Optimizing Graph Transformer Networks with Graph-based Techniques

Loc Hoang †
The University of Texas at Austin
loc@cs.utexas.edu

Udit Agarwal, Gurbinder Gill, Roshan Dathathri
KatanaGraph
{udit, gill, roshan}@katanagraph.com

Abhik Seal, Brian Martin
AbbVie Inc.
{abhik.seal, brian.martin}@abbvie.com

Keshav Pingali
The University of Texas at Austin
pingali@cs.utexas.edu

Abstract

Graph transformer networks (GTN) are a variant of graph convolutional networks (GCN) that are targeted to heterogeneous graphs in which nodes and edges have associated type information that can be exploited to improve inference accuracy. GTNs learn important metapaths in the graph, create weighted edges for these metapaths, and use the resulting graph in a GCN. Currently, the only available implementation of GTNs uses dense matrix multiplication to find metapaths. Unfortunately, the space overhead of this approach can be large, so in practice it is used only for small graphs. In addition, the matrix-based implementation is not fine-grained enough to use random-walk based methods to optimize metapath finding. In this paper, we present a graph-based formulation and implementation of the GTN metapath finding problem. This graph-based formulation has two advantages over the matrix-based approach. First, it is more space efficient than the original GTN implementation and more compute-efficient for metapath sizes of practical interest. Second, it permits us to implement a sampling method that reduces the number of metapaths that must be enumerated, allowing the implementation to be used for larger graphs and larger metapath sizes. Experimental results show that our implementation is 6.5× faster than the original GTN implementation on average for a metapath length of 4, and our sampling implementation is 155× faster on average than this implementation without compromising on the accuracy of the GTN.

1 Introduction

Graph neural networks (GNNs) are used for machine learning on graphs to perform tasks such as node classification and link prediction that require learning features on nodes and/or edges. Many GNN architectures exist such as the graph convolutional network (GCN) [14], GraphSAGE [9], and GIN [20], among others [3, 18, 22]. One limitation of most GNN architectures is that they do not make use of the additional information present in a heterogeneous graph, such as the type information on vertices and/or edges. Being able to operate on such heterogeneous graphs is important: for instance, heterogeneous knowledge graphs have become the preferred choice for representing data in the biomedical domain because they can assimilate data from many sources and model the edge semantics needed to find important relations like drug-target pairs, drug-side-effect pairs, drug-disease

This work was done by this author as part of work with AbbVie.
1Equal contribution

Preprint. Under review.
pairs, disease-pathway pairs, etc. Another example is finding key opinion leaders who can champion a topic, which is often done by using heterogeneous graphs compiled from literature, publications, patents, scientific research areas, and citations.

The graph transformer network (GTN) \cite{21} can leverage type information in heterogeneous graphs by learning important \textit{metapaths} (typed paths) in the graph and encoding this information into a \textit{metapath graph} which can then be used by a regular GCN. This can improve node classification accuracy \cite{21}. In addition, they are able to \textit{find} important metapaths without the need for domain experts to provide the list of metapaths. Existing GTN implementations use dense matrix multiplication to compute metapaths. This is not memory efficient as the size of the matrix grows quadratically with the number of vertices in the graph. As a result, these implementations can be used only for small graphs with fewer than 200K vertices. In addition, these matrix-based approaches do not support fine-grained operations such as sampling paths through random walks to reduce the number of considered paths.

This work makes the following contributions to the area of GTNs.

1. We present a new algorithm for the graph transformer network that formulates the problem as a series of graph operations rather than as matrix operations.
2. We present a random walk based approach that uses this graph-based formulation to sample important metapaths to further reduce memory usage and computation cost.
3. We implement this algorithm and show that it outperforms the original implementation by 6.5× on average. We also show that random-walk sampling improves performance by 155× over the original implementation without compromising accuracy of node classification.
4. We show experimentally that the sampling approach can run and scale on large graphs with up to 1.5 billion edges.

2 Background: Graph Transformer Networks

This section introduces graph neural networks and graph transformer networks, and motivates the need for a graph formulation of GTNs.

2.1 Graph Neural Networks

Graph neural networks (GNNs) \cite{8} extend the deep neural network (DNNs) approach to graphs. In DNNs, an input (typically a tensor) is passed through a series of \textit{layers} where it is transformed via tensor operations like matrix multiplication using learnable parameters. The output at the end of the layers is a \textit{transformed} version of the input used for some downstream task. DNNs are trained in a series of epochs that update the learnable parameters of the layers to achieve better results such as improved accuracy for tasks like node classification. In a GNN, the input to the layers are vertices and their features. To leverage the fact that the input is a graph, the feature passed into a layer is not the vertex feature by itself but an \textit{aggregation} of the features of the vertex’s neighbors. Many GNN architectures exist \cite{2,14,18,20}, and they differ in how they define the \textit{aggregation} and the \textit{update} phases (e.g., layer transformation including and pre-/post-processing). In this paper, we focus on the graph convolutional network (GCN) \cite{14}, a basic GNN which does a sum aggregation of neighbor features normalized by source/destination vertex degrees, followed by a vanilla update.

2.2 Metapaths

A length \(l\) metapath in a heterogeneous graph is a path comprised of edge types \(\langle t_1, t_2, ..., t_l \rangle\) that represents a typed relation between the endpoints. A \textit{metapath edge} can be drawn between the endpoints of the metapath. This explicit representation of a metapath is useful because it (1) captures heterogeneity with a non-typed edge and (2) explicitly encodes a multi-hop relationship beyond a vertex’s immediate neighborhood. Since most GNN architectures do not leverage the heterogeneity of a graph during training, using metapath edges to represent these heterogeneous relationships can increase the information that the GNN can use during training and inference \cite{6,21}. Metapaths are also useful in other machine learning applications such as improved node embeddings with metapath-guided random walks \cite{10,5} and metapath connections serving as predictors of effectiveness in a learning model of drug effectiveness for diseases \cite{11}.
Not all metapaths are meaningful, so typically an expert familiar with the heterogeneous graph defines the important metapath relationships. This can be problematic: it is not the case that an expert can be found for every heterogeneous graph dataset, and even experts can introduce biases into the metapaths. For datasets in a new domain, an expert may not even exist. Therefore, it is useful to have a method to determine important metapaths automatically and leverage them for learning.

2.3 Graph Transformer Networks

GTN is a variant of graph convolutional networks (GCN) that automatically learns important metapaths in a heterogeneous graph. Importance is defined using a scoring function for paths. Usually, the score for a path is computed as the product of the importance scores of its component edges, and the importance score of an edge may depend on the position of that edge in the metapath. Therefore, a length $l$ metapath $m$ comprised of types $(t_1, t_2, ..., t_l)$ has an importance score equal to $s(1, t_1) \cdot s(2, t_2) \cdot \cdots \cdot s(l, t_l)$, where $s$ is a scoring function for an edge in a given position in the metapath.

![Figure 1: Metapath graph construction. The matrix denotes the importance of an edge type for a position in the metapath. The heterogeneous graph’s edges are scored based on this matrix. The metapath graph has edges $(A, C)$ and $(A, E)$: the former is composed of $(A, B, C)$ and $(A, D, C)$ with scores $2 \cdot 2 = 4$ and $1 \cdot 3 = 3$, and the latter is composed of $(A, D, E)$ with score $1 \cdot 2 = 2$.](image1)

![Figure 2: Example of matrix computation that occurs to find the metapaths in Fig. 1. The graph’s adjacency matrix is duplicated, and the scores corresponding to each edge type for a particular on is filled accordingly. A matrix multiply then finds metapaths edges with the correct score: $(A, C) = 7$ and $(A, E) = 2$.](image2)

Given the input graph, the GTN generates a new metapath graph by replacing the original graph’s edges with weighted metapath edges. Fig. 1 illustrates this process for a length 2 metapath. The score matrix on the left is a graphical representation of an edge scoring function $s$. The example has two edge types: solid and dashed. The original graph is shown in the middle, and it has 3 paths: $(A, B, C)$, $(A, D, C)$, and $(A, D, E)$. These correspond to 3 different metapaths: (solid, dashed), (dashed, solid), and (dashed, dashed), respectively, and they get scores of 4, 3, and 2, respectively.

---

3 A GTN implementation includes other details such as addition of self-edges to the original graph to simulate paths of length less than $l$ and softmax normalization of scores, as used in the original GTN implementation. For simplicity of explanation and brevity, we do not delve into these details, but the implementations we evaluate in our experiments do account for them.
The metapath edges are weighted based on scores of the paths and their endpoints: \((A, B, C)\) and \((A, D, C)\) contribute their scores to metapath edge \((A, C)\), and \((A, D, E)\) contributes to edge \((A, E)\). The generated metapath graph will then be used as the input to the GCN in place of the original graph. The metapath graph’s edges are used during GNN aggregations, which are weighted based on the metapath edges’ weight; therefore, if the metapath weights accurately reflect the importance of the metapath, then the GCN is able to correctly leverage the heterogeneity of the original graph and its important relationships through the weights on metapath edges.

The scoring function must be able to score the edges accurately; since the metapath graph construction is part of the inference pipeline, it is possible to use the error of the GCN step for the task it is being trained for to adjust the scoring function. This is the key idea behind GTN training: the error from the GCN is back-propagated to the metapath graph generation step, and the gradients can then be used to adjust the scores so that the next training epoch will result in higher accuracy. There are two main benefits: (1) the GCN will be augmented by heterogeneous metapath information that it did not have access to before, which may improve GCN accuracy for heterogeneous graphs, and (2) the scoring function is trained alongside the GCN, meaning that the scores can identify the important edges of a metapath; in other words, important metapaths are learned without any expert intervention.

2.4 Implementations of GTNs

The only implementation of the GTN we know of is the original one written in PyTorch \[16, 21\]. The metapath graph in this implementation is represented as a dense adjacency matrix computed with a series of dense matrix multiplication operations. Fig. 2 illustrates this for the example in Fig. 1: an edge score matrix is created for every position in the metapath with the appropriate scores for each edge, and the matrix multiplication operation is used to enumerate paths. For an \(l\) length metapath, there are \(l\) matrices and \(l - 1\) matrix multiplies to generate the metapath graph.

In this approach to metapath finding, the computation cost grows linearly with the length of the metapath, and the key computation is a dense matrix multiplication, which has been heavily optimized by BLAS libraries. However, the memory overhead of this approach is extremely high: dense matrices use \(O(n^2)\) memory where \(n\) is the number of graph vertices. Because of this, this implementation fails to run on even average-sized graphs unless the machine has a very large memory.

3 Graph Formulation for Graph Transformer Networks

This section presents our formulation of the graph transformer network as a series of graph operations.

3.1 Metapath Graph Generation via Path-finding

Instead of finding metapaths via matrix multiplies, we find paths via graph traversal and generate the metapath graph using the generated paths. We use dynamic programming to make this process efficient.

Algorithm 1 shows the high level algorithm. For a metapath graph with metapaths of length \(l\), the weight of a metapath edge \((a, b)\) is the sum of the scores of all \(l\)-length metapaths starting at \(a\) and ending at \(b\). Therefore, the algorithm finds all length \(l\) paths in the graph (Line 2); the method of path finding on the graph is left to the implementation, and different path finding methods trade-off memory and compute overheads. Each path is scored by obtaining the individual scores of its edges and multiplying them together as discussed in Section 2.3 (Line 4). This score is added to a running sum for the metapath edge corresponding to that path (Line 6). After all paths are enumerated, scored, and added, the metapath graph MG will be complete and have the correct edge weights.

If \(l\) is sufficiently large, path finding becomes very expensive as the number of paths grows exponentially. Therefore, we formulate Algorithm 3, based on a dynamic programming approach for constructing large paths by concatenating several smaller paths \[1, 4\] to reduce the computational requirement of Algorithm 1 by cutting the length of the generated paths by half in exchange for using more memory to store intermediate metapath graphs, called MG\(_1\) and MG\(_2\) in the pseudocode in Algorithm 3. Instead of enumerating length \(l\) paths, paths of length \(l/2\) are enumerated (Line 2). Then, two scores are generated for each individual path: the first one corresponds to the path starting from edge \((v, x_1)\) at position 1 (Line 4), and the second one corresponds to the one with all edge
positions offset by \( l/2 \) (Line 5). These two scores are added into the metapath edges of two different intermediate metapath graphs (Lines [7][8]). The final step (Lines [9][12]) gets the metapath edge \((a, c)\) of the desired length \( l \) metapath graph by multiplying the scores of metapath edge \((a, b)\) and \((b, c)\) in the two intermediate metapath graphs, respectively, for all \( b \). Algorithm [3] computes the same metapath graph as Algorithm [1] at a high level, it is because the multiplication of the two metapath edge scores computes the sum of the products of the same paths found by Algorithm [1] (a formal proof can be found in the Appendix).

**Algorithm 1** Vanilla Metapath Graph Generation

**Input:** Graph \( G \); Edge Score Function \( ES \); Edge Type Function \( ET \)

**Output:** Metapath Graph \( MG = (V, E, W) \)

1: for all vertices \( v \) in \( G \) do
2: Enumerate length \( l \) paths \( P \) from \( v \)
3: for path \( p = (v, x_1, ..., x_i) \) in \( P \) do
4: \( score = ES(ET(v, x_1), 1) \cdot \prod_{i=2}^{l} ES(ET(x_{i-1}, x_i), i) \)
5: add edge \((v, x_i)\) to \( MG.E \), if it already doesn’t exist
6: \( MG.W(v, x_i) + = score \)

**Algorithm 2** Metapath Graph Generation using Random Walks

**Input:** Graph \( G \); Edge Score Function \( ES \); Edge Type Function \( ET \); Number of walks \( num\_walks \)

**Output:** Metapath Graph \( MG = (V, E, W) \)

1: for all vertices \( v \) in \( G \) do
2: Sample length \( l \) \( num\_walks \) paths \( P \) from \( v \)
3: for path \( p = (v, x_1, ..., x_i) \) in \( P \) do
4: \( score = ES(ET(v, x_1), 1) \cdot \prod_{i=2}^{l} ES(ET(x_{i-1}, x_i), i) \)
5: add edge \((v, x_i)\) to \( MG.E \), if it already doesn’t exist
6: \( MG.W(v, x_i) + = score \)

**Algorithm 3** Metapath Graph Generation with \( l/2 \) Paths

**Input:** Graph \( G \); Edge Score Function \( ES \); Edge Type Function \( ET \)

**Output:** Metapath Graph for first-half \( l/2 \) paths \( MG_1 \); Metapath Graph for second-half \( l/2 \) paths \( MG_2 \); Metapath Graph for full \( l \) paths \( MG \)

1: for all vertices \( v \) in \( G \) do
2: Enumerate length \( l/2 \) paths \( P \) from \( v \)
3: for path \( p = (v, x_1, ..., x_{l/2}) \) in \( P \) do
4: \( score_1 = ES(ET(v, x_1), 1) \cdot \prod_{i=2}^{l/2} ES(ET(x_{i-1}, x_i), i) \)
5: \( score_2 = ES(ET(v, x_1), l/2 + 1) \cdot \prod_{i=2}^{l/2} ES(ET(x_{i-1}, x_i), l/2 + i) \)
6: add edge \((v, x_{l/2})\) to \( MG_1.E \) and \( MG_2.E \), if it already doesn’t exist
7: \( MG_1.W(v, x_{l/2}) + = score_1 \)
8: \( MG_2.W(v, x_{l/2}) + = score_2 \)
9: for metapath edge \( e_1 = (a, b) \) in \( MG_1 \) do
10: for metapath edge \( e_2 = (b, c) \) in \( MG_2 \) do
11: add edge \((a, c)\) to \( MG \), if it already doesn’t exist
12: \( MG.W(a, c) + = MG_1.W(e_1) \cdot MG_2.W(e_2) \)

### 3.2 Implementation Considerations for Pathfinding Formulation

Obtaining an efficient implementation requires careful attention to the following issues, some of which involve space-time tradeoffs.
Going Beyond $1/2$ Splitting the path into two $1/2$ subpaths avoids redundantly finding $1/2$ subpaths while finding the length $1$ path. It is possible to use even smaller subpaths (e.g., $1/4$, $1/8$, $1/16$). We use $1/2$ for two main reasons: (1) breaking a path down further would require another intermediate metapath graph object (e.g., $\text{MG}_{1,2,3,4}$) which could increase the space overhead significantly and (2) in our applications, metapath lengths are not very large.

Enumeration of Paths The performance of metapath-finding depends critically on the method used for path enumeration, and involves a trade-off between time and space. For example, paths from a given node can be enumerated by performing a depth-first walk starting at that node. This is memory-efficient since there are only a limited number of “active path” searches at any given time. The problem with this approach is that there may be redundancy when computing path scores. To illustrate, say there are two paths $\{A, B, C, D, E\}$ and $\{A, F, C, D, E\}$ found by two different threads. Both threads would find the subpath $\{C, D, E\}$ to append to the subpaths $\{A, B, C\}$ and $\{A, F, C\}$. It is more efficient to find this subpath once and multiply its score with the sum of the two prefix paths. An alternative is to perform level-by-level path enumeration. First, find all length $k$ metapaths and their scores and store them all in memory. Then, to get length $k+1$ metapaths, take the length $k$ metapaths, extend them by one edge, and multiply with the score for that edge. This avoids the redundancy problem of the depth-first extension: $\{A, B, C\}$ and $\{A, F, C\}$ will be found at the same time with their contributions present in the length 2 metapath edge $(A, C)$. This approach, however, must store all such intermediate metapaths during computation, and this space overhead quickly becomes infeasible as the path length and the graph grows in size.

Memoization of Paths vs. Recomputation of Paths The gradient update step of GTN training requires that intermediate metapaths of length less than $l$ are available to compute the gradients to update edge scores. PyTorch GTN’s [21] auto-differentiation mechanism stores the intermediate matrices for metapaths of length 2 to length $l$ metapaths, and this becomes prohibitively expensive for large graphs and metapath lengths. In the graph formulation, one can store all length $l$ paths and derive gradients from these paths, but this is also expensive. To avoid memory overhead, our implementation regenerates all paths in the backward gradient update pass. This adds computational overhead but reduces memory overheads, so it permits us to handle much larger graphs.

Storage Format of (Intermediate) Metapath Graphs Graphs are typically stored in memory in a compressed format where non-existing edges do not take up storage. This is in contrast to a dense adjacency matrix in which non-existent edges are stored explicitly as zeroes. The first approach has the disadvantage that the number of edges each vertex has must be known ahead of time, so dynamic allocation of this data structure cannot be done: precomputation must be done to determine how large an intermediate metapath graph will be if this storage format is used. The second approach does not have this disadvantage, but the space requirement is proportional to the square of the number of vertices. The PyTorch implementation [21] uses dense matrices for each intermediate metapath graph, so the memory overhead is impractical for large graphs. Our graph formulation precomputes the space required for the metapath graph and the intermediate metapath graphs.

3.3 Metapath Sampling

As graphs grow in size, the number of metapaths grows exponentially, and as the number of paths grow, the amount of total computation and the overall memory usage also increase. To overcome these issues and generate the metapath graph more efficiently, we use a random walk based approach for sampling important paths based on the edge scores of the paths. This approach allows us to significantly reduce the total amount of computation and memory usage while also allowing us to build a metapath graph that gives comparable accuracy to original GTN formulation. Because we only find a constant number of paths per node, we can explicitly store them as well so recomputation of paths is not needed during the backward step. Algorithm [2] presents the pseudocode of our random walk approach for generating metapath graphs. The appendix contains the details of the random walk implementation. Note that sampling metapaths cannot be easily expressed using a matrix-based API such as PyTorch [21]: sampling is a fine-grained operation while matrix operations are inherently bulk operations.
Table 1: Input graphs and their properties. chem2bio, reddit, ogbn-products, and twitter40 have synthetic data for values it does not explicitly have (e.g., twitter40 has no features); these values are omitted from the table since accuracy is not evaluated. The sum of train, val, and test splits does not amount to 100 since not all the nodes’ labels are used.

4 Experimental Results

4.1 Setup

We implement our graph transformer network (GTN) implementation as well as the graph convolutional network (GCN) [14] subroutine in C++ code using the KatanaGraph graph engine: we refer to it in this paper as Graph-GTN (G-GTN). We also evaluate the random walk variant of G-GTN which we refer to as Walk-GTN (W-GTN). W-GTN-X refers to W-GTN with X sampled metapaths for each vertex. Our GCN implementation is based on the vertex program formulation in DeepGalois [12] with an extension to propagate the gradients to the GTN phase during training; this formulation has been shown to be competitive with the state-of-the-art. We compare our GTN with the PyTorch implementation which we refer to as P-GTN. Table 1 lists the inputs used in our experiments. We use ACM, DBLP, and IMDB [19], three inputs from the original GTN paper [21], to evaluate the runtime and accuracy. In order to evaluate scalability for large graphs, we add synthetic labels/features/edge types (as required) to chem2bio [2, 7], reddit [9, 17], ogbn-products [13], and twitter40 [15]; we do not evaluate accuracy on these graphs because of this synthetic metadata. We were unable to evaluate the P-GTN with these inputs because it failed to run them due to the memory requirements of that implementation.

Experiments are run on a machine with 40 Intel Xeon Gold 5218R (Cascade Lake) CPUs with 256GB DRAM. All networks are run for 300 epochs: the GTNs use a GCN layer followed by 2 dense layers (illustrated in Fig. 3) with a hidden feature size of 64 except for twitter40, which uses 16 due to twitter40’s higher memory cost, and the GCN uses 2 GCN layers with hidden feature size 64. The output layer is a softmax layer in all cases. If the 300 epochs take longer than 8 hours (i.e., average epoch time of 96 seconds), we list the time as “TO”/timeout in the results. Precomputation time (e.g., graph construction, intermediate CSR computation, etc.) for all systems is not included in the runtime results. The accuracy we report is for the node classification problem: test accuracy is evaluated every 5 epochs including the last epoch. Unless otherwise mentioned, GTNs use 3 graph transformer layers (i.e., the metapaths being considered have up to 4 edges). More experimental setup details can be found in the Appendix.
4.2 Comparisons with matrix-based GTN

Overview Table 2 shows the average epoch time and peak accuracy for P-GTN compared to G-GTN, W-GTN, and the basic GCN when metapaths with 4 edges are used. G-GTN and W-GTN, the graph formulations of the GTN problem, are significantly faster than P-GTN: on average, G-GTN is 6.5× faster, W-GTN-10 is 350× faster, W-GTN-50 is 155× faster, and W-GTN-100 is 101× faster than P-GTN for this setting. W-GTN outperforms the other GTN systems: it looks for a constant number of metapaths per node, so for non-trivial graphs with many paths, the reduction in the number of paths results in better runtime.

Differences in accuracy of P-GTN and G-GTN can be attributed to randomness such as weight initialization or the differences in exact computation among the systems (e.g., floating point inaccuracies based on different multiplication order). The important point to note is that accuracy is similar between the two; this should be the case because abstractly, they do the exact same thing. On the other hand, in principle, sampling in W-GTN may affect accuracy since the metapath graph generated will consist of only a constant number of random sampled walks from each vertex. What is noteworthy is that W-GTN does not significantly degrade accuracy even though the metapath graph is constructed from sampled paths; in these results, degradation occurs only when 10 paths per node are sampled, but there is no loss of accuracy when more paths are sampled. In fact, W-GTN can achieve higher peak accuracy in these settings. This can occur because important metapaths are found by sampling, so the resulting graph is less noisy than both the original graph and the full metapath graph. This could also be due to the fact that sampling can avoid overfitting to the training dataset.

Fig. 4 shows the time to accuracy for the ACM graph for the GTN-based systems. G-GTN reaches high accuracy significantly faster than P-GTN because each epoch takes less time. Similarly, the variations of W-GTN reach good accuracy faster than G-GTN because of faster epoch time.

Finally, note that the GCN is the most computationally efficient of the GNN architectures we compare with because it does not find metapaths, and for some of these heterogeneous graphs like ACM, it obtains comparable peak accuracy to the GTNs without any need to use the heterogeneity of the graph. In these cases, a GTN is not required. For graphs like IMDB and DBLP where using heterogeneous
information leads to significantly better accuracy, however, a computationally efficient GTN like G-GTN or W-GTN is vital.

**Scaling with Metapath Length**  Fig. 5 shows the runtime of the GTN systems with varying numbers of metapath lengths. P-GTN’s runtime scales linearly as the metapath length increases: increasing $l$ only adds another dense matrix for matrix multiplication. The trade-off is that memory usage increases significantly (by the size of the dense matrix). G-GTN is faster than P-GTN at lower metapath lengths, but its performance declines as metapath length increases. As explained in Section 3.2 in exchange for memory efficiency, G-GTN must do redundant computation during path search and does not memoize paths, resulting in an increase in compute time as the metapath length (i.e., the number of paths) grows. W-GTN avoids these issues entirely by limiting the number of metapaths to a constant number and storing these paths. W-GTN is significantly faster than the other systems and continues to scale as the metapath length grows because the number of generated metapaths is constant without loss of accuracy.

### 4.3 GTNs on Large Graphs

![Figure 6](image-url)

Figure 6: Scaling of W-GTN for large graphs as metapath length (i.e., number of transformer layers) and number of walks are increased. 0 walks is G-GTN. Note that the scales are different in each plot.

We were unable to run P-GTN on large graphs because the storage requirement for creating the metapath graph (which can have more edges than original graph) was higher than the memory on our machine. G-GTN (i.e., 0 walks) was able to process only chem2bio. Therefore, we believe a sampling-based approach like W-GTN is crucial for doing machine learning with metapaths on large heterogeneous graphs.

Fig. 6 shows the average epoch time for 5 epochs on the larger graphs for varying metapath lengths and number of random walks. The major takeaway is that W-GTN continues to scale as both metapath length and the number of random walks grows. In fact, the increase in runtime as metapath length grows is not high: the number of walks is low and constant, so an increase in length does not add significant work to the system. Only increasing the number of walks increases runtime for W-GTN for these graphs.

### 5 Conclusion

This paper presents (i) a new graph-based formulation of the GTN and (ii) a random walk sampling approach for sampling metapaths to reduce both the computation and memory usage of GTNs without...
compromising the accuracy of the underlying task. The sampling based approach is up to $155 \times$ faster on average than the original matrix-based GTN implementation without accuracy degradation, and it allows running GTNs on larger graphs that cannot be run using the PyTorch implementation.

**Societal Impact**

Heterogeneous knowledge graphs have become the preferred choice for representing data in biomedical domain because they can assimilate data from many sources and model the edge semantics needed for machine reasoning. Metapaths can represent hidden connections in these graphs, but are buried under the complex knowledge graph, and hence can be difficult to interpret. Graph transformer networks (GTNs) provide a solution to this problem, but the current implementations fail to work for any real-size data. These implementations are also very compute-intensive and requires a lot of energy, thus exacerbating the problem of global warming and climate change. This work addresses both these problems by (1) reducing the training time for GTNs by $155 \times$ and (2) extending the usability of GTNs to real-world biomedical datasets, thus helping identify new connections between drug-target pairs, drug-side-effect pairs, drug-disease pairs, disease-pathway pairs etc.

**References**

[1] **Agarwal, U., Ramachandran, V., King, V., and Pontecorvi, M.** A deterministic distributed algorithm for exact weighted all-pairs shortest paths in $\tilde{O}(n^{3/2})$ rounds. In *Proceedings of the 2018 ACM Symposium on Principles of Distributed Computing* (2018), pp. 199–205.

[2] **Chen, B., Dong, X., Jiao, D., Wang, H., Zhu, Q., Ding, Y., and Wild, D. J.** Chem2bio2rdf: a semantic framework for linking and data mining chemogenomic and systems chemical biology data. *BMC Bioinformatics* 11, 1 (2010), 1–13.

[3] **Chen, J., Ma, T., and Xiao, C.** FastGCN: Fast learning with graph convolutional networks via importance sampling. In *International Conference on Learning Representations* (2018).

[4] **Cormen, T. H., Leiserson, C. E., Rivest, R. L., and Stein, C.** *Introduction to algorithms*. MIT press, 2009.

[5] **Dong, Y., Chawla, N. V., and Swami, A.** metapath2vec: Scalable representation learning for heterogeneous networks. In *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining* (2017), pp. 135–144.

[6] **Fu, X., Zhang, J., Meng, Z., and King, I.** Magnn: metapath aggregated graph neural network for heterogeneous graph embedding. In *Proceedings of The Web Conference 2020* (2020), pp. 2331–2341.

[7] **Gao, Z., Fu, G., Ouyang, C., Tsutsui, S., Liu, X., Yang, J., Gessner, C., Foote, B., Wild, D., Ding, Y., et al.** edge2vec: Representation learning using edge semantics for biomedical knowledge discovery. *BMC Bioinformatics* 20, 1 (2019), 1–15.

[8] **Gori, M., Monfardini, G., and Scarselli, F.** A new model for learning in graph domains. In *Proceedings. 2005 IEEE International Joint Conference on Neural Networks*, 2005. (2005), vol. 2, pp. 729–734 vol. 2.

[9] **Hamilton, W. L., Ying, R., and Leskovec, J.** Inductive representation learning on large graphs. In *Proceedings of the 31st International Conference on Neural Information Processing Systems* (Red Hook, NY, USA, 2017), NIPS ’17, Curran Associates Inc., pp. 1025–1035.

[10] **He, Y., Song, Y., Li, J., Ji, C., Peng, J., and Peng, H.** Hetespaceywalk: A heterogeneous spacey random walk for heterogeneous information network embedding. In *Proceedings of the 28th ACM International Conference on Information and Knowledge Management* (2019), pp. 639–648.

[11] **Himmelstein, D. S., Lizée, A., Hessler, C., Brueggeaman, L., Chen, S. L., Hadley, D., Green, A., Khankhianian, P., and Baranzini, S. E.** Systematic integration of biomedical knowledge prioritizes drugs for repurposing. *eLife* 6 (2017), e26726.

[12] **Hoang, L., Chen, X., Lee, H., Dathathri, R., Gill, G., and Pingali, K.** Efficient distribution for deep learning on graphs. In *First MLSys Workshop on Graph Neural Networks and Systems (GNNSys21)* (2021).
H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, Eds., vol. 33, Curran Associates, Inc., pp. 22118–22133.

[14] Kipf, T., and Welling, M. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations* (2016), ICLR ’16.

[15] Kwak, H., Lee, C., Park, H., and Moon, S. What is Twitter, a Social Network or a News Media? In *Proceedings of the 19th International Conference on World Wide Web* (New York, NY, USA, 2010), WWW ’10, ACM, pp. 591–600.

[16] Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Kopf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., Bai, J., and Chintala, S. Pytorch: An imperative style, high-performance deep learning library. In *Advances in Neural Information Processing Systems 32*, H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, Eds., Curran Associates, Inc., 2019, pp. 8026–8037.

[17] pushshift.io. pushshift.io.

[18] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., and Bengio, Y. Graph attention networks. In *International Conference on Learning Representations* (2018), ICLR ’18.

[19] Xiao, W., Houye, J., Chuan, S., Bai, W., Peng, C., P., and Yanfang, Y. Heterogeneous graph attention network. *WWW* (2019).

[20] Xu, K., Hu, W., Leskovec, J., and Jegelka, S. How powerful are graph neural networks? In *International Conference on Learning Representations* (2019), ICLR ’19.

[21] Yoon, S., Jeong, M., Kim, R., Kang, J., and Kim, H. J. Graph transformer networks. In *Advances in Neural Information Processing Systems* (2019), H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, Eds., vol. 32, Curran Associates, Inc.

[22] Zeng, H., Zhou, H., Srivastava, A., Kannan, R., and Prasanna, V. Accurate, efficient and scalable graph embedding. In *2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (May 2019), pp. 462–471.

6 Appendix

6.1 Additional Experimental Setup Details

**Changes to PyTorch GTN to Match Computation** The high level computation changes are described here. We are including a patch file that has the exact changes to the source code as well. These changes were made to make it so that P-GTN was closer to G-/W-GTN in terms of high level computation.

1. Learnable bias in PyTorch’s linear layers was removed.
2. Normalization done over out-edges, not in-edges.
3. Metapath normalization removed.
4. Learning rate/weight decay removed from Adam optimizer.
5. Only 1 channel is used when running P-GTN (G-GTN does not have support for multiple channels, and multiple channels would mean more overhead in any case).

**Hyperparameter Details** The layer composition of 1 GCN layer followed by 2 linear layers for the GTN was chosen because the original GTN paper used these parameters. Similarly, the hidden feature size of 64 on each layer was chosen because that is what the original PyTorch GTN paper used. All systems use the Adam optimizer with a learning rate is 0.01, beta parameters 0.9 and 0.999, epsilon $10^{-8}$, and no weight decay.

**Data Split** The data split used for ACM, DBLP, and IMDB were the same splits used in the original Graph Transformer Network paper as that is where we obtained the inputs.
Synthetic Feature/Label/Edge Type Generation Details  In order to run some inputs with the GTN, we generated synthetic values for things like features, labels, and edge types for the large graphs (chem2bio, reddit, ogbn-products, twitter40). Note that we do not check accuracy for these graphs because it would not make sense due to the generated values; we did this solely in order to illustrate scaling of our GTN implementation on larger graphs and to show that GTNs are very expensive to run in terms of memory and compute time without sampling or some other method of reducing the number of metapaths. The actual synthetic values that we generated should not be interpreted to have any kind of meaning behind them other than filler values in order to make the GTN run. We are including this information here for the sake of completeness.

Synthetic features were generated for chem2bio and twitter40. Every vertex’s feature was a vector of length 50 all with the number 2.

Synthetic edge types were generated for all large graphs but chem2bio: for each edge, we randomly choose 1 of 4 different edge types.

Synthetic labels were generated for chem2bio and twitter40. For each vertex, we choose 1 of 3 labels.

Finally, we also created a train/val/test splits for chem2bio and twitter40: 20% were train nodes, 10% were validation nodes, and 70% were testing nodes.

6.2 Proof of \( l/2 \) Path Split Correctness

**Theorem 1.** Let \( G \) be a graph and let \( MG \) be its metapath graph for some length \( l \). Also, let \( MG_1 \) and \( MG_2 \) be the metapath graphs of \( G \) for first-half \( l/2 \) and second-half \( l/2 \) paths respectively. \( MG(u, v) \) is the weight of the edge \((u, v)\) in the metapath graph \( MG \). Then, \( MG(u, v) = \sum_{k \in V} MG_1(u, k) \cdot MG_2(k, v) \) for every pair of vertices \( u, v \in V \).

**Proof.** Consider a pair of vertices \( u, v \) and let \( P_l(u, v) \) represents the set of metapaths between \( u \) and \( v \) for length \( l \). Then,

\[
MG(u, v) = \sum_{p \in P_l(u, v)} score(p) = \sum_{p \in P_l(u, v)} score_1(u, x) \cdot score_2(x, v) \\
\text{(where } x \text{ is the node at position } l/2 \text{ in } p) \\
= \sum_{x \in V} (\sum_{p_1 \in P_l/2(u, x)} score_1(u, x) \cdot (\sum_{p_2 \in P_l/2(x, v)} score_2(x, v))) \\
= \sum_{x \in V} MG_1(u, x) \cdot MG_2(x, v) \\
\]

\[\blacksquare\]

6.3 Random Walk Algorithm

**Algorithm 4** Random Walk Algorithm

| Input: | Graph \( G \); vertex \( v \); Number of walks \( num\_walks \); Walk-length \( walk\_length \) |
|--------|-------------------------------------------------------------|
| Output:| Set of paths \( P \) |
| 1: \( P \leftarrow \phi \) |
| 2: for \( i \leftarrow 1 \) to \( num\_walks \) do |
| 3: \( p \leftarrow \{v\} \) |
| 4: for \( j \leftarrow 1 \) to \( walk\_length \) do |
| 5: \( \text{last} \leftarrow p[j - 1] \) |
| 6: Randomly sample \( u \) from \( N \cup \{\text{last}\} \) using acceptance-rejection sampling |
| 7: \( p \leftarrow p \cdot (\text{last}, u) \) |
| 8: \( P \leftarrow P \cup p \) |
| 9: return \( P \) |
We give a brief overview of our random walk implementation. The input is a graph $G$ along with a vertex $v$ from which we need to sample $num\_walks$ paths of length $walk\_length$. Each iteration of the for loop (Lines 2-9) samples one path, starting from $v$ of length $walk\_length$. In the inner for loop in lines 4-7, a vertex is sampled randomly using an acceptance-rejection sampling technique, which takes into account the weights of outgoing edges. Edges with higher weights are more likely to get picked, meaning more important metapaths (at that point in training/inferencing) are more likely to be sampled.