Graph Masked Autoencoder

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ABSTRACT

Transformers have achieved state-of-the-art performance in learning graph representations. However, there are still some challenges when applying transformers to real-world scenarios due to the fact that deep transformers are hard to be trained from scratch and the memory consumption is large. To address the two challenges, we propose Graph Masked Autoencoders (GMAE), a self-supervised model for learning graph representations, where vanilla graph transformers are used as the encoder and the decoder. GMAE takes partially masked graphs as input, and reconstructs the features of the masked nodes. We adopt asymmetric encoder-decoder design, where the encoder is a deep graph transformer and the decoder is a shallow graph transformer. The masking mechanism and the asymmetric design make GMAE a memory-efficient model compared with conventional transformers. We show that, compared with training from scratch, the graph transformer pre-trained using GMAE can achieve much better performance after fine-tuning. We also show that, when serving as a conventional self-supervised graph representation model and using an SVM model as the downstream graph classifier, GMAE achieves state-of-the-art performance on 5 of the 7 benchmark datasets.

KEYWORDS

Graph Transformers, Graph Neural Networks, Graph Self-supervised Learning.

1 INTRODUCTION

As the Internet and information technology develop rapidly in recent years, graph-structured data has emerged as a new type of information carrier and becomes more and more important in data mining and information retrieval. Graphs can now be seen everywhere in our daily life, such as citation networks [4, 50], social networks [39], transportation networks [36], molecule networks [16, 48], and e-commercial networks [54], etc. They have many important applications in finance, healthcare, recommendation, etc. Different from traditional data formats such as texts and images, graphs do not have a fixed structure and are highly sparse. To overcome the new challenges and to extract useful information from graphs, a lot of machine learning models have been proposed by the researchers to model graphs. For example, node2vec [17], collaborative filtering [21], graph neural networks [26, 46], etc.

Graph convolutional neural networks (GCNs) [26] have been a dominating model architecture in graph mining. They extract the local information in graphs by aggregating neighborhood representations. However, it is commonly observed that a 2-layer GCN shows the best overall performance in most cases, while deeper GCNs perform worse [29, 57]. That means, GCNs work best when aggregating only 2-hop neighbors. This is believed to be because of the over-smoothing problem [29] introduced by deep GCNs, where the neighborhood aggregating mechanism tends to make all the node representations identical to each other. Although researchers have been attempting to solve this problem in many ways [2, 38, 56], such an over-smoothing problem seems to be an inherent limitation of GCNs and are hard to be eliminated completely. It prevents GCNs from going deeper and thus can only capture local information while ignoring global information. However, such global information have been shown to be also important for learning high-quality graph representations [6, 7, 58]. How to effectively capture the global information becomes an urgent problem waiting to be solved in the broad graph mining community.

Recently, transformers [45] have been applied to the graph domain [51, 55] and have shown promising performance for solving the above challenge. Transformers are a type of neural network. The core design of them is the self-attention mechanism. In the transformer layer, an attention value is calculated for each instance pair. The embeddings are then calculated by aggregating all other instances weighted by the attentions. An illustration of the difference between GCN and transformer is shown in Fig. 1. Therefore, transformers can easily capture global information. Besides, transformers have a multi-head design to enable effective parallel computing. Because of such good properties, transformers have now become the state-of-the-art model in many NLP and CV tasks.

However, there are two key challenges when applying transformers to the graph domain. First, transformers can be very deep with dozens of layers and millions of parameters, which makes them hard to be trained from scratch [55]. Tailored training schemes and

Figure 1: An illustration of different aggregation mechanisms used by GCN and transformer. The red node is the target node. The first picture (left) shows the local aggregation used by a GCN layer, where the embedding of the target node is obtained by aggregating its neighbors. The second picture (right) shows the global aggregation used by a transformer layer, where the embedding is obtained by aggregating all the nodes in the graph.
hyper-parameters are necessary for the model to achieve a satisfying performance. Second, transformers have quadratic memory consumption with respect to the number of instances. Real-world graphs usually contain a large number of nodes, which makes it very easy to run out of memory when training transformers on graphs.

In this work, we aim to solve the above two challenges with our proposed model. Inspired by BERT [10] and MAE [20], we propose a self-supervised graph transformer model named Graph Masked Autoencoders (GMAE). It has an encoder and a decoder, where the encoder encodes a partially masked graph into embeddings and the decoder reconstructs the features of the masked nodes. GMAE can serve as an effective pre-training model to solve the first challenge. After trained with GMAE framework in a self-supervised manner, the encoder can be fine-tuned in an end-to-end supervised manner for specific downstream tasks. Our GMAE pre-training and fine-tuning scheme shows better performance and is much easier to train than training a graph transformer from scratch. To solve the second challenge, we use a mask-and-predict mechanism in GMAE, where some of the nodes in the graph are masked, i.e., the number of input nodes is reduced. Since the memory consumption of transformers is quadratic w.r.t. to the number of instances, the memory consumption of GMAE is much less than a conventional transformer. Besides, we use an asymmetric design of encoder and decoder, where the encoder is a deep transformer and the decoder is a shallow transformer (e.g., 2 layers). Such asymmetric design enables us to train a deeper encoder thanks to the low memory load of the shallow decoder, meanwhile achieving better performance compared with using a deep decoder.

We summarize our contributions as follows:

- We propose Graph Masked Autoencoders (GMAE), a self-supervised model for graph representations.
- GMAE can serve as an effective pre-training method for graph transformers to improve the performance and simplify the training process.
- With the masking mechanism and the asymmetric encoder-decoder design, GMAE has a much less memory consumption compared with conventional graph transformers. Therefore, it can be used to train large graphs and deep transformers.
- Extensive experiments show that GMAE pre-training and fine-tuning outperforms state-of-the-art supervised models. GMAE also achieves state-of-the-art performance on vanilla self-supervised graph classification tasks with linear evaluation protocol.

2 RELATED WORK

2.1 Self-supervised Graph Representation Learning

Early self-supervised graph representation learning methods focus on designing graph kernels. A conventional graph kernel method first decomposes graphs into some subgraphs, then it compares the number of shared subgraphs across different graphs to form graph embeddings. Different graph kernel methods usually differ in the way of extracting subgraphs. Popular graph kernel methods include random walk kernels [23], shortest-path kernels [5], graphlets [33, 41], Weisfeiler-Lehman graph kernels [40], and Deep Graph Kernels [49].

Since graph kernels are handcrafted, they suffer from a poor generalization ability. To overcome this problem, people have explored many self-supervised contrastive methods to learn graph representations. Graph2vec [32] and sub2vec [1] use random walk to generate "corpus" of graphs and use skipgram model to learn representations. Infograph [43] maximizes the mutual information between the graph-level representation and the representations of substructures. Recently, graph contrastive learning has emerged as the new state-of-the-art self-supervised graph representation learning method, which maximizes the agreement between two different views of the original graph. Typical graph-level contrastive learning methods include GraphCL [52], MVGRL [19], GCC [34], etc.

2.2 Transformers

Transformers [45] are one type of neural network which uses the attention mechanism as the core design. It has achieved state-of-the-art performance in many tasks in both natural language processing (NLP) and computer vision (CV). In NLP, a large number of transformer models have been proposed to solve various tasks. For example, MCA [50], sparse transformers [9], Longformer [3], Big-Bird [53], Reformer [27], Linear Transformer [24], etc. Among such a great number of works, BERT [10] should be the most well-known language model built with transformers.

While transformers have become the dominating model in NLP, people have also tried to apply transformers in computer vision domain. They have again achieved state-of-the-art performance in many different vision tasks, such as image classification [12, 35, 44], object detection [8], and few-shot learning [11], etc.

Early applications of transformers in graph domain focus on the sequential recommendation because the positional embeddings are easy to be defined based on the user interaction sequence and timestamps, such as SASRec [22], BERT4Rec [42], SSE-PT [47], TGSRec [15], etc. Some other works have tried to adopt transformers into static graph tasks and have achieved competitive performance compared with state-of-the-art GNN-based models. For example, GROVER [37] incorporates traditional GNNs into the transformer architecture to help process graph-structured data. GT [13] uses the Laplacian eigenvector as the positional embeddings. MAT [31] achieves competitive performance on molecular prediction tasks by altering the attention mechanism in transformers with inter-atomic distances and the molecular graph structure. SAN [28] uses a full Laplacian spectrum to learn the positional embeddings of nodes. Gopherm [51] uses degree centralities, shortest path distances, and edge features as the positional embeddings. Gopherm [55] extends graph transformers into node-level tasks for a single large graph by using the ego-graphs instead of the full-graphs. These works are all done in an end-to-end supervised manner. Most of them are hard to be trained from scratch [55] and suffer from the large quadratic memory consumption with respect to the input length.
3 PRELIMINARIES

3.1 Notations and Definitions

A graph $G$ can be described as $G = (V, E)$, where $V$ is the set of vertices (nodes) and $E$ is the set of edges. Suppose there are $n_V$ nodes and $n_E$ edges in a graph, an adjacency matrix $A \in \mathbb{R}^{n_V \times n_V}$ is used to describe the connections among nodes. Each entry in $A$ is either 1 or 0 representing whether there is a link between the two nodes or not. Some graphs have auxiliary information such as node features $X_V \in \mathbb{R}^{n_V \times d_V}$ and edge features $X_E \in \mathbb{R}^{n_E \times d_E}$ which can be used to facilitate training, where $d_V$ and $d_E$ are the numbers of dimensions of node features and edge features respectively.

Graph self-supervised learning aims to train a model $f$ that takes the graph data (without labels) as input and outputs the embeddings of each node. In this work, we assume that we only have node features and edge features as the auxiliary information. Thus, the model $f$ can be expressed as

$$f(A, X_V, X_E) = H$$

where $H \in \mathbb{R}^{n_V \times d_H}$ is the output embeddings of each node, and $d_H$ is the number of output dimensions.

3.2 Graph Transformers

A transformer is composed of several transformer layers. Each transformer layer contains a self-attention module and a feed-forward network. Suppose the input hidden representation matrix is $H \in \mathbb{R}^{n \times d}$, where $n$ is number of instances (nodes) and $d$ is the hidden dimension. The self-attention module contains three learnable matrices $Q \in \mathbb{R}^{d \times d}$, $K \in \mathbb{R}^{d \times d}$ and $V \in \mathbb{R}^{d \times d}$, which stand for Queries, Keys and Values respectively. Note that we usually have $d_Q = d_K$ due to the self-attention mechanism introduced next. The self-attention module first computes the three matrices as

$$Q = HW_Q, \quad K = HW_K, \quad V = HW_V$$

Then the dot product is applied to the queries with all keys to obtain the weights on the values. The final output matrix is computed by

$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}}V)$$

The obtained output matrix is an $n \times d_o$ matrix where each row represents the output representation of the corresponding instance.

Then a 2-layer feed-forward network (FFN) is used to project the representations and model capacity:

$$\text{FFN}(x) = \text{max}(0, xW_1 + b_1)W_2 + b_2$$

where $W_1$ and $W_2$ are learnable weight matrices. $b_1$ and $b_2$ are learnable biases.

The node feature information is already contained in the input feature matrix and is seen by the transformer. But the above mentioned forward propagation does not contain the structural information of graphs, i.e., each node is treated identically with no ordering. Therefore, positional embeddings are necessary for the transformer to know the relative positions of nodes. In natural language processing and computer vision, the positional embeddings are easy to define based on the absolute positions of words and pixels. However, unlike sentences and images, nodes in a graph do not have an absolute order. We don’t know which node is the “first” node in a graph. Nodes can only be described with relative positions based on their connections. To solve this problem, Graphormer proposed three types of positional encodings to jointly capture the structural information of graphs, which are centrality encoding, spatial encoding, and edge encoding. They encode the degree centralities, the shortest path distances, and the edge features into the three encodings respectively. In this way, the graph structural information can be well captured by the transformer.

4 GRAPH MASKED AUTOENCODER

In this section, we introduce the details of our proposed graph masked autoencoders (GMAE). A GMAE contains an encoder and a decoder. We use Graphormer [51] as our backbone model, i.e., our encoder and decoder are both graph transformers proposed by the Graphormer.

4.1 Training

We first introduce how GMAE works by going through the training process. An illustration of the GMAE framework is shown in Fig. 2. Note that we omit how we deal with the positional embeddings here and it will be introduced afterwards.

The encoder aims to learn the embeddings of each node. During training, for each input graph, we first randomly mask some of the nodes. These masked nodes will not be seen by the encoder. The encoder will only take the features of the observed node as input and then outputs the embeddings of each observed node. For example, suppose the number of nodes in an input graph is $n$ and the number of node features is $d_V$. Conventional end-to-end graph transformers take the full feature matrix $X_V \in \mathbb{R}^{n \times d_V}$ as input. However, the encoder in GMAE only takes partial feature matrix $X_V^o \in \mathbb{R}^{n_o \times d_V}$ as input, where $n_o$ is the number of observed nodes. The output embedding matrix of the encoder is $X_e \in \mathbb{R}^{n_o \times d_e}$, where $d_e$ is the number of output dimensions. Each row in $X_e$ is the embedding of the corresponding observed node.

The decoder aims to reconstruct the masked node features given the observed node embeddings. After we obtain the output embedding matrix $X_e$ from the encoder, we use a learnable mask token $x_m \in \mathbb{R}^{1 \times d_e}$ to replace the masked nodes and insert them into $X_e$ to obtain a new matrix $X_e' \in \mathbb{R}^{n_e \times d_e}$. The mask token $x_e$ is shared.
We follow Graphormer and use their proposed centrality encoding, all compared baselines are supervised methods. For our transformer, then we fine-tune the pre-trained encoder on the same ZINC training set using the labels, and report the mean absolute error on the ZINC test set. Our GMAE pre-training and fine-tuning scheme achieves the best performance.

We first compare GMAE pre-training and fine-tuning scheme with conventional end-to-end graph transformers because of the masking mechanism and the asymmetric encoder-decoder design. They both help save a lot of memory and make it possible for GMAE to be trained on larger graphs and to train deeper graph transformer encoders.

### 4.4 Properties

GMAE has a much less memory consumption compared with conventional end-to-end graph transformers because of the masking mechanism, the asymmetric encoder-decoder design. They both help save a lot of memory and make it possible for GMAE to be trained on larger graphs and to train deeper graph transformer encoders.

#### 4.4.1 Masking mechanism

Because of the masking mechanism, the size of the input feature matrix is largely reduced. We will see in our experiments that masking half of the nodes yields a good overall performance on all the datasets, while for some particular datasets, the best mask ratio can even be 90%. Since graph transformers have quadratic memory consumption with respect to the input length, such a high mask ratio can largely reduce the memory consumption.

#### 4.4.2 Asymmetric encoder-decoder design

In GMAE, the encoder and decoder are asymmetric. The encoder is a deep graph transformer, while the decoder is a shallow graph transformer. For example, in our experiments, a encoder with 16 layers and a decoder with 2 layers can achieve state-of-the-art performance in most cases. Such a design leads to an expressive encoder and meanwhile saves computation resources. Although our encoder is deep, the size of the input feature matrix is reduced because of the masking mechanism. However, a conventional end-to-end graph transformer is a deep transformer just like our encoder, but with a full feature matrix as the input, which makes the memory consumption quite large. On the other hand, the input to our decoder is a full feature matrix with inserted mask tokens, which seems to have a large memory consumption. In fact, since the decoder is very shallow, the computational load is still quite small.

#### 4.4.3 Scalability

Because of the above two designs, GMAE can be potentially used to train large graphs and deep encoders.

**Scalable to large graphs.** By masking half or more nodes, GMAE can be used to learn graphs with a large size while still maintaining a relatively small memory consumption.

**Scalable to deep encoders.** Since the input to the encoder is a masked feature matrix, increasing the number of layers in the encoder will not cause the memory consumption to increase as much as a conventional transformer which takes the full feature matrix as input. Therefore, we can potentially train a deeper encoder which can increase the model expressiveness.

### 5 EXPERIMENTS

We show the performance of GMAE by two groups of experiments. We first compare GMAE pre-training and fine-tuning scheme with state-of-the-art supervised models. Next, we compare GMAE with

| method         | test MAE  |
|----------------|-----------|
| GIN            | 0.526±0.051 |
| GraphSage      | 0.398±0.002 |
| GAT            | 0.384±0.007 |
| GCN            | 0.367±0.011 |
| GatedGCN-PE    | 0.214±0.006 |
| MPNN(sum)      | 0.145±0.007 |
| PNA            | 0.142±0.010 |
| GT             | 0.226±0.014 |
| SAN            | 0.139±0.006 |
| Graphormer     | 0.122±0.006 |
| GMAE           | 0.039±0.002 |

Table 1: GMAE pre-training and fine-tuning result on ZINC. Compared numbers are from the Graphormer paper [51]. All compared baselines are supervised methods. For our GMAE pre-training and fine-tuning, we first pre-train an encoder on the ZINC training set using our GMAE self-supervised training scheme (the encoder has the same architecture with the compared Graphormer baseline, which is a 12-layer graph transformer; the decoder is a 2-layer graph transformer), then we fine-tune the pre-trained encoder on the same ZINC training set using the labels, and report the mean absolute error on the ZINC test set. Our GMAE pre-training and fine-tuning scheme achieves the best performance.

4.2 Positional Embeddings

We follow Graphormer and use their proposed centrality encoding, spatial encoding, and edge encoding as the positional embeddings. To obtain the encodings, we need to know the node degrees, the shortest path distances of all node pairs, and the edge features. Note that edge encoding only works on datasets where edge features are available.

In GMAE, we obtain the positional embeddings of nodes based on the whole graph, i.e., our masking mechanism is only applied to the node features and not to the graph structure. When calculating the node degrees and shortest path distances, the whole graph is presented to us without masking. Then the positional embeddings will be added to the input of the encoder and the decoder, and also to the attention matrix in each transformer layer. Please refer to Graphormer [51] for more details regarding the positional embeddings.

4.3 Evaluation

After training, the decoder is discarded, and we only use the encoder for downstream tasks. At the inference stage, no masking is applied, and the whole graph is fed into the encoder. For graph-level tasks, a readout function can be applied to the node embeddings, such as average pooling. These node embeddings and graph embeddings can be further used for downstream tasks such as classification and clustering. GMAE can be used for both pre-training tasks and vanilla self-supervised tasks. For pre-training tasks, the encoder is fine-tuned in an end-to-end manner, i.e., all the parameters of the encoder are fine-tuned. In self-supervised tasks, the encoder is fixed, and the output node embeddings and graph embeddings are used as the input for downstream models and tasks.
some popular self-supervised graph representation models following
the common linear evaluation protocol, which is to train a
downstream SVM classifier using the learned embeddings.

5.1 GMAE Pre-training & Fine-tuning

We first show the superiority of GMAE by comparing it with state-of-the-art supervised models. We conduct experiments on the ZINC subset dataset [14], which contains 10000 molecular graphs for training, 1000 for validation, and 1000 for testing. Graphormer [51] has shown state-of-the-art performance on ZINC, where the model they used is a 12-layer graph transformer. For a fair comparison, in our GMAE pre-training and fine-tuning, we also use a 12-layer graph transformer as the encoder. We use a 2-layer graph transformer as the decoder in pre-training phase. During pre-training, we train the encoder and decoder in a self-supervised manner as introduced in section 4. Only the training set is used to pre-train the model. The hyper-parameters used in pre-training phase are consistent with Graphormer, except that we early-stop when the loss does not decrease for 50 epochs. In the fine-tuning phase, we discard the decoder, then fine-tune the encoder and an additional linear projection layer in a supervised manner using the training set. We fine-tune it for 300 epochs with 0.001 learning rate. The final result is shown in Table 1. The compared numbers are from the Graphormer paper [51].

Our GMAE shows state-of-the-art performance that outperforms all the compared baselines. Note that even if trained from scratch, Graphormer already outperforms all other baselines, and our GMAE can further boost its performance significantly. This suggests that pre-training is important for graph transformers. With our GMAE pre-training scheme, the transformers learn the important features and patterns contained in graphs effectively. Such information generalizes well when fine-tuned on the ground-truth labels.

5.2 GMAE Self-supervised Training

We further show that GMAE can be treated as a state-of-the-art self-supervised method by comparing it with popular self-supervised graph representation baselines under linear evaluation protocol, where we use a downstream SVM classifier to evaluate the quality of the learned graph embeddings.

5.2.1 Baselines. We choose 6 self-supervised graph representation models as our baselines:

- sub2vec [1]: learning representations for subgraphs using random walks.
- graph2vec [32]: graph-level representation learning using random walks.
- GCN [26]: graph convolutional networks.
- Graphormer [51]: graph-level transformers.
- InfoGraph [43]: mutual information maximization between graph-level representation and the representations of substructures of different scales.
- GraphCL [52]: a graph-level contrastive learning framework.

Sub2vec and graph2vec are representative self-supervised graph representation models based on random walks. InfoGraph and GraphCL are state-of-the-art self-supervised graph contrastive learning models. However, as for GCN and Graphormer, since they are originally semi-supervised and supervised methods respectively, we adopt the graph loss introduced in GraphSage [18] to them to enable self-supervised representation learning.

5.2.2 Datasets. We use 7 benchmark graph classification datasets, namely PROTEINS, BZR, COX2, NCI1, MUTAG, ER_MD, and DHFR. They are collected by the TU Dortmund University [25]. Dataset statistics are listed in Table 2.

5.2.3 Experiment Settings. For all the baseline methods, we follow their codes and default settings and report the best results. For GMAE, we use a 2-layer decoder, while the number of encoder layers is tuned from 1 to 30. The mask ratio is tuned from 0.1 to 0.9 with the step size 0.1. The number of hidden dimensions is 80 and the number of heads in the transformer layers is 8. Following Graphormer [51], we use a linear decay learning rate scheduler with 40000-step warm-up stage. We set the peak learning rate to be 1e-4 and the end learning rate to be 1e-9. The training stops when the loss does not decrease for 50 epochs. After obtaining the learned graph embeddings, we use an SVM classifier to do graph classification with 10-fold cross validation, following [43, 52]. We report the average accuracy of 5 runs.

5.2.4 Results. Table 3 shows the results of all methods. GMAE show state-of-the-art performance by outperforming other methods on 5 of the 7 datasets. This suggests that, without fine-tuning, GMAE also works very well when used in the vanilla self-supervised
representation scenario. We can further observe that, among the 6 baseline methods, graph contrastive learning methods (InfoGraph and GraphCL) achieve the best performance. The self-supervised Graphormer also performs good but is a little bit worse than InfoGraph and GraphCL. Instead, our GMAE outperforms InfoGraph and GraphCL on 5 of the 7 datasets. This suggests that our GMAE framework can effectively boost the performance of self-supervised graph transformers.

5.3 Analysis

We show some basic properties of GMAE, including how much memory it saves compared with conventional transformers, and how the mask ratio and number of decoder layers influence its performance.

5.3.1 Memory Consumption. We first compare the memory consumption of GMAE and Graphormer. For Graphormer, we set the number of layers as 12. For GMAE, the encoder is a 12-layer transformer and the decoder is a 2-layer transformer. We set the mask ratio in GMAE as 0.7. The memory consumption of the two models w.r.t. the number of nodes is shown in Fig. 3. We can observe that, the memory usage of GMAE is significantly less than Graphormer. Therefore, GMAE can be potentially used to train larger graphs and deeper graph transformers.

5.3.2 Mask ratio. Next, we show how the mask ratio influences the performance of GMAE. We conduct experiments on both pre-training & fine-tuning scenario (using ZINC dataset) and self-supervised learning scenario (using 7 benchmark datasets from TU dataset). For each dataset, we tune the mask ratio from 0.1 to 0.9 while keeping other hyperparameters consistent with the ones used in Table 1 and Table 3. We report the mean absolute error for ZINC, and report the downstream graph classification accuracy for the other 7 datasets, which are all averaged over 5 runs. The results are shown in Fig. 4. Note that, for ZINC, since the y axis is the mean

Table 3: Graph classification accuracy of the SVM model trained using the learned graph embeddings under self-supervised setting. The boldfaced ones are the best, and the underlined ones are the second.

|        | PROTEINS | BZR   | COX2  | NCI1  | MUTAG  | ER_MD  | DHFR  |
|--------|----------|-------|-------|-------|--------|--------|-------|
| sub2vec| 67.31±0.50 | 78.52±0.50 | 78.07±0.17 | 59.76±0.35 | 84.47±0.37 | 59.41±0.00 | 60.95±0.21 |
| graph2vec | 67.31±0.41 | 84.00±1.08 | 80.15±0.58 | 69.66±0.26 | 86.44±1.25 | 65.82±1.52 | 77.29±0.87 |
| GCN    | 59.57±0.00 | 78.77±0.00 | 78.16±0.00 | 50.05±0.00 | 66.49±0.33 | 59.41±0.00 | 60.98±0.00 |
| Graphormer | 72.13±0.55 | 83.87±0.25 | 78.21±0.37 | 69.40±0.42 | 87.21±0.56 | 68.43±1.76 | 60.98±0.51 |
| InfoGraph | 74.02±0.40 | 84.84±0.86 | 80.55±0.51 | 77.50±0.74 | 86.07±1.78 | 72.24±0.88 | 80.48±1.34 |
| GraphCL | 74.89±0.65 | 84.20±1.82 | 81.10±0.82 | 78.75±0.28 | 87.66±1.03 | 73.23±0.86 | 68.81±4.15 |
| GMAE   | 75.38±0.85 | 87.43±0.99 | 81.75±0.79 | 82.51±0.31 | 88.97±0.83 | 71.14±0.74 | 80.06±1.73 |

Figure 4: Mask ratios. Note that for ZINC, the y axis is the mean absolute error, where a smaller value indicates a better performance. For the other 7 datasets, the y axis is the accuracy, where a larger value indicates a better performance.
Figure 5: Number of decoder layers. Note that for ZINC, the y axis is the mean absolute error, where a smaller value indicates a better performance. For the other 7 datasets, the y axis is the accuracy, where a larger value indicates a better performance.

absolute error, so a smaller value indicates a better performance. For other 7 datasets, the y axis is the accuracy, so a larger value indicates a better performance.

Generally, the best mask ratio depends on the specific dataset. For example, COX2 and MUTAG prefer a large mask ratio at around 0.8 and 0.9 respectively; ZINC, ER_MD and NCI1 prefer a small mask ratio at around 0.3; PROTEINS, however, has two peak values at 0.4 and 0.7; BZR works well with all the mask ratios ranging from 0.2 to 0.7, while DHFR prefers mask ratios smaller than 0.7. In general, GMAE has a good overall performance when the mask ratio is around 0.4 or 0.7. In other words, GMAE can achieve a very good performance when around half of the nodes are masked, which can lead to a significant memory reduction.

5.3.3 Number of decoder layers. At last, we show how the depth of the decoder influences the performance of GMAE. We follow the settings we used when comparing different mask ratios. However, this time we tune the number of decoder layers instead of the mask ratio. The results are shown in Fig. 5. We can observe that, a shallow decoder with 1 or 2 layers performs better than deeper decoder, which suggests that such an asymmetric encoder-decoder design works good for GMAE. It can not only maintain a good performance, but also help save memory.

6 CONCLUSION

In this paper, we present a novel self-supervised graph representation model named Graph Masked Autoencoders (GMAE) based on graph transformers. It masks a large portion of the nodes in a graph and reconstruct the features of those masked nodes. When serving as a pre-training tool, it can significantly boost the performance of graph transformers. It also has state-of-the-art performance when evaluated under the self-supervised linear evaluation protocol. With the masking mechanism and asymmetric encoder-decoder design, the memory consumption of GMAE is largely reduced compared with conventional graph transformers, and can in turn be used to train large graphs and deep transformers.

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