Unleashing the Power of Transformer for Graphs

Lingbing Guo, Qiang Zhang, Huajun Chen

Abstract
Despite recent successes in natural language processing and computer vision, Transformer suffers from the scalability problem when dealing with graphs. The computational complexity is unacceptable for large-scale graphs, e.g., knowledge graphs. One solution is to consider only the near neighbors, which, however, will lose the key merit of Transformer to attend to the elements at any distance. In this paper, we propose a new Transformer architecture, named dual-encoding Transformer (DET). DET has a structural encoder to aggregate information from connected neighbors and a semantic encoder to focus on semantically useful distant nodes. In comparison with resorting to multi-hop neighbors, DET seeks the desired distant neighbors via self-supervised training. We further find these two encoders can be incorporated to boost each others’ performance. Our experiments demonstrate DET has achieved superior performance compared to the respective state-of-the-art methods in dealing with molecules, networks and knowledge graphs with various sizes.

1. Introduction
Transformer has become one of the most prevalent neural models for natural language processing (NLP) (Vaswani et al., 2017; Devlin et al., 2019). The self-attention mechanism leveraged by Transformer has already been extended to graph neural network (GNN) models, e.g., GAT (Velickovic et al., 2018) and its variants (Wu et al., 2019; Vashishth et al., 2020; Kim & Oh, 2021; Chen et al., 2021). Nevertheless, these models only consider the 1-hop neighbors, which violates the original intention of Transformer that attends to the elements at distant positions. In this regard, they are graph convolutional networks (GCNs) with learnable attention weights for aggregating 1-hop neighborhood.

Recently, Graphormer (Ying et al., 2021) starts to leverage the standard Transformer architecture for graph representation learning and has achieved state-of-the-art performance on many benchmarks. Different from large-scale knowledge graphs (KGs) or networks, the input graph for the graph property prediction tasks are limited with small sizes (e.g., small molecules). Graphormer is thus inapplicable on large-scale graphs. The same problem also appears in the computer vision (CV) area, yet has recently been tackled by patching pixels to patches and then to windows in a hierarchical fashion (Dosovitskiy et al., 2021; Liu et al., 2021). These works inspire us to explore the possibility of using one universal Transformer architecture as the general backbone to model different sizes of graphs.

How to attend to the nodes at arbitrary distance? Is it possible to directly aggregate the embeddings of multi-hop neighbors? Yes, but it is not necessary. As far as we know, there are few GCN-based or GAT-based methods considering the three or more-hop neighbors. Even the improvement brought by the two-hop neighbors is very limited (Sun et al., 2020; Chen et al., 2021). Using one-hop neighbors is sufficient to achieve promising performance in most cases.

However, are all multi-hop neighbors useless? Definitely not, we just lack an effective approach to seek the useful distant neighbors from the enormous noise. In this paper, we propose dual-encoding Transformer (DET) to tackle the above problem. In DET, we consider two types of neighbors, i.e., structural neighbors and semantic neighbors. Structural neighbors are usually the one-hop neighbors leveraged by existing GNN models (Vashishth et al., 2020; Kim & Oh, 2021; Chen et al., 2021). Nevertheless, these models only consider the 1-hop neighbors, which violates the original intention of Transformer that attends to the elements at distant positions. In this regard, they are graph convolutional networks (GCNs) with learnable attention weights for aggregating 1-hop neighborhood.

Figure 1 shows the basic idea of DET to let two encoders continuously improve each other. For structural encoding, we use the standard self-attention layer to encode the graph structure information. The attention scores of semantic encoder is incorporated as the semantic attention bias to assist the structural encoder. We then model semantic encoding as the dual process, with the semantic encoder as the main attention model and the structural encoder as an assistant model. Therefore, DET ensures efficient neighborhood aggregation while encouraging global node connections.

The key is learning a semantic encoder to identify useful
distant nodes as semantic neighbors. The one-hop neighbors usually contribute the most valuable information to represent the node of interest. Therefore, the problem can be converted to find the distant nodes that are as important as the one-hop neighbors. Towards this end, we add a contrastive loss in structural encoding. We use the near neighbors as positive examples and randomly sampled distant nodes as negative examples, such that the training process can be fully unsupervised.

Another key design is the semantic operator \( \odot \) used to estimate the semantic score between the node of interest and others. We consider a learnable similarity function rather than directly feeding the encoder with raw embeddings. This is because that the similarity is one of the most important metrics for clustering embeddings, which compels the encoder to value the semantically close yet structurally distant nodes. The idea of considering semantically close neighbors is similar to MSA Transformer (Rao et al., 2021) and AlphaFold 2 (Jumper et al., 2021) for proteins, except that the family members (i.e., semantic neighbors in this paper) are obtained from self-supervised learning rather than querying the genetic datasets.

The proposed DET is capable of achieving superior performance on various learning tasks oriented to graphs with different sizes: (1) For the graph property prediction task, DET outperforms the best-performing methods on the PCQM4M-LSC (Nakata & Shimazaki, 2017) and ZINC (Dwivedi et al., 2020) datasets; (2) For the node classification task, DET has competitive or better performance than the state-of-the-art attention-based methods, on the Cora, CiteSeer, PubMed and PPI benchmarks (Yang et al., 2016; Zitnik & Leskovec, 2017); (3) For the KG completion (a.k.a., entity prediction) task, DET achieves the state-of-the-art performance on both FB15K-237 (Toutanova & Chen, 2015) and WN18RR (Dettmers et al., 2018) datasets. We also present in-depth model analysis to provide more insights.

2. Related Works

We split the related literature into two parts: self-attention and position embeddings.

2.1. Self-attention

Self-attention-based neural models, such as Transformer, have recently become the de facto choice in NLP tasks, ranging from language modeling and machine translation (Vaswani et al., 2017; Devlin et al., 2019) to question answering (Yang et al., 2019) and sentiment analysis (Xu et al., 2019a). Transformer has significant advantages over conventional sequential models like recurrent neural networks (RNNs) (Williams & Zipser, 1989; Hochreiter & Schmidhuber, 1997) in both scalability and efficiency.

When modelling graph data, another well-used self-attention mechanism is proposed by GAT (Velickovic et al., 2018), which we call the linear attention in this paper. Compared with the dot-product calculation in the original implementation, the linear attention performs concatenation of query and key nodes for the query node, which is efficient when ranking candidate nodes on large graphs. Therefore, it has become the primal choice for modeling graph data (Wu et al., 2019; Sun et al., 2020; Vashishth et al., 2020; Wang et al., 2019a; Kim & Oh, 2021).

In this paper, we use the dot-product attention to encode the structural neighbors and the modified linear attention to encode semantic neighbors.

2.2. Position Embedding

Position embeddings are one of the most important attributes to Transformer. Transformer variants adapted to different areas usually customize this attribute. For example, ViT (Dosovitskiy et al., 2021) sequentially indexes the patches and encodes the indices as 1D position embeddings.
SwinTransformer (Liu et al., 2021) proposes the 2D-aware relative position biases, which employs a learnable matrix to record pairwise patch position information in the window.

In addition to the position information, other prior knowledge can also be injected as attention biases or embeddings into Transformer. For example, Graphformer (Ying et al., 2021) encodes centrality and shortest path distance into embeddings, and then incorporates them as “position embeddings” into Transformer. HittER (Chen et al., 2021) adds the edge type (i.e., relation) information of KGs when encoding entity embeddings.

Specially, MSA Transformer (Rao et al., 2021; Jumper et al., 2021) leverages the multiple sequence alignment (MSA) information, which is closely related to our work. When aggregating the information of one site, it does not only consider the others along the protein sequence, but also the same site within the evolutionary family members. The semantic encoding proposed in this paper also exploits such “family” information, except that the family members is selected based on the semantic scores.

3. Methodology

In this section, we will illustrate the detail and insight of DET. We start from the preliminaries, and then introduce the dual-encoding process leveraged by DET, after which we illustrate how to train the semantic encoder to obtain the semantic neighbors. Finally, we present the implementation of the whole architecture.

3.1. Preliminaries

We first introduce the terminologies and notations that will be used in the following sections.

**Graph** We define a graph as \( G = (\mathcal{V}, \mathcal{E}) \), where \( \mathcal{V} = \{v_1, v_2, ..., v_n\} \) is the node set, and \( \mathcal{E} = \{e_1, e_2, ..., e_m\} \) is the edge set. \( n \) and \( m \) denote the numbers of nodes and edges, respectively. In practice, different tasks often have more complicated graph structures. For example, molecular graphs and KGs have typed edges (i.e., chemical bonds and relations). We do not discuss these details in the main paper, and follow the general setting to process these specific features (Ying et al., 2021; Chen et al., 2021).

**GNN and Self-attention** Without loss of generality, we define a GNN as a neural network that learns a group of weights to aggregate the embeddings of the one-hop or multi-hop neighbors for the node of interest. In this sense, self-attention can be naturally treated as a GNN model. Let \( Q \in \mathbb{R}^{n \times h} \), \( K \in \mathbb{R}^{n \times h} \), \( V \in \mathbb{R}^{n \times h} \) denote the query, key, and value matrices, respectively. \( h \) denotes the hidden-size. In this paper, they are the same node embedding matrix.

Self-attention calculates the attention scores as follows:

\[
A = \text{Softmax}\left(\frac{QK^\top}{\sqrt{h}}\right),
\]

where \( A \in \mathbb{R}^{n \times n} \) records the node-to-node attention scores. We then aggregate the node embeddings with the following equation:

\[
H = AV,
\]

where \( H \in \mathbb{R}^{n \times h} \) is the output embedding matrix, with each row denoting the output embedding of a node in \( \mathcal{V} \).

**Linear Attention** The computational complexity of the above dot-product implementation is \( \omega(n^2) \) (without considering hidden-size). As the number of nodes increases, the cost becomes unacceptable. GAT (Velickovic et al., 2018) proposes a linear self-attention implementation to mitigate this problem by only considering the one-hop neighbors:

\[
B_{ij} = \sigma(b^\top(v_iW \parallel v_jW)),
\]

where \( B_{ij} \) denotes the attention score from the node of interest \( v_i \) to a neighbor \( v_j \). \( v_i, v_j \in \mathbb{R}^h \) are the embeddings of \( v_i \) and \( v_j \), respectively. \( b \in \mathbb{R}^h \) and \( W \in \mathbb{R}^{h \times h} \) are weight vector and matrix, respectively. \( \sigma \) is the activation function and \( \parallel \) denotes the concatenation operation. The linear attention does not consider the correlations within neighbors, and thus its computational complexity is cut down from \( \Omega(n^2) \) to \( \Omega(n + m) \).

3.2. Dual Encoding

The well-used two attention mechanisms have different pros and cons. To fulfill our goal of designing a universal graph Transformer architecture, we propose to combine their advantages to effectively and efficiently encode graphs with different sizes.

**Structural Encoding** The standard dot-product attention can be easily extended on the small graphs. We add a virtual node \( v_c \) (Devlin et al., 2019) as the context node connected with all nodes in \( G \). Then, the output representation for \( v_c \) can be regarded as the representation of \( G \). For the large graphs like KGs or networks, we can perform self-attention on the one-hop ego graph \( G_i \) given the node of interest \( v_i \). Therefore, the output embedding for node \( v_i \) is

\[
h_i^{st} = \sum_{v_j \in \mathcal{N}(v_i)} A_{ij}v_j,
\]

where \( h_i^{st} \) denotes the output of structural encoder for \( v_i \). \( A_{ij} \) denotes the attention score for the context node \( v_c \) to the neighbor \( v_j \). \( \mathcal{N}(v_i) \) denotes the structural one-hop neighbor set for \( v_i \). With multiple stacked layers, the correlations within the one-hop neighbors will be leveraged.
Therefore, we can use one universal encoder layer to model the graph structural information to obtain the node representation and graph representation. Note that, the encoder itself does not consider the difference of nodes in the graph structure (e.g., distance to the node of interest). Follow the exiting works (Ying et al., 2021; Chen et al., 2021), we accordingly add the centrality, relation type, or shortest distance path information as special position embeddings to the encoder. The details can be found in Appendix A.

**Semantic Encoding** The structural features may be less discriminative to identify a neighbor. For example, if the node of interest has a large amount of neighbors, it is inevitable that many neighbors will have similar or identical structural features (e.g., shortest path distance to $v_i$). This problem is even more serious when we only consider the one or two hop neighbors. However, if we consider more than two hop neighbors, the sheer quantity of available information will overwhelm the neural network.

In this paper, we seek the distant neighbors not based on paths but the semantic scores estimated by the semantic encoder. Specifically, the semantic similarity is estimated by a learnable neural function $f_s: \mathbb{R}^h \times \mathbb{R}^h \rightarrow \mathbb{R}$:

$$f_s(v_i, v_j) = \sigma(v_i \odot v_j) = \sigma(W_s(v_i - v_j) + b_s), \quad (5)$$

where $\odot$ is the semantic difference operator. The choice of $\odot$ is flexible, as long as it can reflect the similarity between $v_i$ and $v_j$. Here, we use a weighted $L1$ distance as $\odot$, which is simple and can be easily extended to matrix operation. $W_s \in \mathbb{R}^{1 \times h}$ and $b_s \in \mathbb{R}$ (for single head attention) are the weight matrix and bias, respectively.

**Dual-encoding Transformer** In DET, the structural encoder encodes the graph structural information into node embeddings, while the semantic encoder calculates the attention scores based on the semantic similarity. It is worth incorporating these two encoders to achieve better performance. As shown in Figure 1, when the structural encoder fails to estimate which neighbors are more important, the attention bias provided by the semantic encoder may be helpful. For example, in a citation network, the semantic similarity may be a more effective metric than structural distance when aggregating the neighboring papers for classification.

| Hops   | FB15K-237 | WN18RR |
|--------|-----------|--------|
| 1-hop  | 20.3      | 2.7    |
| 2-hop  | 1,781.4   | 8.9    |
| 3-hop  | 64,774.9  | 30.5   |
| 5-hop  | -         | 483.8  |

Figure 2. Comparing MSA with semantic neighbors. The left figure is sliced from (Jumper et al., 2021).

### 3.3. Exploiting the Semantic Neighbors

To establish a stable dual-encoding process, the key is seeking reliable semantic neighbors. In this paper, we propose a self-supervised training method to exploit the semantic neighbors of the node of interest, which is based on the following two hypotheses:

**Hypothesis 1** *The one-hop neighbors are the most informative sources to identify and represent the node of interest.*

Intuitively, if a node appears as a neighbor of other nodes for many times, the information provided by this node may not be helpful to make the node of interest *unique*. Table 1 shows the average appearing times for different hops of neighbors. We can find that the two or more-hop neighbors of a node are shared by more others, which is why current GNN models rarely consider the multi-hop neighbors. This is also known as the over-smoothing problem. Therefore, it is reasonable to regard the one-hop neighbors as the most informative sources.

**Hypothesis 2** *The distant nodes with similar embeddings to that of the node of interest are important sources to the node of interest.*

It has been proven that the information provided by the family members is useful for protein structure prediction in MSA Transformer (Rao et al., 2021) and AlphaFold2 (Jumper et al., 2021). Although the idea of the semantic encoder is not directly inspired by these two existing works, we actually find the close correlations between the semantic neighbors and the MSA information, which may explain why DET works.
We first initialize all parameters of DET and embeddings. We illustrate the implementation of DET by Algorithm 1.

**Algorithm 1 Dual-encoding Transformer**

**Input:** graph \( G = (V, E) \), the prediction loss \( L_{\text{main}} \), structural encoder \( M_{\text{st}} \) and semantic encoder \( M_{\text{se}} \)

Initialize all parameters.

repeat

Select the semantic neighbors for each node.

for each batch data \((X, Y)\) do

\[ H_{\text{st}} \leftarrow M_{\text{st}}(X) | M_{\text{se}}(X) \]
\[ H_{\text{se}} \leftarrow M_{\text{se}}(X) | M_{\text{st}}(X) \]
\[ H \leftarrow H_{\text{st}} \oplus H_{\text{se}} \]

Compute \( L_{\text{sn}} \) according to Equation (6)

\[ L \leftarrow L_{\text{main}}(H, Y) + L_{\text{sn}} \]

Update the parameters according to \( L \)

end for

until the performance on validation set converges

Multiple sequence alignment (MSA) can be regarded as the results of biological sequence alignment. The protein sequences in the same family are assumed to have a common ancestor or an evolutionary relationship. The semantic neighbors of the node of interest, on the other hand, are also assumed to have similar semantic characteristics to the node of interest. We compare MSA and semantic neighbors in Figure 2. The MSA results are obtained by searching the genetic database, while the semantic neighbors are obtained by searching the node embedding set with the semantic encoder. Therefore, the semantic encoder in this sense is equivalent to a column attention layer leveraged by MSA Transformer and AlphaFold 2.

Based on the above two hypotheses, we define the semantic neighbor fetching loss as:

\[
L_{\text{sn}}(v_i) = - \frac{1}{|\mathcal{N}(v_i)|} \sum_{v_j \in \mathcal{N}(v_i)} \ln(f_s(v_i, v_j)) + \frac{1}{|\mathcal{N}^{-}(v_i)|} \sum_{v_k \in \mathcal{N}^{-}(v_i)} \ln(f_s(v_i, v_k)), \tag{6}
\]

where \( \mathcal{N}^{-}(v_i) \) is the negative neighbor set where the negative examples are randomly sampled distant nodes to \( v_i \).

### 3.4. Implementation

We illustrate the implementation of DET by Algorithm 1. We first initialize all parameters of DET and embeddings. For better efficiency, the semantic neighbors of each node are only updated at the beginning of each epoch. Then, for each batch, the structural output embeddings are generated by the structural encoder conditioned on the semantic encoder bias, and verse visa. Finally, we combine the main prediction loss and the semantic neighbor fetching loss, and update all parameters by back-propagation.

### Table 2. Graph property prediction results on PCQM4M-LSC.

| Model     | #param. | train MAE | validate MAE |
|-----------|---------|-----------|--------------|
| GCN       | 2.0M    | 0.1318    | 0.1691       |
| DeeperGCN | 25.5M   | 0.1059    | 0.1398       |
| GraphSage | -       | -         | -            |
| GIN       | 3.8M    | 0.1203    | 0.1537       |
| GT        | 83.2M   | 0.0955    | 0.1408       |
| Graphormer| 47.1M   | **0.0546**| **0.121**    |

### Table 3. Graph property prediction results on ZINC.

| Model   | #param. | test MAE |
|---------|---------|----------|
| GCN     | 505,079 | 0.367    |
| GraphSage | 505,341 | 0.398    |
| GIN     | 509,549 | 0.526    |
| PNA     | 387,155 | 0.142    |
| GAT     | 531,345 | 0.384    |
| SAN     | 508,577 | 0.139    |
| GT      | 588,929 | 0.226    |
| Graphormer | 489,321 | 0.122    |
| DET     | 489,562 | **0.113**|

### 4. Experiment

In this section, we conducted experiments on a variety of benchmarks, ranging from graph property prediction to node classification and KG completion, to verify the effectiveness of DET. The source code was uploaded and will be available online. Please see Appendix B for dataset statistics.

#### 4.1. Graph Property Prediction

**Settings** We evaluated DET on the graph property prediction benchmarks PCQM4M-LSC (Hu et al., 2021) and ZINC (Dwivedi et al., 2020). The former is used in recent Open Graph Benchmark Large-Scale Challenge1, while the later is a popular dataset used to evaluate graph representation learning methods.

We employed a 12-layer DET with hidden-sizes 768 and 80, for PCQM4M-LSC and ZINC, respectively. Due to the number of nodes for each graph is very small (usually less than 50), we directly perform attention operations on the whole graph rather than on one-hop or semantic neighbors. Therefore, we removed the semantic neighbor fetching loss in this experiment.

**Baselines** We compared DET with state-of-the-art GNN methods on the dataset leader-boards: the attention-based methods SAN (Kreuzer et al., 2021), GT (Dwivedi & Bresson, 2021) and Graphormer (Ying et al., 2021); and other

1https://ogb.stanford.edu/kddcup2021/pcqm4m/
recently developed GNN methods GCN (Kipf & Welling, 2017), GraphSage (Hamilton et al., 2017), GIN (Xu et al., 2019b), DeeperGCN (Gilmer et al., 2017), and PNA (Corso et al., 2020).

**Results** Table 2 and Table 3 summarize the experimental results measured by mean average error (MAE) on two datasets. Due to the inaccessibility of the testing data on PCQM4M-LSC, we alternatively report the MAE results on training and validation sets.

Overall, DET outperformed all the baseline methods, achieving a new state-of-the-art on both two datasets. Compared with Graphormer that only considers encoding structural information with Transformers, DET significantly improved the performance, with 6.2% and 7.4% MAE decline on PCQM4M-LSC and ZINC, respectively. Furthermore, the number of model parameters was still relatively equivalent to that of baselines. We also observe that DET had more significant advantages over other methods on ZINC. This is because the restriction of the model size on the ZINC benchmark severely limited the capability of modeling structural information. Leveraging the semantic information becomes a more efficient choice. If we do not limit the model size of DET, it can easily achieve a MAE of 0.006.

### 4.2. Node Classification

**Settings** We evaluated DET on four benchmarks that are generally used for node representation learning. Specifically, Cora, CiteSeer, and PubMed (Yang et al., 2016) are three citation network datasets used for the transductive setting, while PPI (Zitnik & Leskovec, 2017) is a well-used protein-protein interaction dataset for the inductive setting. Following (Kim & Oh, 2021), we repeated experiments 100 times on Cora, CiteSeer, and PubMed with random seeds, and 30 times on PPI, to produce reliable results.

We followed a general GAT model setting defined in the PyTorch Geometric (Fey & Lenssen, 2019) framework. We used a stacked two-layer DET, with a learning-rate of 0.005, optimized with an Adam optimizer (Kingma & Ba, 2015). We used the standard dot-product attention mechanism when encoding one-hop structural information, which performed better than the linear attention proposed by GAT in our implementation.

**Baselines** We selected the attention-base methods GAT (Veličković et al., 2018), CGAT (Wang et al., 2019a), and SuperGATSD (Kim & Oh, 2021) as baseline methods. Particularly, SuperGATSD also uses the standard dot-product attention rather than that used in original GAT. In addition, other GNN methods GCN (Kipf & Welling, 2017), GraphSage (Hamilton et al., 2017) and GCN+NS (Zheng et al., 2020) were also added for comparison.

| Model       | Cora  | CiteSeer | PubMed | PPI    |
|-------------|-------|----------|--------|--------|
| GCN         | 81.5  | 70.3     | 79.0   | 61.5 ± 0.4 |
| GraphSage   | 82.1 ± 0.6 | 71.9 ± 0.9 | 78.0 ± 0.7 | 59.0 ± 1.2 |
| GCN+NS      | 83.7 ± 1.4 | 74.1 ± 1.4 | -     | -     |
| GAT         | 83.0 ± 0.7 | 72.5 ± 0.7 | 79.0 ± 0.4 | 72.2 ± 0.6 |
| CGAT        | 81.4 ± 1.1 | 70.1 ± 0.9 | 78.1 ± 1.0 | 68.3 ± 1.7 |
| SuperGATSD  | 82.7 ± 0.6 | 72.5 ± 0.8 | 81.3 ± 0.5 | 74.4 ± 0.4 |
| DET         | 84.6 ± 0.4 | 72.8 ± 0.5 | 81.8 ± 0.3 | 73.7 ± 0.3 |

**Results** The results are shown in Table 4, from which we can observe that DET outperformed the attention-based methods on most datasets except PPI. Although SuperGATSD had better performance on this dataset, we argue that it is no contradiction to incorporate SuperGATSD as structural encoder into DET to obtain a stronger model.

Interestingly, the attention-based methods unanimously performed worse than the GCN-based method GCN+NS on CiteSeer. SuperGATSD and CGAT even had the same or worse results compared with the original GAT. Nevertheless, we observe significant improvement from GAT to DET. This result empirically demonstrates the strength of leveraging semantic neighbors.

### 4.3. KG Completion

**Settings** We conducted experiments on the entity prediction task to evaluate DET for KG representation learning. The main target of entity prediction is to predict the subject entity (or object entity) for a given triple. We evaluated DET on the current benchmarks FB15K-237 (Toutanova & Chen, 2015) and WN18RR (Dettmers et al., 2018), which are sampled from the real-world KG Freebase (Bollacker et al., 2008) and WordNet (Miller, 1995), respectively.

The training setting mostly followed (Kim & Oh, 2021) as baseline methods. SuperGATSD had better performance on this dataset, we argue that it is no contradiction to incorporate SuperGATSD as structural encoder into DET to obtain a stronger model.

| Model      | FB15K-237 | WN18RR |
|------------|-----------|--------|
| MRR MR Hits@1 | MRR MR Hits@1 |
| TransE     | .310 199 .218 .232 1.706 .061 |
| RotatE     | .338 177 .241 .476 3.340 .428 |
| TuckER     | .358 180 .266 .470 1.043 .443 |
| CoKE       | .364 197 .272 .484 - .450 |
| CompGCN    | .355 197 .264 .479 3.533 .443 |
| HintER     | .373 158 .279 .503 2.268 .462 |
| DET        | .376 150 .281 .507 2.255 .465 |
Unleashing the Power of Transformer for Graphs

Table 6. Ablation study results on different datasets (metrics: MAE for ZINC; Accuracy for Cora, CiteSeer and PubMed; MR for FB15K-237 and WN18RR. ↑: higher is better; ↓: lower is better. ×: unavailable entry).

| Structural encoder | Semantic encoder | Semantic neighbor fetching | ZINC↑ | Cora† | CiteSeer† | PubMed↑ | FB15K-237↓ | WN18RR↓ |
|--------------------|------------------|---------------------------|-------|-------|----------|---------|----------|---------|
| ✓                  | ✓                | ✓                        | ×     | 84.6  | 72.8     | 81.8    | 150      | 2.255   |
| ✓                  | ✓                | ✓                        | 0.113 | 82.6  | 72.7     | 78.1    | 151      | 2.305   |
| ✓                  | ✓                | ×                        | 0.122 | 84.0  | 71.6     | 80.9    | 158      | 2.268   |
| ✓                  | ✓                | ×                        | 0.515 | 83.1  | 72.6     | 77.7    | ×        | ×       |

Figure 3. Accuracy on three citation network datasets, in term of hyper-parameter \( \tau \) (average results of 7 runs).

Baselines We chose the best-performing entity prediction methods as our baselines: the TransE-family methods TransE (Bordes et al., 2013), RotatE (Sun et al., 2019), and TuckER (Balazevic et al., 2019), and the attention-based methods CoKE (Wang et al., 2019b), CompGCN (Vashishth et al., 2020), and HittER (Chen et al., 2021). Specifically, CoKE and HittER also leverage Transformer to encode structural information.

Results We report the main results on Table 5. It can be clearly observed that DET surpassed all the baselines across all datasets and metrics. The improvement on MR (mean rank) is most significant, which implies that DET learned better embeddings for all entities, not only for top ones that valued by Hits@1. By comparing the results with those in Table 3 and Table 4, we actually find that the performance superiority of DET is slim in the entity prediction task. We believe this is because KGs perhaps have the most complicated graph structures in real world. They have much more different edge types than networks or molecules. Encoding the structural information is thus more important for KGs. Even though, we still observe considerable improvement on two datasets.

5. Further Analysis

The superior performance inspires us to explore and evaluate DET in depth. In this section, we design three experiments to help us better understand the idea of DET.

5.1. Is Every Module in DET Useful?

We first conducted ablation study experiments to verify the effectiveness of each module in DET. We picked up six datasets in different representation learning tasks and present the results in Table 6. We removed the modules from DET step-by-step while kept identical hyper-parameter setting along the experiments.

Semantic Neighbor Fetching The semantic neighbor fetching loss is undoubtedly important to DET. No matter combining two encoders or only using semantic encoder, integrating with the semantic fetching module had better performance in most cases. The improvement was most notable on PubMed, where it yielded 3.7% and 3.8% of accuracy increases, respectively. The mean rank results on WN18RR also got worse without the fetching loss.

Semantic Encoder If we do not consider the semantic neighbor fetching loss, is semantic encoder itself useful for DET? Unfortunately, we find the answer ambiguous. For Cora, PubMed, and WN18RR, when we did not employ the fetching loss, DET with the semantic encoder performed much worse than DET without the semantic encoder. But we observe that the situation reversed on CiteSeer and FB15K-237. In fact, when we only consider one-hop neighbors, the semantic encoder without fetching loss is just a “minus” attention layer. It may have its pros and cons compared with the standard dot-product attention layer on different datasets. In this sense, the semantic fetching loss is who endows the semantic encoder with the characteristic.

On the ZINC dataset, when it is capable of applying attention operations on the whole graph, the semantic encoder could estimate the semantic similarity between distant nodes without the help of the fetching loss. Therefore, we can see that the dual-encoding version of DET greatly outperformed the structural encoder only version on ZINC. Overall, the effectiveness of the semantic encoder is conditioned: it must get in touch with the distant nodes.
Structural Encoder The structural encoder also has merits. From the results of the 3-rd and 5-th rows in Table 6, we can find that it had better performance than the semantic encoder on most datasets except CiteSeer. The dot-product attention is worthy of analysis. We also noticed that the worst MAE on ZINC was obtained by only using the semantic encoder, due to the absence of all structural information.

5.2. Does the Semantic Encoder Perform Better in Citation Networks?

In Section 3, we mention that the semantic encoding may be more helpful in citation networks, where the semantically close neighbors are the key components to predict the label of the node of interest. In this section, we conducted experiment to verify this assumption empirically. In DET, we set a hyper-parameter $\tau$ to control the combination of the structural encoder and the semantic encoder, which can be written in the following equation:

$$h = \tau h^s + (1 - \tau) h^e,$$

where $h$, $h^s$, $h^e$ denote the combined output, structural output, and semantic output, respectively. By assigning different $\tau$, we can control the importance of each encoder in the combination.

The experimental results are shown in Figure 3. Although the performance gap among three datasets was significant, we observe a similar trend: the accuracy first increased steadily from $\tau = 0$ to $\tau = 0.1$, and then peaked around $\tau = 0.15$, after which dropped rapidly until $\tau = 1$. When $\tau = 0$ or $\tau = 1$, we used only the semantic encoder or the structural encoder in training. The performance at $\tau = 0$ is significantly better than that at $\tau = 1$, which empirically demonstrates the advantage of leveraging semantic neighbor information. We further find that best performance was achieved at $\tau = 0.15$, 0.15, and 0.05, respectively. This observation suggests that properly combining the output of two encoders may be the best choice. However, we should notice that, averaging the results (i.e., $\tau = 0.5$) was not a good idea on all dataset, as the semantic encoder always performed better than the structural encoder.

5.3. How does the Semantic Encoder Help the Structural Encoder?

It is worth exploring how the semantic encoder affects the structural encoder. In Figure 4, we illustrate two examples on FB15K-237 and WN18RR, respectively. For the structural one-hop neighbors, we find that the scores calculated by the semantic encoder are in line with human intuition. For example, in the left figure, the entity USA has a very low score although it is directly connected to Nintendo by relation service_location. The verb precede and accompany also obtain relatively low scores in the right figure. These neighbors are not very related to the entities of interest from human perspective. On the other hand, some one-hop neighbors get high semantic scores, e.g., the well-known director Shigeru Miyamoto of Nintendo in FB15K-237 and the verb walk in WN18. They are the entities that should gain more attentions. On the other hand, for the semantic neighbors, we can see that the exploited distant neighbors are closely related to the entity of interest. For example, Atlas is an important game developer to Nintendo. Aggregating such information may be helpful when the model is asked to predict the games related to Nintendo. For the verb travel in WN18RR, move also shares many key features with it. We also conducted experiment to analysis the effects of the semantic encoder to the structural encoder during the training phase. Limited by paper length, we refer the interested readers to Appendix C.

6. Conclusion and Future Work

In this paper, we proposed a new Transformer architecture, called DET, to deal with different types of graphs. In DET, the structural encoder aggregates information from connected nodes while the semantic encoder seeks the distant nodes with useful semantics. The experimental results demonstrate the strong performance of DET on three prevalent GNN tasks across 8 benchmarks. We hope DET can bring more insights and inspirations in developing unified Transformer architectures. In future, we plan to adapt DET to NLP and CV areas.
Unleashing the Power of Transformer for Graphs

References

Balazevic, I., Allen, C., and Hospedales, T. M. Tucker: Tensor factorization for knowledge graph completion. In EMNLP-IJCNLP, pp. 5184–5193, 2019.

Bollacker, K. D., Evans, C., Paritosh, P., Sturge, T., and Taylor, J. Freebase: A collaboratively created graph database for structuring human knowledge. In SIGMOD, pp. 1247–1250, 2008.

Bordes, A., Usunier, N., Garcia-Durán, A., Weston, J., and Yakhnenko, O. Translating embeddings for modeling multi-relational data. In EMNLP, pp. 10395–10407, 2021.

Chen, S., Liu, X., Gao, J., Jiao, J., Zhang, R., and Ji, Y. Hitter: Hierarchical transformers for knowledge graph embeddings. In EMNLP, pp. 10395–10407, 2021.

Corso, G., Cavalleri, L., Beaini, D., Liò, P., and Veličković, P. Principal neighbourhood aggregation for graph nets. NeurIPS, 33:13260–13271, 2020.

Dettmers, T., Minervini, P., Stenetorp, P., and Riedel, S. Convolutional 2D knowledge graph embeddings. In AAAI, pp. 1811–1818, 2018.

Devlin, J., Chang, M., Lee, K., and Toutanova, K. BERT: pre-training of deep bidirectional transformers for language understanding. In NAACL-HLT, pp. 4171–4186, 2019.

Dosovitskiy, A., Beyer, L., Kolesnikov, A., Weissenborn, D., Zhai, X., Unterthiner, T., Dehghani, M., Minderer, M., Heigold, G., Gelly, S., Uszkoreit, J., and Houlsby, N. An image is worth 16x16 words: Transformers for image recognition at scale. In ICLR, 2021. URL https://openreview.net/forum?id=YicbFdNTTy.

Dwivedi, V. P. and Bresson, X. A generalization of transformer networks to graphs. AAAI Workshop on Deep Learning on Graphs: Methods and Applications, 2021.

Dwivedi, V. P., Joshi, C. K., Laurent, T., Bengio, Y., and Bresson, X. Benchmarking graph neural networks. arXiv preprint arXiv:2003.00982, 2020. URL https://arxiv.org/abs/2003.00982.

Fey, M. and Lenssen, J. E. Fast graph representation learning with PyTorch Geometric. In ICLR Workshop on Representation Learning on Graphs and Manifolds, 2019.

Gilmer, J., Schoenholz, S. S., Riley, P. F., Vinyals, O., and Dahl, G. E. Neural message passing for quantum chemistry. In ICML, pp. 1263–1272, 2017.

Hamilton, W. L., Ying, Z., and Leskovec, J. Inductive representation learning on large graphs. In NIPS, pp. 1024–1034, 2017.

Hochreiter, S. and Schmidhuber, J. Long short-term memory. Neural Computation, 9:1735–1780, 1997.

Hu, W., Fey, M., Ren, H., Nakata, M., Dong, Y., and Leskovec, J. Ogb-lsc: A large-scale challenge for machine learning on graphs. arXiv preprint arXiv:2103.09430, 2021.

Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., Bridglan, A., Meyer, C., Kohl, S. A. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., Back, T., Petersen, S., Reiman, D., Clancy, E., Zielinski, M., Steinegger, M., Pacholska, M., Berghammer, T., Bodenstein, S., Silver, D., Vinyals, O., Senior, A. W., Kavukcuoglu, K., Kohli, P., and Hassabis, D. Highly accurate protein structure prediction with AlphaFold. Nature, 596(7873):583–589, 2021.

Kim, D. and Oh, A. H. How to find your friendly neighborhood: Graph attention design with self-supervision. In ICLR, 2021. URL https://openreview.net/forum?id=Wi5KUNlqWty.

Kingma, D. P. and Ba, J. Adam: A method for stochastic optimization. In ICLR, 2015. URL http://arxiv.org/abs/1412.6980.

Kipf, T. N. and Welling, M. Semi-supervised classification with graph convolutional networks. In ICLR, 2017. URL https://openreview.net/forum?id=SJU4ayYgl.

Kreuzer, D., Beaini, D., Hamilton, W., Létourneau, V., and Tossou, P. Rethinking graph transformers with spectral attention. arXiv preprint arXiv:2106.03893, 2021.

Liu, Z., Lin, Y., Cao, Y., Hu, H., Wei, Y., Zhang, Z., Lin, S., and Guo, B. Swin transformer: Hierarchical vision transformer using shifted windows. In ICCV, pp. 10012–10022, 2021.

Miller, G. A. WordNet: An electronic lexical database. Communications of the ACM, 38, 1995.

Nakata, M. and Shimazaki, T. Pubchemqc project: a large-scale first-principles electronic structure database for data-driven chemistry. Journal of chemical information and modeling, 57(6):1300–1308, 2017.

Rao, R., Liu, J., Verkuijl, R., Meier, J., Canny, J. F., Abbeel, P., Sercu, T., and Rives, A. Msa transformer. bioRxiv, 2021. URL https://www.biorxiv.org/content/10.1101/2021.02.12.430858v1.

Sun, Z., Deng, Z.-H., Nie, J.-Y., and Tang, J. Rotate: Knowledge graph embedding by relational rotation in complex...
Unleashing the Power of Transformer for Graphs

space. In ICLR, 2019. URL https://openreview.net/forum?id=HkgE9nRqYQ.

Sun, Z., Wang, C., Hu, W., Chen, M., Dai, J., Zhang, W., and Qu, Y. Knowledge graph alignment network with gated multi-hop neighborhood aggregation. In AAAI, pp. 222–229, 2020.

Toutanova, K. and Chen, D. Observed versus latent features for knowledge base and text inference. In CVSC, pp. 57–66, 2015.

Vashishth, S., Sanyal, S., Nitin, V., and Talukdar, P. P. Composition-based multi-relational graph convolutional networks. In ICLR, 2020. URL https://openreview.net/forum?id=By1A_C4tPr.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., and Polosukhin, I. Attention is all you need. In NIPS, pp. 5998–6008, 2017.

Velickovic, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., and Bengio, Y. Graph attention networks. In ICLR, 2018. URL https://openreview.net/forum?id=rJXMpikCZ.

Wang, G., Ying, R., Huang, J., and Leskovec, J. Improving graph attention networks with large margin-based constraints. CoRR, abs/1910.11945, 2019a.

Wang, Q., Huang, P., Wang, H., Dai, S., Jiang, W., Liu, J., Lyu, Y., Zhu, Y., and Wu, H. Coke: Contextualized knowledge graph embedding. arXiv preprint arXiv:1911.02168, 2019b.

Williams, R. J. and Zipser, D. A learning algorithm for continually running fully recurrent neural networks. Neural computation, 1:243–248, 1989.

Wu, Y., Liu, X., Feng, Y., Wang, Z., Yan, R., and Zhao, D. Relation-aware entity alignment for heterogeneous knowledge graphs. In IJCAI, pp. 5278–5284, 2019.

Xu, H., Liu, B., Shu, L., and Yu, P. S. BERT post-training for review reading comprehension and aspect-based sentiment analysis. In NAACL-HLT, pp. 2324–2335, 2019a.

Xu, K., Hu, W., Leskovec, J., and Jegelka, S. How powerful are graph neural networks? In ICLR, 2019b. URL https://openreview.net/forum?id=ryGs6iA5Km.

Yang, W., Xie, Y., Lin, A., Li, X., Tan, L., Xiong, K., Li, M., and Lin, J. End-to-end open-domain question answering with bertserini. In NAACL-HLT, pp. 72–77, 2019.

Yang, Z., Cohen, W. W., and Salakhutdinov, R. Revisiting semi-supervised learning with graph embeddings. In ICML, volume 48, pp. 40–48, 2016.
A. Position Embedding

In graphs, there are many important features that are used to identify different nodes. Thanks to learnable position embedding, these discrete features now can be encoding into embeddings and then combined with the raw embedding of nodes.

Specifically, for graph representation learning task, we use the same method proposed by (Ying et al., 2021) to encode degree centrality of an arbitrary node $v_i$ as:

$$c_i = f_c(\text{deg}(v_i)),$$

where $\text{deg}(v_i)$ denotes the degree of the node $v_i$, and $f_c : \mathbb{R} \rightarrow \mathbb{R}^h$ is the mapping function that converts the node degree to a learnable embedding. We further consider encoding the distances to different neighbors for the node of interest $v_i$ by the following equation:

$$d_{v_i,v_j} = f_d(\text{spd}(v_i,v_j)),$$

where $\text{spd}(v_i,v_j)$ denotes the shortest path distance from $v_i$ to $v_j$, and $f_d : \mathbb{R} \rightarrow \mathbb{R}^h$ is a similar function that converts the distance to a learnable embedding.

For KG representation learning task, we follow (Chen et al., 2021) to encoder the edge types into node embeddings, which is implemented by an additional atom transformer $\mathcal{M}_A$ to encode triples. Specifically, for a given triple $(v_i, r_{ij}, v_j)$ for the node of interest $v_i$, where $r_{ij}$ denote the edge type (i.e., relationship) between $v_i$ and $v_j$. The edge type information can be encoded by the following equation:

$$e_{ij} = \mathcal{M}_A([c_A, v_i, r_{ij}, v_j]),$$

where $[c_A, v_i, r_{ij}, v_j]$ is the input embedding sequence. $c_A$ is the virtual node for the atom Transformer, whose output represents the edge encoding embedding.

B. Dataset Details

We present the overall dataset statistics in Table 7.

B.1. Graph Property Prediction

For PCQM4M-LSC, the model is asked to predict the DFT (density functional theory)-calculated HOMO-LUMO energy gap of given molecules. It contains more than 3.8M 2D molecular graphs as input, which is especially appropriate to evaluate the performance of model in large scale scenarios. On other hand, ZINC is a relative small datasets, where the main target is to predict the graph property regression for constrained solubility. It is one of the most popular real-world molecular datasets for graph representation learning.

![Figure 5. The validate MAE results on the ZINC dataset, in term of training step.](image)

B.2. Node Classification

Cora, CiteSeer and PubMed are three citation network datasets proposed by (Yang et al., 2016). They are typically used for transductive node classification task. PPI on the other hand is used for inductive evaluation. It consists of 24 graphs, with 20 graphs for training, and 2 for validation and 2 for testing. All four datasets are the prevalent benchmarks used for node classification.

B.3. KG Completion

FB15K-237 is the revised version of the original FB15K dataset (Bordes et al., 2013) that was used as entity prediction benchmark in last ten years. However, recent studies (Toutanova & Chen, 2015; Dettmers et al., 2018) find that the original FB15K contains a large proportion of redundant data, some of which may incur testing data leakage, the same to another well-used dataset WN18. Therefore, most latest studies only use the revised datasets FB15K-237 and WN18RR for evaluation. FB15K-237 has more different relationships, while WN18RR is more sparse and has more different entities.

C. Analysis on the Training Process

We conducted experiments to compare the performance of structural encoder with and without the semantic encoder, in term of training steps.

We depict the valid MAE results on ZINC in Figure 5. At the beginning of the training, we find that the two methods do not have a visible performance gap. The curves are tightly overlapped during step 0 to 74, 000.

As the performance starts to be converged, i.e., step 74, 000 to 148, 000, only using structural encoder is better than combining the two encoders. However, as the valid MAE tends
Figure 6. The validate MAE results on the PCQM4M-LSC dataset, in term of training step.

It is worth-noting that the turning point appears at the performance starts to be converged, where the input embeddings also approach the ideal positions. Therefore, the semantic similarity among embeddings can be estimated more precisely, and contribute to a better semantic encoder. Therefore, DET can obtain a lower MAE than the single structural encoder. We present the result on PCQM4M-LSC in Figure 6, which supports the same conclusion.