times d_z} \).

\[
q = W^{\text{query}}x, \quad k = W^{\text{key}}x, \quad \text{and} \quad v = W^{\text{value}}x.
\]

The attention map is computed by applying a scaled-dot product between the queries and the keys.

\[
a_{ij} = \frac{q_i \cdot k_j}{\sqrt{d_z}} \quad \text{and} \quad \hat{a}_{ij} = \frac{\exp(a_{ij})}{\sum_{k=1}^{N} \exp(a_{ik})}.
\]

The self-attention module outputs the next hidden feature by applying weighted summation on the values.

\[
z_i = \sum_{j=1}^{N} \hat{a}_{ij} v_j.
\]

\( z \) is later fed into a feed-forward neural network (FFN) with a residual connection [He et al., 2016]. However, we defer detailed explanations since it is out of the scope of our paper. In practice, multi-head self-attention module that exploits multiple self-attention maps in parallel is adopted.

### 3.2 Previous Approaches for Learning Graph with Transformer

To encode graph structure in Transformer, previous methods focus on encoding graph information into either the attention map or the hidden representations of Transformer. Graphormer (Ying et al., 2021) adopted two special learnable terms on the self-attention module to encode graph information on the attention map.

\[
a_{ij}^{\text{Graphormer}} = \frac{q_i \cdot k_j}{\sqrt{d_z}} + b_{\psi(i,j)} + \mathcal{E}_{e_{ij}} \cdot w.
\]

Learnable scalar bias \( b_{\psi(i,j)} \) encodes structural relationship between two nodes, e.g., \( b_{1} \) is a bias representing two nodes that are \( l \)-hop apart. \( \mathcal{E}_{e_{ij}} \cdot w \) encodes edge information between nodes. An embedding vector \( \mathcal{E}_{e_{ij}} \) is a feature representing edge between the node \( n_i \) and the node \( n_j \), and \( w \) is a learnable vector. To encode graph structure on the hidden representation, Graphormer adds Centrality encoding into the input \( x \) which represents the number of edges of a node.

Graphormer integrates graph structure directly on the attention map with the bias terms. However, our method encodes graph information on the attention map considering contextual relationship between node features and graph information. We will explain the details in Section 4.1.

Some approaches (Dwivedi & Bresson, 2020; Kreuzer et al., 2021) utilize graph Laplacian (Belkin & Niyogi, 2003) \( \lambda \in \mathbb{R}^{N \times d_z} \) as positional encodings on the input feature \( x \); \( \lambda \) are the top-\( d_z \) smallest eigenvectors of \( I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} \) where \( I \) is an identity matrix, \( A \) is an adjacency matrix and \( D \) is a degree matrix. The graph Laplacian \( \lambda_i \) represents the structure of a graph with respect to node \( n_i \).

\[
\hat{x}_i = x_i + \lambda_i.
\]

In the case of (Kreuzer et al., 2021), an additional Transformer model \( f \) which outputs the learnable positional encoding when the graph Laplacian is given: \( \hat{x}_i = x_i + \hat{\lambda}_i \) where \( \hat{\lambda} = f(\lambda) \).

By adding the graph Laplacian into input \( x \), graph information can be encoded in both the attention map and the hidden representations. However, our method encode graph information directly on the features of the value. We will explain the details in Section 4.2.

### 4 Our Approach

We define structure embeddings \( \mathcal{P} \) for query, key, and value to encode the graph structure: \( \mathcal{P}^{\text{query}}, \mathcal{P}^{\text{key}}, \mathcal{P}^{\text{value}} \in \mathbb{R}^{L \times d_z} \). Each embedding vector of \( \mathcal{P} \) represents the structural relationship between nodes in a graph, e.g., \( \mathcal{P}_l \) represents the structural relationship of two nodes where their shortest path distance is \( l \). \( d_z \) is the dimension size of hidden features and \( L \) is the maximum shortest path distance that our method considers.
Figure 2: Illustration of the proposed Graph Self-Attention (GSA) module. The structural relationship between the nodes in a graph is represented with the shortest path distance, and the relationship is encoded with structure embedding. The maximum shortest path distance, that we considered in this example, is two. Edges between the nodes are encoded with the edge embedding. The equation with red-colored text denotes our context-aware attention which encodes graph structure in the attention map. The equation with blue-colored text denotes our graph-embedded value.

We define edge embeddings $\mathcal{E}$ for query, key, and value to encode edge information between two nodes in a graph: $\mathcal{E}_{\text{query}}, \mathcal{E}_{\text{key}}, \mathcal{E}_{\text{value}} \in \mathbb{R}^{E \times d_z}$. $\mathcal{E}_{ij}$ is a vector representing edge between two nodes $n_i$ and $n_j$. $E$ is the number of types of edge. The structure embeddings and the edge embeddings are shared throughout GSA modules.

### 4.1 Context-aware attention

We propose two terms to build our context-aware attention map. The first term $b_{ij}^{\text{query-context}}$ is query contextualized bias that considers the interaction between the query feature and the graph information; structural relationship and edge feature.

$$b_{ij}^{\text{query-context}} = q_i \cdot \mathcal{P}_{\text{key}}^{(1)}(i,j) + q_i \cdot \mathcal{E}_{ij}$$

(6)

Likewise, the second term $b_{ij}^{\text{key-context}}$ is a key contextualized bias that considers the interaction between the key feature and the graph information.

$$b_{ij}^{\text{key-context}} = k_j \cdot \mathcal{P}_{\text{query}}^{(1)}(i,j) + k_j \cdot \mathcal{E}_{ij}$$

(7)

Finally, the attention map is computed by summing the two biases and scaled-dot product between query and key:

$$a_{ij} = \frac{q_i \cdot k_j + b_{ij}^{\text{query-context}} + b_{ij}^{\text{key-context}}}{\sqrt{d_z}}.$$ 

(8)

Our two biases are parameterized by the hidden features (query and key) and graph information (structural relationship and edge) using the dot-product operations. Unlike Eq. (4) where any two nodes with the same distance apart share the same bias $b_{\psi(i,j)}$, our method deploys different bias according to the context of the query or key features.

### 4.2 Graph-embedded value

For natural language processing (Brown et al., 2020; Devlin et al., 2018) or computer vision tasks (Dosovitskiy et al., 2020, 2020), Transformer adopts positional encoding $\mathcal{P}_{\text{pos}}$ as the input of self-attention module to represent sequential data structure. The input features can be factorized into two terms: $W_i(x_i + \mathcal{P}_{i\text{pos}}) = v_i + \mathcal{P}_{i\text{pos}}$ where $\mathcal{P}_{i\text{pos}} = W_i \mathcal{P}_{i\text{pos}}$. By adding the two terms, the positional information is encoded in the hidden features of value with a summation. Likewise, we propose to encode graph structure in the value with a summation.
| Model Configurations | # Params | # Layers | Hidden dim | FFN layer dim | # Heads |
|----------------------|----------|----------|------------|---------------|---------|
| GSA-Tiny             | 106k     | 4        | 64         | 64            | 8       |
| GSA-Tiny2x           | 409k     | 4        | 128        | 128           | 16      |
| GSA-Small            | 489k     | 12       | 80         | 80            | 8       |
| GSA-Standard         | 46.2M    | 12       | 768        | 768           | 32      |
| GSA-Large            | 118.3M   | 18       | 1024       | 1024          | 32      |

Likewise, we add structure embeddings into the hidden features of value to encode structural information of a graph. Also, we add edge embeddings into value to encode edge features between two nodes:

\[
    z_i = \sum_{j=1}^{N} \hat{a}_{ij} (v_j + P_{\psi(i,j)} + E_{e_{ij}}).
\]  

Unlike the feeding structural information in the input \( x \), e.g., centrality encoding (Ying et al., 2021) or graph Laplacian of (Kreuzer et al., 2021; Dwivedi & Bresson, 2020), our method directly encodes graph information with learnable embeddings into the hidden features of value.

### 4.3 Implementation details

#### 4.3.1 Virtual node

Following (Gilmer et al., 2017; Ying et al., 2021), we adopt a special node called virtual node which is connected to all other nodes. The role of a virtual node is similar to the classification token (Devlin et al., 2018), where its output feature \( z \) is used as an input for the branch that predicts downstream tasks. Note that, the virtual node is not used for finding the shortest path between two nodes. Throughout all experiments, we add an additional virtual node to a graph to perform the downstream tasks.

#### 4.3.2 Structural relationship

We utilize the shortest path distance \( \psi(i,j) \) to describe the structural relationships between the two nodes \( n_i \) and \( n_j \). \( L \) is the maximum distance of the shortest path that we consider, and we utilize a special embedding vector \( P_{\text{far}} \) on context-aware attention for the node pairs with distance more than \( L \). For the nodes pairs that are unreachable, we utilize another special embedding vector \( P_{\text{unreachable}} \). Finally, for the pairs that are connected with the virtual node, we utilize another special embedding vector \( P_{\text{virtual}} \).

#### 4.3.3 Edge feature

Every pair of nodes does not have edge features, because some nodes are not connected. Therefore, we utilize a special embedding vector \( E_{\text{no}} \) for the pairs of node that are not connected with an edge: \( \{(n_i, n_j) | i \neq j \text{ and } j \notin N_i\}_{i=1:|N|} \). For the pair of two identical nodes, i.e., \( i = j \), we use a special embedding vector \( E_{\text{self}} \). Finally, for the pairs that are connected with the virtual node, we utilize another special embedding vector \( E_{\text{virtual}} \).

### 5 Experiment

† indicates the models adopted Transformer for learning graph representation. Bold faced text indicates the best result.

**Model Configurations.** We summarize the configurations of all the models we use in our experiments in Table 1. We carefully choose the hyper-parameters of the models for fair comparison with other methods. For instance, it is a convention to keep the number of parameters of a model to 100k or 500k for the MNIST, CIFAR10 from benchmarking-GNN (Dwivedi et al., 2020). For the models with 100k parameters, we design the GSA-tiny. For the models with 500k parameters,
Table 2: Results on MNIST graph classification accuracy. The higher the better.

| Method                  | #Params | ACC (%)     |
|-------------------------|---------|-------------|
| GCN Kipf & Welling (2016) | 101k    | 90.71 ± 0.22 |
| MoNet Monti et al. (2017)   | 104k    | 90.81 ± 0.03 |
| 3WLGNN Maron et al. (2019)  | 108k    | 95.08 ± 0.96 |
| GAT Velićković et al. (2017) | 110k    | 95.54 ± 0.21 |
| GIN Xu et al. (2018)       | 105k    | 96.49 ± 0.25 |
| GraphSage Hamilton et al. (2017) | 104k    | 97.31 ± 0.10 |
| GatedGCN Bresson & Laurent (2017) | 104k    | 97.34 ± 0.14 |
| EGT Hussain et al. (2021)  | ~100k   | 97.94 ± 0.19 |
| PNA Corso et al. (2020)    | ~100k   | 97.94 ± 0.12 |
| †GSA-Tiny (Ours)          | 106k    | 98.15 ± 0.14 |
| †GSA-Tiny2x (Ours)        | 409k    | 98.20 ± 0.08 |
| †GSA-Standard(Ours)       | 46.2M   | 98.18 ± 0.05 |

We simply double the embedding size, feature dimensions and the number of heads, resulting GSA-Tiny2x have 409k parameters in total. For molecule property prediction datasets such as ZINC, OGBG-MolPCBA, OGBG-MolHIV and PCQM4M datasets (Hu et al., 2020), we referenced the model configuration from Graphormer (Ying et al., 2021) for fair comparison.

5.1 Classification on Superpixel Graph of Images

We have demonstrated our method for the task of graph classification on image. We tested on two medium-scale datasets, MNIST (70K superpixel graphs, 40-75 nodes/graph), CIFAR10 (60K superpixel graphs, 85-150 nodes/graph) with the MIT License. These datasets are a semi-artificially generated datasets in which the nodes of each graph are created with the SLIC (Achanta et al., 2012) algorithm and the superpixel coordinates and intensity are assigned as node features. Each node forms edges by connecting with the 8 nodes closest to them.

We quantize the distance feature provided by (Dwivedi et al., 2020) with the number of the first decimal place and used it as an edge feature index, \( e_{ij} \). The evaluation metric is classification accuracy (ACC). All experiments are conducted for 5 times, and we report the mean and the standard deviation of the experiments. To benchmark the previous methods, we reference the existing results reported on (Dwivedi et al., 2020).

We set \( L \) to 3 for CIFAR10 throughout subsequent experiments. We adopt the linear learning rate decay, and the learning rate starts from \( 2 \times 10^{-4} \) and ends at \( 1 \times 10^{-9} \). We train the model 400 epoch with 3 epochs warm-up step, and measure test performance when validation loss hit the local minimum. In addition, we randomly dropout the attention map and the input to feed-forward neural networks with the probability of 0.1. We adopt GSA-Tiny and GSA-Tiny2x on Table 1 which have the similar number of parameters to the compared methods. We also adopt GSA-Standard to validate that the generalization ability of our method improves with the increased number of parameters.

Table 2 shows the results on MNIST graph classification benchmark. We achieve the state-of-the-art results in the MNIST dataset compared to the existing GCN-based methods. In the MNIST dataset, small models tend to achieve better accuracy than the large model due to overfitting incurred by over-parameterization. In the MNIST dataset, although the small models show better accuracy than the large model, most of the results converge at high accuracy showing that our models achieve good performance regardless of the model size.

Table 3 shows the results on CIFAR10 graph classification benchmark. Overall, our small model shows competitive accuracy compared to GCN-based methods. However, unlike GCN, the models of Transformer does not suffer from over smoothing (Li et al., 2020) issue even though multiple layers are stacked. Thus we trained our large model with the CIFAR10 dataset. This experiment demonstrate a superior accuracy that is 4.94% points higher than that of the existing GCN-based DGN (Beani et al., 2021) method. The model performance tends to increase as the model size increases. Moreover, our models with large learning parameters have less standard deviation compared to the GCN-based methods.
Table 3: Results on CIFAR10 graph classification accuracy. The higher the better.

| Method                  | #Params | ACC (%) |
|-------------------------|---------|---------|
| MoNet Monti et al. (2017) | 101k    | 54.66±0.52 |
| GIN Xud et al. (2018)    | 106k    | 55.26±1.53 |
| GCN Kipf & Welling (2016)| 101k    | 55.71±0.38 |
| 3WLGNN Maron et al. (2019)| 109k    | 59.18±1.59 |
| GAT Velickovic et al. (2017)| 111k    | 64.22±0.46 |
| 3WLGNN Maron et al. (2019)| 106k    | 55.26±1.53 |
| GIN Xu et al. (2018)    | 111k    | 64.22±0.46 |
| GAT Veličković et al. (2017) | 105k    | 65.77±0.31 |
| 3WLGNN Maron et al. (2019)| 109k    | 67.00±0.62 |
| GAT Veličković et al. (2017) | 104k    | 67.31±0.31 |
| GCN Kipf & Welling (2016)| 101k    | 67.31±0.31 |
| GatedGCN Bresson & Laurent (2017) | 104k    | 67.31±0.31 |
| PNA Corso et al. (2020) | 105k    | 67.31±0.31 |
| DGN Bresson & Laurent (2017) | 109k    | 67.31±0.31 |
| GSA-Tiny (Ours)          | 107k    | 68.13±0.23 |
| RingGNN Chen et al. (2019)| 505k    | 39.17±17.1 |
| 3WLGNN Maron et al. (2019)| 503k    | 58.04±2.51 |
| GSA-Tiny2x (Ours)        | 409k    | 70.05±0.24 |
| GSA-Standard (Ours)      | 46.2M   | 77.78±0.07 |

Table 4: Results on ZINC. * indicates a fine-tuned model. The lower the better.

| Method                  | #Params | MAE |
|-------------------------|---------|-----|
| GIN Xu et al. (2018)    | 505k    | 0.526±0.051 |
| GAT Velickovic et al. (2017) | 531k    | 0.384±0.007 |
| GCN Kipf & Welling (2016)| 505k    | 0.367±0.011 |
| GatedGCN Bresson & Laurent (2017) | 505k    | 0.214±0.006 |
| MPNN * (sum) Grimner et al. (2017)| 481k    | 0.145±0.007 |
| PNA Corso et al. (2020) | 387k    | 0.142±0.010 |
| GSA-Small (Ours)        | 489k    | 0.094±0.002 |

5.2 MOLECULE PROPERTY PREDICTION

We validate our method on the task of the graph-level property prediction with benchmarking datasets with MIT license: OGBG-MolPCBA (MolPCBA) [Hu et al. 2020], and ZINC from the benchmarking GNN [Dwivedi et al. 2020]. MolPCBA consists of 437,929 graphs and the task is to predict multiple binary labels indicating various molecule properties. The evaluation metric is average precision (AP). ZINC is also a small dataset that consists of 12,000 graphs and the task is to regress a molecule property. Note that we follow the dataset split from the [Dwivedi et al. 2020]. The evaluation metric is mean absolute error (MAE). All experiments are conducted for 5 times, and we report the mean and the standard deviation of the experiments.

We adopt the linear learning rate decay, and the learning rate starts from $2 \times 10^{-4}$ and ends at $1 \times 10^{-9}$. Throughout experiments, we set $L$ to 5. For ZINC dataset, we adopt GSA-Small configuration with less than 500k parameters for fair comparison. We dropout the attention map and the input to feed-forward neural networks with the probability of 0.1. For MolPCBA dataset, we adopt GSA-Standard and GSA-Large configurations. We dropout the attention map and the input to feed-forward neural networks with the probability of 0.3 only for MolPCBA. Following [Ying et al. 2021], we initialize the parameter of the models with the weight of a pretrained model trained on PCQM4M [Hu et al. 2020] dataset.

Table 4 shows the results on ZINC dataset, our models achieve state-of-the-art MAE score. Our method achieves far better score than GCN-based methods, and achieves significantly better score than Transformer-based methods. Table 5 shows the results on MolPCBA dataset, our model achieves state-of-the-art AP score.
Table 5: Results on MolPCBA. * indicates a fine-tuned model. The higher the better.

| Method | #Params | AP (%) |
|--------|---------|--------|
| DeeperGCN-VN+FLAG Li et al. (2020) | 5.6M | 28.42 ± 0.43 |
| DGN Beani et al. (2021) | 6.7M | 28.85 ± 0.30 |
| GINE-VN Brossard et al. (2020) | 6.1M | 29.17 ± 0.15 |
| PHC-GNN Le et al. (2021) | 1.7M | 29.47 ± 0.26 |
| GINE-APPNP Brossard et al. (2020) | 6.1M | 29.79 ± 0.30 |
| GIN-VN Xu et al. 2018 | 3.4M | 29.02 ± 0.17 |
| **Graphormer-FLAG** Ying et al. (2021) | 119.5M | 31.39 ± 0.32 |
| **GSA-Standard** (Ours) | 46.2M | 30.77 ± 0.07 |
| **GSA-Large** (Ours) | 118.3M | 31.50 ± 0.10 |

Table 6: Results on PCQM4M. * indicates the results are cited from the official leaderboard. VN indicates that the model used the virtual node. The lower the better.

| Method | #Params | Train MAE | Validate MAE | Test MAE |
|--------|---------|-----------|--------------|----------|
| GCN Kipf & Welling (2016) | 2.0M | 0.1318 | 0.1691 (0.1684*) | 0.1838* |
| GIN Xu et al. (2018) | 3.8M | 0.1203 | 0.1537 (0.1536*) | 0.1678* |
| GCN-VN Kipf & Welling (2016) | 4.9M | 0.1225 | 0.1485 (0.1510*) | 0.1579* |
| GIN-VN Xu et al. (2018) | 6.7M | 0.1150 | 0.1395 (0.1396*) | 0.1487* |
| GINE-VN Brossard et al. (2020) | 13.2M | 0.1248 | 0.1430 | - |
| DeeperGCN-VN Li et al. 2020 | 25.5M | 0.1059 | 0.1398 | - |
| **GT Dwivedi & Bresson (2020)** | 0.6M | 0.0944 | 0.1400 | - |
| **GT-wide Dwivedi & Bresson (2020)** | 83.2M | 0.0955 | 0.1408 | - |
| **Graphormer (small) Ying et al. (2021)** | 12.5M | 0.0778 | 0.1264 | - |
| **Graphormer (small) Ying et al. (2021)** | 47.1M | 0.0778 | 0.1264 | - |
| **GSA-Standard** (Ours) | 46.2M | 0.0349 | 0.1225 | - |

5.3 OGB Large Scale Challenge

We validate our method on two datasets for quantum chemistry regression from OGB large scale challenge (Hu et al., 2020). The two datasets aims to predict DFT-calculated HOMO-LUMO energy gap of molecules given their molecular graphs. We conduct experiments on both the PCQM4M (Hu et al., 2020) and PCQM4Mv2 (Hu et al., 2020) datasets, which are currently the biggest graph-level prediction datasets containing about 4 millions graphs in total and their license is MIT. PCQM4Mv2 is a updated version of PCQM4M which contains DFT-calculated 3D strcure of molecules. For our experiments, we only utilize molecular graphs not 3D structure. We achieve the-state-of-the-art MAE on the validation set of both datasets.

Throughout experiments, we set L to 5. We adopt a GSA-Standard for fair comparisons with Graphormer (Ying et al., 2021). We dropout the attention map and the input to feed-forward neural networks with the probability of 0.1. We linearly increase learning rate upto $2 \times 10^{-4}$ for 3 epochs and linearly decay learning rate upto $1 \times 10^{-9}$ for 400 epochs. We are unable to measure test MAE of PCQM4M, since the test dataset is removed because PCQM4Mv2 is newly released.

Table 6 shows the results on PCQM4M dataset. Our model obtain the best train MAE showing that our model successfully memorizes training datasets with less parameters than Graphormer (Ying et al., 2021) or GT (Dwivedi & Bresson, 2020). Moreover, our model achieves the state-of-the-art validation MAE. Note that, methods with the lower validation MAE obtain the better test MAE on both datasets.

Table 7: Results on PCQM4Mv2. The results of other methods are cited from the official leaderboard. VN indicates that the model used the virtual node. The lower the better.

| Method | #Params | Validate MAE | Test-dev MAE |
|--------|---------|--------------|--------------|
| GCN Kipf & Welling (2016) | 2.0M | 0.1379 | 0.1398 |
| GIN Xu et al. 2018 | 3.8M | 0.1195 | 0.1218 |
| GCN-VN Kipf & Welling (2016) | 4.9M | 0.1225 | 0.1153 |
| GIN-VN Xu et al. (2018) | 6.7M | 0.1083 | 0.1084 |
| **GSA-Standard** (Ours) | 46.2M | 0.0349 | 0.1225 |

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A Appendix

You may include other additional sections here.