DAGFORMER: DIRECTED ACYCLIC GRAPH TRANSFORMER

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ABSTRACT

In many fields, such as natural language processing and computer vision, the Transformer architecture has become the standard. Recently, the Transformer architecture has also attracted a growing amount of interest in graph representation learning since it naturally overcomes some graph neural network (GNNs) restrictions. In this work, we focus on a special yet widely used class of graphs—DAGs. We propose the directed acyclic graph Transformer, DAGformer, a Transformer architecture that processes information according to the reachability relation defined by the partial order. DAGformer is simple and flexible, allowing it to be used with various transformer-based models. We show that our architecture achieves state-of-the-art performance on representative DAG datasets, outperforming all previous approaches. The source code is available at https://github.com/LUOyk1999/DAGformer.

1. INTRODUCTION

Graph neural networks (GNNs) have shown to be an efficient representation learning framework for graph-structured data. A broad family of GNNs construct multilayer models in which each layer operates on the previous layer to generate new representations utilizing a message-passing mechanism [1] to aggregate neighborhood-specific information. Among different graph types, directed acyclic graphs (DAGs) are of special interest to machine learning researchers since many machine learning models, such as abstract syntax trees and neural architectures. A directed graph is a DAG if and only if the edges define a partial ordering over the nodes. The partial order is an additional strong inductive bias that one would naturally like to integrate into the neural network. By the information flow from predecessors to successors through edges, DAGs could gather information like a recurrence structure. A number of neural networks that employ DAGs architecture have been proposed, such as Tree-LSTM [2], DAG-RNN [3], D-VAE [4] and DAGNN [5]. Specifically, DAGNN conducts information aggregation using graph attention.

Even though those message-passing mechanisms have been developed, critical limits have been found. These include the limited expressiveness of GNNs as well as known problems such as over-smoothing and oversquashing [6, 7]. Recently, graph Transformers alleviate these basic constraints of the sparse message passing mechanism by enabling nodes to attend to all other nodes in a graph (global attention). However, most existing approaches are designed for undirected graphs, and they perform generally in DAGs.

In this work, we try to address the question of how to encode DAGs information into a Transformer architecture. We propose DAGformer—directed acyclic graph Transformer—that produce a representation for a DAG. Our principal contribution is to introduce a self-attention mechanism that considers the DAG reachability relation and thus captures effective interaction between nodes. In particular, we have modified the global attention mechanism by only allowing nodes to attend to their ancestors and descendants in a DAG. Furthermore, we propose an efficient positional encoding that can be implemented in linear time for DAGs. We show that our architecture can be used for any transformer-based graph representation model. Using our novel architecture DAGformer, we obtain state-of-the-art results on OpenGraphBenchmark-CODE2 dataset [8] and the NA dataset [4].

2. RELATED WORK

In this section, we present our notation and then review relevant prior work. We refer to a graph as $G = (V, E, X)$, where $V$ and $E \subset V \times V$ are respectively the node set and the edge set. Node features are stored in $X \in \mathbb{R}^{n \times d}$ with each row representing the feature vector of one node, where $n$ is the number of nodes and $d$ is the dimension of the features, while the attributes of node $v$ is denoted by $x_v \in \mathbb{R}^d$.

2.1. Message Passing Graph Neural Networks

Recently, message passing graph neural networks have become one of the leading approaches to learning graph representations. The GCN [9], which was based on executing convolutions on the graph, is an early seminal example. Gilmer et al. [1] reformulated the early GNNs into a framework of message passing GNNs, which computes representations $h_v^\ell$ for all nodes $v$ in every layer $\ell$, and a final graph representation $h_G$ as

$$h_v^\ell = U^\ell (h_v^{\ell-1}, M^\ell \{h_u^{\ell-1} | u \in N(v)\}), \quad (1)$$
in the self-attention module, the input node features $a$ self-attention module and a feed-forward neural network. The Transformer itself is composed of two main parts: eigenvectors for the PE and computing attention on the full graph. The Transformer incorporates the partial ordering entailed by DAGs as a strong inductive bias towards representation learning. However, as mentioned above, they have issues with limited expressiveness, over-smoothing, and over-squashing \[6, 7\].

2.2. Transformers on Graphs

In light of the tremendous success of Transformers in natural language processing (NLP) \[10\], it is reasonable to investigate their applicability in the graph domain. Particularly, they are anticipated to ease the difficulties of over-smoothing and over-squashing in message passing GNNs.

2.2.1. Transformers on DAGs

A Transformer can be seen as a GNN processing a fully-connected graph \[14\]. Using a single self-attention layer, it is able to gather interaction information between any pair of nodes. However, such a mechanism may allow nodes to get some irrelevant information. We want to explore the meaningful information between nodes. As for DAGs, the reachability relation is a strong inductive bias. So we naturally could incorporate it into the self-attention layer. To materialize this idea, we formally define the set of reachable relations of node $v$ as $R_v = \{u | u \leq v \text{ or } v \leq u\}$. And we aggregate information only from $R_v$ at every node $v$. For this, Equation (5) is modified to

$$
\text{DAGAttn}(x_v) = \sum_{u \in R_v} \frac{k(x_v, x_u)}{\sum_{w \in V} k(x_v, x_w)} f(x_u), \forall v \in V
$$

We call this module DAG attention. Fig. 1 shows an illustration of DAG attention.

3.2. Incorporating Positional Encoding

Positional encodings (PE) are intended to convey the position in space of a specific node inside the graph. It refers to the process of concatenating or adding the positional representations of the graph to the input node features before the
main Transformer model, such as the Laplacian positional encoding [11] or random walk positional encoding [17]. For DAGs, we propose a simpler positional encoding called directed acyclic graph positional encodings (DAGPE) that can be computed in linear time. Formally, DAGPE are defined as:

\[ PE_{(pos, 2i)} = \sin \left( \frac{level_{pos}}{10000} \right), \]
\[ PE_{(pos, 2i+1)} = \cos \left( \frac{level_{pos}}{10000} \right), \]

where \( pos \) is the position, \( i \) is the dimension and \( level_{pos} \) is the level of topological equivalence [18], as shown in Fig. 2.

![Fig. 2](image2.png)

**Fig. 2.** An illustration of topological level.

In our architecture, we incorporate PE in DAG attention and modify Equation (6) to

\[ k(x, x') = \exp \left( \left\langle (x + PE_x)W_Q (x' + PE_{x'})W_K \right\rangle \right), \]

where \( W_{Q_{PE}}, W_{K_{PE}} \in \mathbb{R}^{d \times dk} \) are the query and key projection matrices of DAGPE, respectively.

4. EXPERIMENTS

In this section, we evaluate our architecture versus several SOTA methods for graph representation learning, including GNNs and Transformers, on two DAGs prediction tasks. And DAGformer outperforms these benchmarks, demonstrating the framework’s generality and efficacy.

4.1. Datasets and Baselines

The OGBG-CODE2 dataset [8] is comprised of abstract syntax trees (ASTs) derived from about 450k Python method definitions. It is a large dataset, which has 452741 graphs each with 125 nodes on average. The task is to predict the first 5 sub-tokens of the original function’s name. We adopt the standard dataset splitting from the benchmark. We compare our method to the following GNNs: GCN [9], GIN [19], PNA [20] and DAGNN [5], and the Transformer baselines: Transformer [10], GraphTrans [13] and SAT [16] (SOTA). All baseline performances are as reported on the OGB leaderboard.

The NA dataset [4] contains 19,020 neural architectures generated by the ENAS software. The task is to predict the architecture performance on CIFAR-10 under the weight-sharing scheme. Since this is a regression task, the metrics are RMSE and Pearson’s \( r \). We compare to DAGNN [5], D-VAE [4] and S-VAE [21].

4.2. Experimental Setup

4.2.1. The OGBG-CODE2 dataset

For our proposed architecture, we implement DAGformer upon vanilla Transformer, GraphTrans and SAT. For fair comparisons, we use the same hyper-parameters (including training schedule, optimizer, batch size, etc.) as baseline models for all of our three versions. And we repeat the experiments 10 times using different random seeds.

4.2.2. The NA dataset

To measure performance with [4], we put the Transformer with 2 heads, 2 layers and 128 hidden dimension in front of DAGNN [5]. Then we similarly train autoencoders and use sparse Gaussian process regression on the latent representation to predict the architecture performance.

4.3. Evaluation Results

The evaluation results of our experiments are summarized in Table 1 and Table 2. The experiment results successfully demonstrate that our models outperform the baselines across all datasets.
Table 1. OGBG-CODE2 dataset. All the baselines are collected from the OGB leaderboard. We denote it as DAG+Transformer if the backbone is Transformer. DAG+SAT outperforms the state-of-the-art SAT.

| Model            | Valid F1 score | Test F1 score |
|------------------|----------------|---------------|
| GIN              | 0.1376±0.0016  | 0.1495±0.0023 |
| GCN              | 0.1399±0.0017  | 0.1507±0.0018 |
| GIN-Virtual      | 0.1439±0.0026  | 0.1581±0.0020 |
| GCN-Virtual      | 0.1461±0.0013  | 0.1595±0.0018 |
| PNA              | 0.1453±0.0025  | 0.1570±0.0032 |
| DAGNN            | 0.1607±0.0040  | 0.1751±0.0049 |
| Transformer      | 0.1546±0.0018  | 0.1670±0.0015 |
| DAG+Transformer  | 0.1731±0.0014  | 0.1895±0.0014 |
| GraphTrans       | 0.1661±0.0012  | 0.1830±0.0024 |
| DAG+GraphTrans   | 0.1700±0.0021  | 0.1864±0.0018 |
| SAT (SOTA)       | 0.1773±0.0023  | 0.1937±0.0028 |
| DAG+SAT          | 0.1821±0.0013  | 0.1982±0.0010 |

Table 2. Predictive performance of latent representations for dataset NA.

| Model            | RMSE ↓  | Pearson’s r ↑  |
|------------------|---------|----------------|
| S-VAE            | 0.52±0.002 | 0.847±0.001  |
| D-VAE            | 0.375±0.003 | 0.924±0.001  |
| DAGNN            | 0.264±0.004 | 0.964±0.001  |
| Transformer      | 0.266±0.004 | 0.963±0.001  |
| DAG+Transformer  | 0.259±0.003 | 0.965±0.001  |

5. CONCLUSION

We have introduced DAGformer, a Transformer-based model for a special yet widely used class of graphs—DAGs. Our architecture is simple and universal to be used with any transformer-based models as demonstrated by three models in our experiments. It incorporates the reachability relation implied by DAGs as a powerful inductive bias towards representation learning. In addition, we propose a positional encoding for DAGs that is efficient and can be implemented in linear time. We show that DAGformer outperforms the baselines on two datasets with the assistance of this inductive bias.

6. REFERENCES

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