Transformer: Transformer-based Graph Generation
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Abstract—Transformers have become widely used in various tasks, such as natural language processing and machine vision. This paper proposes Gransformer, an algorithm based on Transformer for generating graphs. We modify the Transformer encoder to exploit the structural information of the given graph. The attention mechanism is adapted to consider the presence or absence of edges between each pair of nodes. We also introduce a graph-based familiarity measure between node pairs that applies to both the attention and the positional encoding. This measure of familiarity is based on message-passing algorithms and contains structural information about the graph. Also, this measure is autoregressive, which allows our model to acquire the necessary conditional probabilities in a single forward pass. In the remainder of this section, we will describe prior autoregressive models, their shortcomings and an overview of our proposed model.

The first autoregressive model proposed for graph generation used graph neural networks (GNN) in a very time-consuming manner to generate graphs [1]. You et al. proposed a method for generating larger graphs autoregressively using recurrent neural networks [1]. A few number of prior studies have used transformers instead of recurrent neural networks for graph generation. Fan and Huang [2] used a simple encoder-decoder transformer model for conditional graph generation, where the goal is to generate a graph, given another graph as input. Kawai et al. [3] tackled the problem of unconditional graph generation, using a modified transformer encoder, which was enriched by graph convolutional layers.

Graph convolutional layers are common tools for extracting structural information from graphs, and the idea of using them in autoregressive models was previously proposed in [2]. Since a graph convolutional layer collects the data from all neighboring nodes of each node, it violates the autoregressive property. Thus, to satisfy the autoregressive property, these models need a separate forward pass on a subset of the input graph to compute the conditional probability of each node given the preceding nodes. Therefore, they need to perform $O(n)$ forward passes to compute the likelihood of an input graph with $n$ nodes. Our goal is to propose an alternative model for injecting structural information into a transformer-based model that retains the autoregressive property and can compute all conditional probabilities in a single forward pass for the entire graph.

In this paper, we propose Gransformer, which is an autoregressive transformer-based graph generation model. Gransformer uses a single masked transformer encoder to compute all the required conditional probabilities in one forward pass. Nodes in the network are represented by their preceding adjacency vectors, that is, the vectors that indicate their connections to the preceding nodes. There is a unit corresponding to each graph node in each self-attention layer of the transformer encoder. To determine the output of each unit, we apply a lower triangular mask to the layers of self-attention, so that only the information from the preceding nodes is taken into account.

In addition, we use a shared Masked Autoencoder for Distribution Estimation (MADE) [6] in the output layer to model the sequential dependency between the edge probabilities of each node to all the preceding nodes. MADE is a well-known and efficient autoregressive model that has inspired other generative models such as [7], [8]; MADE helps us

I. INTRODUCTION

Deep graph generation models are currently used for various applications ranging from biology to drug discovery to social network analysis. Among different graph generation methods, autoregressive models have shown promising results in generating diverse graphs. These models generate graphs by sequentially generating nodes and edges based on previously generated components.

Some autoregressive models are based on recurrent neural networks and do not use the structural properties of the graph [1], while some other methods use graph convolutional networks to directly benefit from the structural information [2]. There is also a prior study that substitutes recurrent neural networks with transformer networks and meanwhile tries to incorporate graph convolutional networks to use the graph structural information [3]. A basic challenge for autoregressive models that use graph convolutional networks for graph generation is that during their training process, they need to run a separate forward pass for each component (node, edge, or subgraph) to compute the likelihood of that component based on the preceding components. In this paper, we propose an autoregressive model based on transformers, that benefits from graph structural information by using some alternative method to the graph convolutional layers, which enables it to compute the likelihood of the input graph in a single forward pass. In the remainder of this section, we will describe prior autoregressive models, their shortcomings and an overview of our proposed model.

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1Alternatively, we can consider our model as a single decoder of a transformer model with no cross-attention layers.
easily model the dependency of edge generation and efficiently generate edge probabilities all at once.

In order to integrate the structural properties of the graph to the single forward pass of a transformer encoder, we use the following two techniques: first, we change the attention formulation of the model according to the presence or absence of edges between each pair of nodes. Second, we introduce a measure of familiarity between each pair of nodes and use it to modify the attention mechanism and the positional encoding formula. This measure is derived from the message-passing algorithm and represents the structural proximity between two nodes. This measure is also autoregressive since the familiarity function of nodes \( j \) and \( i \) \((j \geq i)\) is computed only from the subgraph that contains the first \( j \) nodes of the graph.

As with some other autoregressive models, such as the models in [1], we use the BFS ordering of the nodes and then reorder the adjacency matrix based on this ordering. Therefore, in a sequence of nodes, it is not possible to have a node that is not connected to any of the preceding nodes. Due to this fact, we need to modify the predicted likelihoods of our model in a way that prevents generating nodes with no connection to the preceding ones. During the training, it can be obtained by a simple modification in the loss function. For the generation phase, we propose a sampling method for generating nodes from the corresponding probability distribution, to avoid generating nodes that are not connected to any of the preceding nodes. The major contributions of this paper can be summarized as follows:

- We propose a graph generation model with a single transformer encoder that utilizes the graph’s structural properties.
- To model edge dependencies efficiently, we propose using a shared MADE in the output layer.
- With the help of the presence or absence of edges between each pair of nodes, we modify the attention mechanism of the transformer model.
- An autoregressive familiarity measure between nodes is introduced to represent the structural properties of the graphs. In both attention layers and positional encoding, we use this measure.
- The model is prevented from generating isolated nodes using a proper sampling method based on the corresponding probability distribution.

In this paper, we only consider generating simple undirected graphs, with no self-loops, no duplicate edges, and no node or edge labels. However, Transformers can be easily extended to handle these cases.

It is worth noting that from a general point of view, deep models for graph generation can be categorized into autoregressive models [1–5], [10], autoencoder-based ones [11–13], adversarial models [14–16], reinforcement learning-based methods [17], [18], flow-based models [19–21], autoregressive models [1–5], [10], and diffusion-based models [22–26].

The models can also be classified by the type of graphs they can generate. Some models generate graphs with node or edge features [3], [28], [29], [32], while some others only generate graphs without any feature [1], [2], [30], [31]. In addition, some models may incorporate specific constraints in their construction process to generate some graphs with certain features, such as chemical rules in molecule generation [17].

Another distinguishing feature is how these models use the structural properties of the input graphs. Some models use either the graph convolutional layers [2], [11], [12] or other graph neural networks [4], and some other ones use random walks on the graph [14], [34]. The models that generate the graph sequentially also benefit from the structural information using node orders based on specific graph traversals such as breath-first search (BFS [1], [2]). Furthermore, autoencoder-based graph generators can be divided into methods that use a single graph as training data [11], [35], [36] and those that use a collection of graphs as training data [12], [27].

It is worth noting that the graph generation problem is closely related to the node embedding problem, as many graph generation models use node embedding as an intermediate step [17], [37]. Furthermore, many graph generation models use similar graph processing techniques as node embedding models, such as deep node embedding models based on random walks [38–40] and graph convolutional networks [41], [42].

The rest of this paper is organized as follows: In Section III we present the proposed method. First, we discuss the transformer and the basic skeleton of the model. Then we state how MADE is used for dependent edge generation, explain our ideas for integrating graph structural properties, and discuss the strategy to avoid generating all zers adjacency vectors. Experimental results are presented in Section IV. Finally, Section V concludes the paper.

II. RELATED WORK

In this section, we briefly review research in graph generation. Existing models for generating deep graphs can be categorized from different points of view. Some models generate an entire graph at once [11], [12], [27], while others generate a graph node by node [1], [28], [29], edge by edge [30–32], or block by block [2], [33]. As mentioned in the previous section, graph generation models can also be divided into autoencoder-based models [11–13], adversarial models [14–16], reinforcement learning-based methods [17], [18], flow-based models [19–21], autoregressive models [1–5], [10], and diffusion-based models [22–26].

In the rest of this section, we briefly explain how previous autoregressive models work. Li et al. modeled the graph generation as a sequence of decisions [4]. They assign a feature vector to each node and update them after each step of the decision-making sequence, using their and their neighbors’ values. Decision-making is made by sampling from probability mass functions computed from these feature vectors. The sequence of decisions is as follows:

1. The model decides to add a new node or finish the process. When it adds a new node, it goes to step 2.
2. It adds a new node, and the model iteratively decides to add a new edge to this node (the last node) or finishes adding edges to this new node and returns to step 1. For adding a new edge to the last node, the model goes to step 3.
3) The model computes a score for each node except the last node. Then, a softmax function is run on the scores to compute the probability of selecting each node. A node is selected using the corresponding probability and connected to the last node. Then, the model returns to step 2.

Although this research [4] opened the direction of autoregressive graph generation, their functions were too time-consuming, and their method is not usable for large-scale graph generation. You et al. simplified the sequence of graph generation by the collaboration of two recurrent neural networks [1]: a graph-level RNN and an edge-level one. Each forward step of the graph-level RNN corresponds to adding a new node to the graph, and this RNN encodes the ”graph state” vector $h_i$ in its hidden state after its $i$-th step. After each forward step of the graph-level RNN, a complete forward pass of the edge-level RNN is run. This edge-level RNN outputs the binary adjacency vector $S_i$ of length $(i-1)$ in $i-1$ steps. The $j$-th element of $S_i$ shows whether the $i$-th node is connected to the $j$-th node or not. The hidden state of the edge-level RNN is initialized by $h_i$. After running the forward pass of the edge-level RNN, $S_i$ is passed to the graph-level RNN to take its next step and compute $h_{i+1}$ using $h_i$ and $S_i$. Also, the graph-level RNN is responsible for deciding when to terminate the graph generation.

Since they do not use the structural information of the graph explicitly, an autoregressive method based on the graph convolutional neural networks presented in [2], which is faster than the method given in [4], and can generate large graphs block-wise. Each iteration of this method adds a new block of $B$ nodes to the current generated graph. Suppose that the sub-graph of the first $(t-1)B$ nodes is generated, and a hidden vector is assigned to each of these $(t-1)B$ nodes. This algorithm first extends this graph of $(t-1)B$ nodes to a hypothetical graph of $tB$ nodes by assuming the $t$-th block as a fully connected graph of $B$ nodes, which are all connected to all the preceding $(t-1)B$ nodes as well. It also initializes the hidden vectors on the nodes of the $t$-th block to some predefined values. Then, several layers of a spatial GCN network are run on this graph to update the hidden vectors on all the $tB$ nodes. After that, for each edge connecting to the nodes of the $t$-th block, the model decides to keep or remove that edge, based on the hidden vectors on the two ends of that edge. The remaining graph is the sub-graph of the first $tB$ nodes.

The model proposed in [3] substitutes the recurrent neural networks used in [1] with transformers and meanwhile uses the graph convolutional networks for structural information similar to the method given in [2]. They combine the features extracted from a graph convolutional layer with the attention layer of the transformer. A beneficial property of transformers is that it is easy to satisfy their autoregressive property, using a simple autoregressive mask on the attention layer. But, when combining transformers with graph convolutional layers, they cannot make them autoregressive by using a simple mask, because graph convolutional layers transfer the graph information between different nodes and violate the autoregressive property. Therefore, to calculate the adjacency vector of the $i$-th node, GRAM runs a separate forward pass on the sub-graph of the first $i$ nodes of the graph. This issue makes this method time-consuming. Here, in this paper, we propose a new way to address this issue. In fact, we present a model to substitute the recurrent neural networks used in [1] with transformers and use the structural information of the graph similarly to the method given in [2] while not having the time-consuming issue of this method.

III. THE PROPOSED METHOD

In this section, we first discuss transformers and how they are related to graph neural networks. Then, we present a method that uses a transformer for graph generation tasks. Two main challenges are the generation of dependent edges and the usage of structural information, which we will address. Finally, we discuss how to prevent the model from generating isolated nodes.

A. Transformer and Graph Generation

The typical form of a transformer model adopts an encoder-decoder architecture. The encoder transforms the input sequence into an embedding one. The decoder generates the output sequence in an autoregressive manner. The decoder generates the output sequence by utilizing the encoder’s output and an extra input sequence. Encoders and decoders can also be used independently to solve different problems. For instance, BERT is a transformer encoder for language understanding [43], while GPT-3 is a state-of-the-art natural language generative model based on a transformer decoder [44].

Transformer decoder takes two sequences, the output of the encoder and the target sequence aims to generate. Since we have only one sequence in our task that works both as the input and output of the model, we use the encoder of the transformer structure. However, we use the decoder’s mask to satisfy the autoregressive property. This mask restricts the $i$-th unit in each layer to be computed just from the first $i$ units of the previous layer. Alternatively, one can consider our model as a single decoder without attention to an encoder’s output.

The main building block of the transformer encoder is the self-attention layer that learns a weighting function to compute the weighted sum of input values $V$. The proposed method computes the weights assigned to $V$ by using a compatibility function between queries $Q$ and the corresponding keys $K$ [45]. For the $t$-th attention layer, input vectors $v_1^{(t)}$, $v_2^{(t)}$, ..., $v_n^{(t)}$ (the rows of matrix $V^{(t)}$) will be transformed to output vectors $v_1^{(t+1)}$, $v_2^{(t+1)}$, ..., $v_n^{(t+1)}$ (the rows of matrix $V^{(t+1)}$) through the following equations.

$$
\text{Att}^{(t)} = M \odot \text{softmax} \left( \frac{Q^{(t)} \times K^{(t)T}}{\sqrt{d_k}} \right),
$$

$$
Q^{(t)} = V^{(t)} \times W_Q^{(t)} + b_Q^{(t)},
$$

$$
K^{(t)} = V^{(t)} \times W_K^{(t)} + b_K^{(t)},
$$

$$
V^{(t+1)} = \text{Att}^{(t)} \times \left( V^{(t)} \times W_V^{(t)} + b_V^{(t)} \right),
$$

where $\text{Att}^{(t)}$ is the attention of the units in the $(t+1)$-th layer to the units in the $t$-th layer. $W_Q^{(t)}$, $W_K^{(t)}$, $W_V^{(t)}$, $b_Q^{(t)}$, $b_K^{(t)}$, $b_V^{(t)}$
and $v_{K}^{(i)}$ are trainable parameters of the model. $M$ is the mask matrix, and $\odot$ denotes the element-wise multiplication.

Based on the graph convolutional networks paradigm, the Transformer encoder is similar to an attention-based spatial graph convolutional network on a fully connected graph. Let us map the $n$ units in each self-attention layer of the transformer encoder to the $n$ nodes of a hypothetical graph. In each self-attention layer, the attention of each unit to another unit assumes a hypothetical edge between the corresponding pair of nodes in the graph. Since without considering a mask, every unit in the encoder has attention to all the units, this structure is similar to the graph convolution on a fully connected graph i.e., there is a directed edge from each node to each other node. Using the decoder’s mask, this structure would be similar to graph convolution on a directed graph in which there are edges from each node to all subsequent nodes (see figure 1). We will use this GCN-based viewpoint to the transformers in section III-C1 to use graph structural information in the process of graph generation.

\[
P(G|\pi) = P(A^\pi|\pi) = \prod_{i} P(L_i^\pi|L_1^\pi, \ldots, L_{i-1}^\pi)
\]  

Therefore, we need the transformer model to estimate every one of these $n$ conditional probabilities. The sequence of the input vectors to the transformer encoder would be $Start, L_1^\pi, L_2^\pi, \ldots, L_n^\pi$ and its output vectors would be $y_1^\pi, y_2^\pi, \ldots, y_n^\pi, End$, where $Start$ and $End$ are the padding vectors. The $i$-th element of $y_k$ ($i < k$) determines the probability of putting an edge between the $k$-th node and the $i$-th node. Therefore, since $L_1^\pi, \ldots, L_n^\pi$ are binary vectors, the target sequence of the vectors in the output layer is $L_1^\pi, L_2^\pi, \ldots, L_n^\pi, End$. We use a lower triangular matrix as the mask matrix i.e., $M$ in Equation (1), to guarantee that $y_k$ is computed only from the first $k$ inputs i.e., from $L_1^\pi, \ldots, L_k^\pi$. Figure 2 shows the schema of the proposed model. The model described so far is similar to the encoder part of the transformer network. However, it uses the decoder’s mask, so that unit $i$ in each layer would be allowed to have attended only to the first $i$ units of the previous layer. In the following subsection, we describe the proposed extensions for the task of graph generation.

**B. Dependent Edge Generation**

Suppose that we only use a masked transformer encoder, without using any extra layers at its output layer. Then, the output sequence of the vectors from the transformer encoder will act as the probability estimation of the adjacency vectors. In other words, the first $i-1$ elements of the $i$-th output vector would represent the probability of the presence of the edges between node $i$ and nodes $1, 2, \ldots, i-1$. All these $i-1$ values are computed from the first $i-1$ input vectors. Therefore, the resulting probability for connecting node $i$ to node $j$ ($j < i$) Suppose we use only a masked transformer encoder without using additional layers on the output layer. Then the output sequence of vectors from the transformer encoder serves as the probability estimate for the adjacency vectors. In other words, the first $(i-1)$ elements of the $i$-th output vector would represent the probability of the presence of edges between node $i$ and nodes $1, 2, \ldots, (i-1)$. All of these $(i-1)$ values are calculated from the first $(i-1)$ input vectors. Therefore,
the resulting probability of connecting node $i$ to node $j$ ($j$) depends only on the edges such as ($i, s$) that $i, s \neq i$. However, it is obvious that knowing the existence or absence of the edges $\langle 1, i \rangle$, $\langle 2, i \rangle$, $\langle (j - 1), i \rangle$ has a significant impact on the decision about the existence of the edge $\langle j, i \rangle$. Therefore, we can extend equation (6) to capture the sequential generation of edges:

$$P(G|\pi) = \prod_{i=1}^{n} \prod_{j=1, s \neq i} P(L_{i}^{s} | L_{1}^{s}, \ldots, L_{i-1}^{s}, L_{i+1}^{s}, \ldots, L_{n}^{s}) \ (7)$$

To model this dependency, You et al. used an additional recurrent neural network in their model for sequential edge generation, which means additional training time [8]. Also, Liao et al. proposed using a mixture to capture the correlation between edges [9]. However, this only increases the ability of their method to model more complex edge distributions. However, it does not fully model the dependence between edges of individual nodes (or blocks in their proposed approach).

We propose to use the Masked Autoencoder for Density Estimation (MADE) [6] for sequential edge generation. MADE is a fully connected feed-forward autoencoder where each unit has a tag in $\{1, 2, \ldots, n\}$. Also, the $n$ units in the input layer and the $n$ units in the output layer have labels $1, 2, \ldots, n$. Connection from a node with label $i$ to another node labeled $j$ in the following layer will be masked if $i > j$. All paths from input nodes that have labels $j, j + 1, j + 2, \ldots, n$ to nodes with labels $j$ in the following layers will be blocked using this mask set. In the same way, it can be shown that the label of each node determines the subset of input units that are allowed to have a path to that node. Therefore, this masking strategy satisfies the autoregressive property.

We use a single MADE with shared parameters for generating the edges of all nodes. In the original MADE network, the input is exactly the target vector, which is supposed to be estimated in the output layer. Here, the target vector for the $i$-th node is the adjacency vector of the node $i$ that we want to see in the output layer of MADE. Therefore, for node $i$, we feed $L_i$ into the MADE network, and it tries to estimate $L_i$ in the output. But, as shown in figure 2, in addition to the target vector, we feed two more inputs to the MADE network: $n$, which is the number of nodes and the $i$-th output vector of the transformer encoder. Additional information from the other two inputs can be incorporated fully into the reconstruction of the target vector in the output layer, so they are tagged as 0 in the input layer, despite the target vector in the input layer which should have tags from 1 to $n$. The experimental results
show that adding direct links from the input units of MADE to the output units with larger tags has a significant impact on the results. Figure [1] illustrates how we use the MADE network to generate the $i$-th output vector.

C. Using Graph Structural Properties

As mentioned earlier, the Transformer is based on the Transformer, which was originally proposed for natural language processing. In NLP tasks, the input text to the Transformer model is represented by a sequence of one-hot vectors. Similarly, we represent an input graph for our model by a sequence of vectors, $L_1, L_2, \ldots, L_n$. However, this representation does not explicitly specify the structural information of the graph that can be used during the training and generation process.

In prior work, graph convolutional networks have been used for this purpose [2]–[4]. To infer a new node (or a new block of nodes) and its connecting edges to the previous nodes, these models consider the subgraph of the existing nodes and apply multiple graph convolutional layers to it. Therefore, $O(n)$ forward passes are needed to compute the loss function. However, we intend to combine the structural graph information with our transformer-based model such that the loss function can be calculated in a single forward pass.

In Sections III-C1 and III-C2 we will discuss two techniques we have proposed for this goal.

1) Using Presence/Absence of Edges: In a regular transformer encoder, each node can attend to all the nodes in the previous layer. As with the transformer decoder, we restrict it to have attention to the preceding nodes using autoregressive masks. But even in this way, we do not use the structural information of the graph and ignore the edges.

Using different sets of key/query/value parameters for pairs of nodes with an edge between them and pairs of nodes without an edge between them allows us to import the structural information of the graph into our proposed model. To be more specific, we can rewrite the Equations (1), (2), (3) and (4) in the following form:

$$\text{Att}_1^{(t)} = M \odot \text{softmax} \left( \frac{Q_1^{(t)} \times K_1^{(t)^T}}{\sqrt{d_k}} \right),$$

$$\text{Att}_2^{(t)} = M \odot \text{softmax} \left( \frac{Q_2^{(t)} \times K_2^{(t)^T}}{\sqrt{d_k}} \right),$$

$$Q_1^{(t)} = V_1^{(t)} \times W_{Q1}^{(t)} + b_{Q1},$$

$$Q_2^{(t)} = V_2^{(t)} \times W_{Q2}^{(t)} + b_{Q2},$$

$$K_1^{(t)} = V_1^{(t)} \times W_{K1}^{(t)} + b_{K1},$$

$$K_2^{(t)} = V_2^{(t)} \times W_{K2}^{(t)} + b_{K2},$$

$$V_1^{(t+1)} = \text{Attn}_1^{(t)} \times (V_1^{(t)} \times W_{V1}^{(t)} + b_{V1}),$$

$$V_2^{(t+1)} = \text{Attn}_2^{(t)} \times (V_2^{(t)} \times W_{V2}^{(t)} + b_{V2}),$$

$$V_1^{(t+1)}(i,j) = V_1^{(t+1)}(i,j) \quad \text{if } A(i,j) = 1,$$

$$V_1^{(t+1)}(i,j) = V_1^{(t+1)}(i,j) \quad \text{if } A(i,j) = 0.$$ (16)

This concept duplicates the computation time without changing the order of time steps. We will see in Section IV-D that the idea of using presence/absence of edges in the attention layer as described above does not necessarily improve our model in practice. Actually, the model needs to collect the information from a longer distance neighborhood for each node, to benefit from the graph structural information. However, we will propose our second idea for injecting graph structural information into our model in Section III-C2. Our experiments in Section IV-D confirm improvement of our model using the latter method.

2) Autoregressive Graph-based Familiarities: This section aims to define a familiarity function $K$ with desired properties between pairs of nodes. To be more precise, $K$ would be

1) based on the graph structure, or represent the graph structural information,

2) autoregressive; i.e., if $i > j$ then $K(i,j)$ is a constant value and if $i \leq j$ then $K(i,j)$ is computed only from the subgraph of the first $j$ nodes.

3) efficiently computable for all the node pairs.

We define $K$ as follows:

$$K(i,j) = \text{sigmoid}(f(g_0(i,j),\ldots,g_n(i,j)), h_{n_k}(i,j),\ldots,h_{0}(i,j)))$$ (17)

$$g_k(i,j) = m_k(i,j)/\max(1,\sum_i m_k(t,j))$$ (18)

$$h_k(i,j) = m_k(i,j)/\max(1, s_k(i,j))$$ (19)

where $f(.)$ is a two-layers MLP with a ReLU activation function in the first layer and a linear activation function in the second layer. The scalar variable $m_k(i,j)$ denotes the number of paths of length $k$ from node $i$ to node $j$ in the subgraph containing nodes 1 to $j$. Also $s_k(i,j)$ denotes the number of paths of length $k$ starting from node $i$ (to any node) in the subgraph containing nodes 1 to $j$. Here, a path means any sequence of nodes in which every two consecutive nodes are connected (so a node can appear more than once in a path). It is clear that if $j < i$, then according to the definition, $m_k(i,j) = 0$ for all values of $k$, and consequently $K(i,j)$ will be a constant value, independent of $i$ and $j$.

Here we briefly justify why the number of paths of length $k$ between pairs of nodes is an appropriate value to represent the structural information of the graph. We consider a process of message passing on a subgraph of the first $j$ nodes in which each node passes its value to all its neighbors at each step. Following this algorithm, the initial message on node $i$ is received exactly $m_k(i,j)$ times by the $j$-th node in step $k$. It is worth noting that most graph convolutional layers and graph kernels based on random walks can be restated by special forms of message passing. For example, in spatial graph convolutional layers, the vector at each node is computed by aggregating the vectors (or equivalent messages) from its neighboring nodes, followed by a nonlinear activation function.

In fact $g_k(i,j)$ and $h_k(i,j)$ are two different normalizations of $m_k(i,j)$. On one hand, these normalizations bound the input values to network $f$; otherwise, it may face numerical overflows for its parameter values during the training process. On the other hand, these normalizations have some probabilistic meaning from a random walk-based point of view. In other
words, if we consider the subgraph of the first \( j \) nodes of an undirected graph, then \( g_k(i, j) \) is the probability of stopping at node \( i \) if we start a random walk of length \( k \) from node \( j \). Also \( h_k(i, j) \) is the probability of stopping at node \( j \) if we start a random walk of length \( k \) from node \( i \).

We now explain how to calculate \( m_0(\ldots), \ldots, m_{n_k}(\ldots) \) efficiently. We define \( M_k \) as an upper triangular matrix whose element in the \( i \)-th row and \( j \)-th column is equal to \( m_k(i, j) \). \( M_0 \) is an identity matrix. Let \( A \) be the adjacency matrix of the graph and \( A(i, j) \) be the element in row \( i \) and column \( j \). Assume that we have computed the function \( m_{k-1}(\ldots) \) or equivalently \( M_{k-1} \). Each path of length \( k \) from \( i \) to \( j \) that uses only the first \( j \) nodes constitutes a first step from node \( i \) to a node \( t \in \{1, 2, \ldots, j\} \) and a path of length \( k-1 \) from node \( t \) to node \( j \) that uses only the first \( j \) nodes. Therefore for \( i \leq j \) we have:

\[
m_k(i, j) = \sum_{1 \leq t \leq j} A(i, t) \times m_{k-1}(t, j) = \sum_{1 \leq t \leq n} A(i, t) \times m_{k-1}(t, j) = [A \times M_{k-1}](i, j) \quad \text{if} \quad i \leq j
\]  

The second line of the above equation is because, for \( t > j \), we have \( m_{k-1}(t, j) = 0 \). Similarly, for \( m_k \) we must have \( i > j \Rightarrow m_k(i, j) = 0 \). Therefore

\[
M_k = \text{tri}_{up}(A \times M_{k-1}),
\]  

where the operator \( \text{tri}_{up} \) converts its input matrix to an upper triangular matrix.

Computing this measure for all node pairs needs \( k \) multiplications of \( n \times n \) matrices, which can theoretically be run either in \( O(k n^2.3728596) \) [46] but practically in \( O(k n^2.8074) \) [47] or \( O(k n e) \) for sparse graphs, where \( e \) is the number of edges (because one of the matrices in each multiplication is the adjacency matrix). In addition, \( n_k \) is an integer parameter in the familiarity measure, which we set to 16 in our experiments.

We can compute \( s_0(\ldots), \ldots, s_{n_k}(\ldots) \) in a very similar way to \( m_0(\ldots), \ldots, m_{n_k}(\ldots) \). If we define \( S_k \) as an upper triangular matrix whose elements in the \( i \)-th row and \( j \)-th column is equal to \( s_k(i, j) \), then \( S_0 \) will be an upper triangular all one matrix. Then using a similar discussion as above we can see that:

\[
S_k = \text{tri}_{up}(A \times S_{k-1}),
\]  

Finally, we will indicate the utilization of the familiarity measure [17] in our model. We multiply the familiarity function by the attention in each layer. In other words, we modify the attention defined in Equation [1] in the following form:

\[
\text{Att}^{(l)} \leftarrow \text{Att}^{(l)} \odot K^T,
\]  

where \( K \) is an \( n \times n \) matrix containing \( K(i, j) \) for all values of \( i \) and \( j \). It is worth noting that the familiarity function defined in Equation [17] contains a two-layer neural network \( f \). This neural network can have different parameter values in different layers of our model. These parameters will be learned with other network parameters through the training process.

Similarly, we propose a positional encoding for the nodes based on \( m_k(\ldots) \) for \( k \in \{0, 2, \ldots, n_k\} \). The intuition is that if we put a one-hot vector on each vector representing its index and let these vectors propagate over the subgraph of the first \( j \) nodes for \( k \) times, then the \( i \)-th element of the final vector (after \( k \) steps of message passing) on the \( j \)-th node will be \( m_k(i, j) \). So we define the positional encoding of node \( j \) as follows:

\[
pos_{\text{enc}}(j) = f_1(z_0(j), z_1(j), \ldots, z_{n_k}(j)),
\]

\[
z_k(j) = f_2(g_k(1, j), g_k(2, j), \ldots, g_k(j, j), h_k(1, j), h_k(2, j), \ldots, h_k(j, j))
\]

where \( f_1 \) is a one-layer MLP (a linear projection with a bias) and \( f_2 \) is a two layers MLP with a ReLU activation function in the first layer and a sigmoid activation function in the second layer. Also, \( g_k \) and \( h_k \) are given in Equations [18] and [19].

D. Avoiding Isolated Nodes

When generating the \( k \)-th node, our model should decide its connection to the preceding \((k-1)\) nodes. In other words, it should try to estimate the first \((k-1)\) elements of \( L_k^* \) (because the other elements of this vector are equal to zero according to the definition.) Since we use BFS orders for training, we should generate graphs in the BFS sequences. However, when we consider a BFS ordering of the nodes of a graph, each node like \( v \) (except the root node) has a parent node in the BFS tree \( (p_v) \). In this ordering, \( p_v \) appears at a position before \( v \). Therefore, adding an isolated node, which does not connect to any of the preceding nodes, is not allowed. However, our model so far has nothing to satisfy this condition. You et al. [1] allows the isolated nodes to be generated and remove them after generating the graph. However, it will disturb the distribution of the generated graph sizes. In this section, we tackle this problem by distributing the probability of the all-zeros vector among valid vectors. Let the binary vector \( y = (y_1, y_2, \ldots, y_{k-1}) \) denote the model estimation of the first \( k-1 \) bits of \( L_k^* \), and \( P(y) \) denote the probability of generation of \( y \).

We define the new density function \( \tilde{P} \) over \( k-1 \)-bits binary vectors as follows:

\[
\tilde{P}(y) = \begin{cases} 0 & \text{if } y_1 = \ldots = y_{k-1} = 0 \\ 1 & \text{otherwise} \end{cases}
\]  

Computation of the new loss function (the new negative log-likelihood) during the training process is easy; it just needs an extra computation of \( P(\tilde{y}) \). However, generation is a bit challenging. A simple method for generating samples from \( \tilde{P} \) is generating samples from \( P \) and rejecting all-zeros samples. But this sampling method is likely to be trapped in long-lasting rejection loops, especially for generating sparse graphs. In order to sample from \( \tilde{P}(y) \) sequentially, it is sufficient to compute \( \tilde{P}(Y_1|y_1, y_2, \ldots, y_{k-1}) \). We prove the following theorem to show how we can efficiently sample binary vectors from \( \tilde{P} \).
\textbf{Theorem 1.} For a fixed set of values for \(y_1, y_2, \ldots, y_{i-1}\), let \(P(Y_i = 1|y_1, \ldots, y_{i-1})\) denoted by \(\hat{P}_i\) then

\[
\hat{P}(Y_i = 1|y_1, \ldots, y_{i-1}) = \begin{cases} P_i, & \text{if } \exists j < i \text{ s.t. } y_j = 1 \\ \prod_{1 \leq j < i} P_i \cdot P(y_j|y_1, \ldots, y_{j-1}) - P(0), & \text{otherwise.} \end{cases}
\]

(27)

For the special case of \(i = 1\),

\[
\hat{P}(Y_1 = 1) = P(Y_1 = 1) \times \frac{1}{1 - P(0)}.
\]

(28)

\textbf{Proof:} We first define the following sets:

\[ A^{(i)}_y = \{a_1, \ldots, a_{k-1}\} \in \{0, 1\}^{k-1}|a_j = y_j \}

(29)

\[ A^{(i)}_0 = \{a_1, \ldots, a_{k-1}\} \in \{0, 1\}^{k-1}|a_i = 0 \}

(30)

\[ A^{(i)}_1 = \{a_1, \ldots, a_{k-1}\} \in \{0, 1\}^{k-1}|a_i = 1 \}

(31)

In other words, \(A^{(i)}_y\) is the set of all binary sequences of length \(k-1\) whose first \(i\) elements are equal to \(y_1, y_2, \ldots, y_{i-1}\). \(A^{(i)}_0\) represents all binary sequences of length \(k-1\) whose \(i\)-th element is equal to 0, and \(A^{(i)}_1\) represents all binary sequences of length \(k-1\) whose \(i\)-th element is equal to 1. As a result, it follows that

\[
\hat{P}(Y_i = 1|y_1, \ldots, y_{i-1}) = \frac{\hat{P}(A^{(i)}_y \cap A^{(i)}_1)}{\hat{P}(A^{(i)}_y \cap A^{(i)}_0) + \hat{P}(A^{(i)}_y \cap A^{(i)}_1)}.
\]

Since \(A^{(i)}_y \cap A^{(i)}_1\) does not include the zero vector, and respecting the definition of the probability mass function \(\hat{P}(\cdot)\) in Equation (26), we infer that

\[
\hat{P}(A^{(i)}_y \cap A^{(i)}_1) = \sum_{e \in \hat{A}_y^{(i)} \cap A^{(i)}_1} \hat{P}(e) = \sum_{e \in \hat{A}_y^{(i)} \cap A^{(i)}_1} \frac{P(e)}{1 - P(0)}.
\]

(33)

\[
= \frac{P(A^{(i)}_y \cap A^{(i)}_1)}{1 - P(0)} = \frac{1}{1 - P(0)} P(Y_i = 1|y_1, \ldots, y_{i-1}) \times \prod_{1 \leq j < i} P(y_j|y_1, \ldots, y_{j-1}).
\]

(34)

If at least one of \(y_1, \ldots, y_{i-1}\) is equal to 1, then \(A^{(i)}_y \cap A^{(i)}_1\) does not include the zero vector as well, and we can infer in a similar way that

\[
\hat{P}(A^{(i)}_y \cap A^{(i)}_0) = \frac{1}{1 - P(0)} P(Y_i = 0|y_1, \ldots, y_{i-1}) \times \prod_{1 \leq j < i} P(a_j|y_1, \ldots, y_{j-1}).
\]

(35)

Hence, respecting Equation (32), we conclude that if there exists \(j < i\) such that for \(y_j = 1\), then we have

\[
\hat{P}(Y_i = 1|y_1, \ldots, y_{i-1}) = \hat{P}(Y_i = 1|y_1, \ldots, y_{i-1}),
\]

(36)

which equals to \(P_i\) by definition. But if \(A^{(i)}_y \cap A^{(i)}_0\) contains the zero vector, it means that \(y_1 = y_2 = \ldots = y_{i-1} = 0\). In this case, we have:

\[
\hat{P}(A^{(i)}_y \cap A^{(i)}_1) = \sum_{e \in A^{(i)}_y \cap A^{(i)}_0} \hat{P}(e) = \sum_{e \in A^{(i)}_y \cap A^{(i)}_0} \frac{P(e)}{1 - P(0)}.
\]

(37)

Putting Equations (34) and (37) into Equation (32), it follows that when \(y_1 = \ldots = y_{i-1} = 0\), then we have

\[
\hat{P}(Y_i = 1|y_1, \ldots, y_{i-1}) = \frac{P_i \cdot \prod_{1 \leq j < i} P(y_j|y_1, \ldots, y_{j-1}) - P(0)}{1 - P(0)}.
\]

(38)

For the special case of \(i = 1\), it is clear that \(\hat{P}(Y_1 = 1) = \hat{P}(A^{(1)}_1)\), and since \(A^{(1)}_1\) does not include the zero vector, according to the definition of the probability mass function \(\hat{P}(\cdot)\) in Equation (26) we have

\[
\hat{P}(A^{(1)}_1) = \sum_{e \in A^{(1)}_1} \hat{P}(e) = \sum_{e \in A^{(1)}_1} \frac{P(e)}{1 - P(0)} = P(Y_i = 1) \times \frac{1}{1 - P(0)}.
\]

(39)

This completes the proof of the theorem. \qed

Therefore, it is obvious that using theorem 1 the model can sequentially sample \(k-1\) bits \(y_1, \ldots, y_{k-1}\) in time of \(O(k)\).

\section{Experimental results}

In order to evaluate the proposed Gransformer, we conduct computer experiments. This section presents our experiments to compare Gransformer with state-of-the-art methods. The implementation of the proposed model and the datasets used in our experiments are available anonymously from [https://github.com/Gransformer/Gransformer](https://github.com/Gransformer/Gransformer).

\subsection{Datasets}

We run the experiments on the following datasets: a synthetic and two real-world. We used 20\% of each dataset as test data and the other 80\% as the training set. For these datasets, we used models with six attention layers (\(T = 6\)) with a hidden size of 400.  

**Ego:** A real-world dataset, containing 757 graphs representing documents (as nodes) and their citations (as edges) extracted from the Citeseer network [48]. Graphs have from 50 up to 399 nodes.  

**Protein:** A real-world dataset of 918 protein graphs [49]. Nodes are amino acids and geometrically close nodes are connected in the graph. Graph sizes vary from 100 to 500.  

**Lobster:** A synthetic dataset of 100 lobsters of at most 100 nodes (average number of nodes equals 80). A lobster is a
TABLE I
MMD SCORES OF DIFFERENT GENERATIVE MODELS. IN EACH COLUMN, THE BEST RESULT IS IN BOLD DIGITS, AND THE BEST TWO RESULTS ARE SHADEd.

| Method      | Deg.   | Clus.  | Orbit  | Deg.   | Clus.  | Orbit  | Deg.   | Clus.  | Orbit  |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Ego dataset |        |        |        | Protein dataset |        |        | Lobster |        |        |
| GraphRNN-S  | 0.16 (0.08) | 0.06 (0.06) | 0.13 (0.09) | 0.21 (0.02) | **0.19 (0.05)** | 0.15 (0.02) | 0.08 (0.02) | 0.17 (0.05) | 0.22 (0.18) |
| GraphRNN    | 0.13 (0.03) | 0.50 (0.03) | **0.03 (0.001)** | 0.03 (0.004) | 1.05 (0.01) | 0.53 (0.02) | **0.01 (0.01)** | **0.00 (0.00)** | **0.01 (0.01)** |
| GRAN        | 0.29 (0.03) | **0.05 (0.02)** | 0.06 (0.01) | 0.04 (0.03) | 0.31 (0.17) | 0.25 (0.07) | 0.56 (0.06) | 0.06 (0.03) | 0.93 (0.14) |
| Transformer | **0.04 (0.001)** | 0.08 (0.01) | 0.04 (0.002) | **0.03 (0.003)** | 0.35 (0.03) | **0.08 (0.01)** | 0.12 (0.07) | **0.00 (0.00)** | 0.34 (0.22) |

Original Gransformer GRAN GraphRNN GraphRNN-S

Fig. 4. Some original samples and generated graphs by different methods, for each dataset.
B. Evaluation Metrics

To compare the generated set of graphs with the actual test data, You et al. [1] suggested using the maximum mean discrepancy (MMD) of several graph statistics to compare all moments of the empirical distribution of the graphs. Similar to [1], we report MMD score for degree and cluster coefficient distributions, as well as average orbit, counts statistics. In addition, to study the effect of different ideas proposed in this paper, we report training and test the negative log-likelihood of GraphRNN and Gransformer without some of its modules.

C. Comparison With Other Generative Methods

In this section, we compare the statistical performance of Gransformer with GraphRNN, GraphRNN-S [1], and GRAN [2] as three baseline autoregressive graph generation models. GraphRNN and GraphRNN-S are based on recurrent neural networks, GRAN is designed based on graph convolutional networks, and Gransformer is transformer-based. Table II presents the results of different methods. It reports the mean and the standard deviation of the MMD scores for the graphs generated by each method after 2600, 2800, and 3000 training epochs. In each column, the best result is represented in bold digits, and the best two cells are shaded. Table II shows that in most of the columns Gransformer is among the two best results. Moreover, Gransformer is the only method that does not achieve the worst MMD value in any of the columns.

Moreover, Table II shows that neither GraphRNN nor GraphRNN-S outperforms the other one by achieving lower MMD values in all cases. There are some cases where their MMD values differ by an order of magnitude, e.g., the MMD of their clustering coefficients for Ego, or the MMD of their degree distributions for Protein.

From the reported results on Lobster dataset in Table II, it is clear that both graphRNN and Gransformer have detected a tree graph that reduces to a caterpillar if we eliminate all its leaf nodes. A caterpillar is a tree that reduces to a path if we eliminate all its leaf nodes. We used parameters $p_1 = 0.7$ and $p_2 = 0.7$ for adding nodes of level 1 and 2 to a path to generate a lobster.

D. Ablation Study

We ablate different components of the proposed method to investigate the impact of each one. Table II reports the negative log-likelihood of the ablated models on both train and test data. The columns “using MADE”, “using K”, “pres/abs of edges” and “graph positional encoding” respectively correspond to the components described in Section III-C1, Equation [17], Section III-C1, and Equation [24].

Comparing row 2 with row 1, it is clear that using graph positional encoding causes a significant improvement in our model. Although our proposed graph positional encoding is computed in a similar way to how the graph-based familiarity matrix $K$ is computed, comparing row 6 with row 5 reveals that even when using $K$, the proposed graph positional encoding causes some improvement in the results.

Comparison between row 3 and row 2, and also between row 6 and row 6 indicates that using presence and absence of edges, as described in Section III-C1 does not necessarily have any gain in practice. It just duplicates the complexity of the attention layers and may even worsen the results. This observation emphasizes the necessity of using higher-order proximity of nodes in the graph to extract its structural information. This is exactly what our proposed graph-based familiarity measure $K$ and our proposed graph-based positional encoding were defined based on, in Equations [17] and [24].

The significant improvement in NLL values in row 7 against all rows 1 to 6 confirms the significant impact of dependent edge generation using MADE in Gransformer. Also, comparing row 7 with rows 8 and 9 verifies that other components are still advantageous in the presence of MADE.

Finally, since the results in rows 8 and 9 are very similar, we keep using the idea of utilizing presence and absence of edges (Section III-C1) in our model, although it does not necessarily have a significant impact on the performance of the model.

V. Conclusion

In this paper, we proposed Gransformer, an autoregressive graph generation model based on a single transformer encoder. We extended the transformer encoder using several techniques. We put an autoregressive mask on the encoder and modified the attention mechanism to utilize the presence or absence of edges between nodes. We also imported graph structural properties to the model by defining a familiarity measure between node pairs inspired by message-passing algorithms. We used the proposed familiarity measure both in the attention layer and for graph-based positional encoding. Our experiments showed that our method is competitive with other methods respecting the MMD scores.

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