Graph Trees with Attention

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Abstract

When dealing with tabular data, models based on regression and decision trees are a popular choice due to the high accuracy they provide on such tasks and their ease of application as compared to other model classes. Yet, when it comes to graph-structure data, current tree learning algorithms do not provide tools to manage the structure of the data other than relying on feature engineering. In this work we address the above gap, and introduce Graph Trees with Attention (GTA), a new family of tree-based learning algorithms that are designed to operate on graphs. GTA leverages both the graph structure and the features at the vertices and employs an attention mechanism that allows decisions to concentrate on sub-structures of the graph. We analyze GTA models and show that they are strictly more expressive than plain decision trees. We also demonstrate the benefits of GTA empirically on multiple graph and node prediction benchmarks. In these experiments, GTA always outperformed other tree-based models and often outperformed other types of graph-learning algorithms such as Graph Neural Networks (GNNs) and Graph Kernels. Finally, we also provide an explainability mechanism for GTA, and demonstrate it can provide intuitive explanations.

1 Introduction

Tree-based methods (TBMs) are a cornerstone of modern data-science and are a leading alternative to neural networks, especially in tabular data settings, where TBMs often outperform deep learning models [1–3]. TBMs are popular with practitioners due to their ease of use, out-of-the-box high performance, and explainability properties. In a large survey conducted by Kaggle in 2021 with more than 25,000 data scientists participants worldwide, 74.1% of the participants reported using decision trees or Random Forests (RF) on a regular basis [4] and more than 50.5% reported using Gradient Boosted Trees (GBT) [5,6]. Overall, there were 32% more participants who reported using TBMs on a regular basis than participants reporting the use of neural networks on a regular basis.

Graph structured data emerges in diverse domains including social studies, molecular biology, drug discovery, and communication [7,8]. It is often of interest to infer properties of these graphs, and thus graph regression and classification has been studied extensively by machine learning researchers in recent years [9,20]. Owing to the popularity and advantage of TBMs in other machine learning...
tasks, it would seem natural that they would be popular for graph related tasks too, but it turns out that applying TBMs on graphs is challenging.

Decision and regression trees split the input space by placing thresholds on the values of features. When operating on graphs, these split criteria should incorporate both the features on the vertices of the graph as well as its topological structure. Moreover, these split criteria should be cognizant of the varying sizes of graphs and of graph isomorphisms. To address these problems, many existing methods extract topology features inspired by graph-theory and combine them with features engineering techniques (also known as feature augmentation) which use domain specific knowledge. However, these approaches are labor intensive, require great amount of domain knowledge, and ignore the way vertex features and topology structure intertwine. This problem is demonstrated in Theorem 3.2 where a pair of non-isomorphic graphs over 4 vertices and 2 features are shown to be inseparable by common tree methods. Moreover, these methods handle only graph-tasks, which are tasks in which a property of the entire graph should be predicted, whereas other tasks, such as predicting properties of vertices or edges are not managed by these solutions.

The success of TBMs on tabular data suggests that they can potentially perform well on graph-based data, given appropriate design modifications to capture the graph structure and features. Hence, the main goal of this work is to introduce such modifications that will allow TBMs to be applied to graph related tasks. In this work we introduce Graph Trees with Attention (GTA), a novel method for implementing TBMs on graphs. GTA can be applied to graphs of varying sizes and are invariant to graph isomorphisms, as shown in Theorem 3.1. GTA modifies standard decision trees, which assume a fixed size feature vector, by introducing novel split criteria that leverage both the topology (structure) and the features of the vertices, and by introducing an attention mechanism that allows predictions to use sub-structures of the given graph. Additionally, GTA can be combined with ensemble methods, such as Random Forests and Gradient Boosted Trees. To evaluate the performance of GTA we present empirical results on 12 well-known graph and node classification benchmarks and show that GTA, when combined with GBT, consistently outperforms other tree-based models. Moreover, in 5 out of 8 graph classification benchmarks, GTA outperforms all other popular methods for graph learning including graph kernels and deep-learning approaches, while being on par on the rest. In node classification tasks, GTA was on par with GNNs on all 4 benchmarks and outperformed these in one case. Our theoretical analysis shows that the attention component of GTA results in strictly more expressive models, and that GTA can separate graphs that GNNs fail to tell apart.

The main contributions of this work are: (1) We present GTA - a new type of trees, specialized for tasks over graph data. (2) We show that GTA based ensembles outperform existing tree-based methods and are competitive with popular GNNs and graph kernels. (3) We provide theoretical results that highlight the expressive power of GTA. (4) We introduce an explainability mechanism, which highlights the vertices and edges in the graph that contribute to the prediction.

2 Related Work

Machine Learning on Graphs Many methods for learning on graphs have been proposed. Among these, an important line of work are Graph Kernel methods which measure the similarity between two graphs by creating vector representations of graphs and computing the cosine similarities between these representations. A more recent line of work is focused on deep-learning approaches: Graph Neural Networks (GNNs) learn a representation vector for the vertices of a given graph using an iterative neighborhood aggregation process. These representations are used in downstream tasks. We refer the reader to Wu et al. and Nikolentzos et al. for recent surveys.

TBMs for graph learning As discussed in the introduction, several approaches were introduced to allow TBMs to operate on graphs. These approaches combine domain specific feature engineering with graph-theory derived features. Other approaches combine GNNs with TBMs in various ways, and were mostly designed for specific problems. XGraphBoost was demonstrated for a drug discovery task. It uses GNNs to embed the graph into a vector and applies GBT to make predictions using this vector representation. A similar method has been used for link prediction between Human Phenotypes and Genes. The recently proposed BGNN

2For the sake of clarity, we ignore edge-features in this work.
model [43] predicts vertex attributes by alternating between training GBT and GNNs. Therefore, existing solutions focus on specific domains and in many cases require domain expertise to use.

In Set-Trees [44] TBMs were extended to operate on data that has a set structure by introducing an attention mechanism. Sets can be viewed as graphs with no edges, and therefore, some ingredients of Set-Trees can be extended for other types of graphs. For example, the use of permutation invariant aggregation functions and the concept of attention. However, Set-Trees do not provide a way to integrate features with the topological structure of the graph. Moreover, for graphs there are different prediction task types (e.g., graph prediction, node prediction, and link prediction), a diversity that does not exist when operating on sets. Therefore, GTA, presented in the following section, attempts to provide a “pure” TBM solution specialized for graph and node prediction tasks that handles both the topology of these graphs and features available on vertices. As such, it is generic in the sense that it does not require much domain knowledge or feature engineering to be used.

3 Graph Trees with Attention

In this section we describe the construction of GTA. Section 3.2 describes the “Graph Walk Features” that are used by GTA. Then, in Section 3.3 we present an attention mechanism that allows applying split criteria to parts of the original graph.

3.1 Preliminaries

Let $G = (V, E)$ be a graph over $n$ vertices which is represented by an adjacency matrix $A$. GTA operates on both directed and undirected graphs where the latter is expressed by constraining the adjacency matrix $A$ to be symmetric. Note that $(A^d)_{ij}$ is the number of walks of length $d$ between vertex $i$ and vertex $j$. Each vertex in $G$ has a feature vector in $\mathbb{R}^a$ associated with it. The value of these features are represented in the matrix $F \in \mathbb{R}^{n \times a}$. Let $f_k \in \mathbb{R}^n$ be a vector containing the values of the $k$th feature over all vertices, i.e., $f_k$ is the $k$th column of $F$. For a vector $v \in \mathbb{R}^n$ we denote its $i$th entry by $(v)_i$. To avoid ambiguity we refer to the decision tree nodes as root, node, inner-node/split-node, leaf, and to the graph vertices as vertex, vertices.

Key differences exist between graph-level tasks and vertex-level tasks. In the former, the goal is to predict a property of an entire graph and hence each example is a different graph with its features. However, in vertex-level tasks, the goal is to predict a property of individual vertices where the graph
When used for graph-level predictions, the vector $v$ should be summarized by a single value to which a threshold can be applied. This aggregation should be permutation invariant to compensate for graph isomorphisms. Therefore, GTA considers the following family of permutation-invariant aggregation functions: sum, mean, min, and max. Hence, when GTA is applied to graph-level tasks, a split criterion in a split-node of GTA takes the form:

$$\left(A^df_k\right)_i \leq \theta \quad (1)$$

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$$\text{AGG} \left(A^df_k\right) \leq \theta \quad (2)$$

### 3.2 Graph Walk Features and Split Criteria

Motivated by the message-passing procedure in GNNs [31], GTA considers split criteria that first propagate feature values through the graph before making decisions based on the values acquired. The propagation of feature values on the graphs is computed using the function $A^df_k$ where $k$ is an index of a feature and $d$ is the depth of the propagation. To understand this function it is helpful to look at some specific examples. If $d = 0$ then $A^0f_k = f_k$ which means that the topology of the graph is ignored, and the values of the feature are taken as is. For $d = 1$ we have that $(A^1f_k)_i$ is the sum of the values of the $k$th feature over the neighbors of the $i$th vertex. For larger values of $d$, all the walks of length $d$ are considered in the following way: if $n_{ji}$ is the number of walks of length $d$ from $j$ to $i$ and $f_k(j)$ is the value of the $k$th feature on the $j$th vertex, then $\left(A^df_k\right)_i = \sum_j n_{ji}f_k(j)$. Therefore, if the feature vector $f_0$ is the constant vector 1, then $A^df_0$ computes, for every vertex $i$, the number of walks of length $d$ in the graph that end in $i$. For this reason, in the experiments, we always add to the set of features a feature with a constant value of 1. The vector $v = A^df_k$ is a vector of size $n$. Therefore, when making vertex-level predictions for the $i$th vertex, a threshold is applied to $i$th coordinate of $A^df_k$, and the criterion in a split-node of GTA takes the form:

$$\left(A^df_k\right)_i \leq \theta \quad (3)$$

The split criterion described above considers topological properties of the graph, and features computed over all its vertices. Nonetheless, there are cases where predictions should rely on substructures of the graph. For example, given a graph of a molecule, predicting its toxicity level may require detecting the presence or absence of a sub-molecule which corresponds to a sub-graph [45]. However, it might be impossible to express rules that are based on properties of subsets of the vertices using the split criteria described above. For example, as proved in Theorem 3.2 for graphs with only one edge and 4 vertices that are positioned on the plane at \{±1\} x \{±1\}, it is impossible to determine if the edge connects (1,−1) and (−1,1) or (1,1) and (−1,−1). To overcome this shortcoming an attention mechanism is used in GTA, as described below.

The attention in GTA is inspired by the attention mechanism in deep-learning [46,47] but uses a different mathematical formulation. The motivation for attention in deep-learning is to allow models to focus on relevant parts of the input [46]. Thus, the attention mechanism in GTA allows the split criteria presented in Section 3.2 to operate on parts of the graph marked by an attention-set [44].

An attention-set is a subset of the vertices $S \subseteq V$. Given the attention-set $S$, a mask matrix $M = 1_S(1_S)^T$ is formed (here $1_S$ is an indicator vector of the attention-set). For example, if there are 5 vertices in the graph and the attention-set $S$ contains only the first 3 vertices, then $1_S = (1,1,1,0,0)$. This mask is applied to the adjacency matrix by using element-wise multiplication denoted by $\odot$. In addition to masks that are induced by attention sets, the mask $I_{|V|}$ is also considered. When applying the attention, the feature values $f_k$ are therefore propagated only through walks of length $d$ that begin and end in vertices of the attention-set. Formally, for vertex-level tasks, this results in the split criterion:

$$\left(\left(A^d \odot M\right)f_k\right)_i \leq \theta \quad (3)$$

3In directed graphs it may be useful to consider negative $d$ values to consider walks in the opposite direction.
and for graph-level tasks:

\[
\text{AGG} \left( \left( A^d \odot M \right) f_k \right) \leq \theta
\]

(4)

It is possible to consider additional types of attentions, for example, where \( A^d f_k \) is first computed and then the result is restricted to the attention-set. In this work we consider only the attention in Eq. (4). Other types as well as a detailed example are discussed in the supplementary materials.

**Generation and Selection of Attention-sets**

Next we present the mechanism that selects which attention-sets should be considered at every split node. Notice that considering every possible subset of the vertices as a candidate attention-set is computationally intractable and may lead to overfitting. Therefore, in GTA the candidate attention-sets are generated while traversing the tree such that the number of candidate attention-sets is at most linear with respect to the depth of the tree. Every tree node \( u \) holds a set of candidate attention-sets \( Att_u \). When searching for the optimal split of \( u \) during the training process, only the attention-sets in \( Att_u \) are considered. The candidate sets are created as follows. In the root node, the only candidate attention-set is the set of all vertices (i.e., \( Att_{\text{root}} = \{ V \} \)). The optimal split for a node \( u \) always uses exactly one attention-set from \( Att_u \). We denote this attention-set by \( S_u \) and refer to it as the active attention-set of node \( u \). In the root node we have that \( Att_{\text{root}} = \{ V \} \) and therefore \( S_{\text{root}} = V \). When applying the optimal split to a node \( u \), two new candidate attention-sets are generated, by splitting \( S_u \) to two disjoint subsets defined as follows:

\[
\left\{ i \in S_u : \left( \left( A^d \odot \left( \mathbf{1}_{S_u} (1_{S_u})^T \right) \right) f_k \right)_i > \theta \right\} \quad \text{and} \quad \left\{ i \in S_u : \left( \left( A^d \odot \left( \mathbf{1}_{S_u} (1_{S_u})^T \right) \right) f_k \right)_i \leq \theta \right\}
\]

(5)

where the parameters \( d, k \) are the parameters chosen for the optimal split of \( u \). These two sets are then added to the candidate sets of the children nodes of \( u \). The rationale for constructing these sets is as follows: the split criterion in Eq. (2) requires that the aggregation of \( (A^d f_k)_i \) over all vertices \( i \in V \) is greater than \( \theta \). If, for example, the aggregation uses the max function, then the vertices whose values \( > \theta \) contribute towards satisfying the condition while the vertices whose values \( \leq \theta \) do not contribute towards satisfying the condition. Therefore, these groups may benefit from further focus (attention) down the tree.

For a node \( u \), the mask \( l_{|V|} \) is always considered as a candidate mask, and the set of candidate attention-sets \( Att_u \) contains \( V \) and all the attention-sets generated along the path from the root to \( u \). Therefore, if \( u \) is at depth \( \delta \) in the tree, then \( |Att_u| \leq 2\delta \). Hence, the size of \( Att_u \) grows linearly with respect to the tree depth. Nevertheless, to further reduce the computational complexity it is possible to limit \( Att_u \) to hold only \( V \) and the candidates generated in the last nodes in the path from the root to \( u \). This guarantees that the size of \( Att_u \) is bounded by a constant.

Figure 2 demonstrates how the candidate attention-sets are generated and used during the training process. Since the node \( u \) is the root we have \( Att_u = \{ V \} \), \( S_u = V \). Node \( v \) has 3 candidate attention-sets, the set of all vertices \( V \), and the two candidates generated in \( u \). Its active attention-set is the two blue and two green vertices, and is then split into two new candidate attentions. Node \( w \) has 5 candidate attention-sets: \( V \), the two candidates generated in \( u \), and the two candidates generated in \( v \).

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4If sum aggregation is used, \( \theta \) is normalized by the size of \( S_u \) when defining the attention sets in Eq. (5).
3.4 Properties of GTA

In this section we discuss some theoretical properties of GTA as well as the computational complexity of training a GTA tree. We first consider invariance properties of GTA. Recall that a graph is described via its feature matrix $F$ and adjacency matrix $A$. If we apply a permutation $P$ to the vertices we obtain a new adjacency matrix $PAP^T$ and features $PF$. Clearly, we would like a graph classifier to provide the same output for the original and permuted graphs. In the graph prediction task this means we would like the output of GTA to be invariant to $P$. In the case of node-prediction, the output of GTA is a vector in $\mathbb{R}^{|V|}$ and we would like it to be equivariant to the permutation. The next lemma shows that this is the case for GTA.

**Lemma 3.1.** GTA trees are invariant to permutations in the case of graph-level tasks, and equivariant in the case of vertex-level tasks.

To prove Lemma 3.1, we show that all GTA’s components are either invariant or equivariant under permutation of the vertices. For example, Graph Walk features are equivariant, and the aggregation function is invariant. The proof is provided in the supplementary materials.

Next, we present results about the expressive power of GTA, when compared to other architectures.

**Lemma 3.2.** There exist graphs which cannot be separated by GTA without the attention mechanism but can be separated by GTA with attention.

**Lemma 3.3.** There exist graphs which cannot be separated by GNNs but can be separated by GTA.

To prove Lemma 3.2, we show a simple example of two graphs over 4 vertices that GTA without attention fails to separate while GTA can, and to prove Lemma 3.3, we consider a well-known example of two regular graphs that GNNs fail to distinguish, and show GTA is able to separate these graphs [48, 49]. Due to space limitations, the proofs are deferred to the supplementary materials.

Next, we turn to analyze the computational complexity of GTA. When training a decision tree, most of the computational effort is in selecting the split criterion at every tree inner-node. The cost of this operation is proportional to the number of possible splits one considers. Since a split criterion is defined by the aggregation function $AGG$, the depth parameter $d$, the selected feature $k$, the selected attention-set $S$ and the threshold $\theta$, then the computational complexity depends on the number of options one has in selecting each of these parameters.

The selection of the feature $k$ and threshold $\theta$ have the same complexity in GTA as in standard trees. The depth parameter $d$ can be bounded by a hyper-parameter $max_depth$. The number of candidate attention-sets for a node $u$ is $2^{depth(u)}$ where $depth(u)$ is the depth of the node $u$ in the tree. This can be further reduced by introducing another hyper-parameter $max_attention$ and limiting the candidate attention-sets to be either full set of vertices or the attention-sets generated in a node in the path to $u$ that is not more than $max_attention$ far from $u$. This will reduce the number of candidate attention-sets to $2^{max_attention}$ at most. Recall that in addition to masks that are induced by the candidate attention sets, the mask $I_{|V|}$ is always considered in a split node. Finally, we have just 4 candidates for the aggregation function. Hence, the complexity of GTA is $8 \times max\_attention \times max\_depth$ the complexity of training standard trees. Interestingly, we show in the supplementary that GTA with $max\_depth = 1$ and $max\_attention = 1$, is sufficient to achieve competitive performance to graph kernels and GNNs and in some cases outperform them.

3.5 Training and Inference

GTA is trained similarly to the way CART models are trained [50]. Nodes are split recursively using a greedy approach, until a stop condition is met (e.g., the maximum tree depth has been reached or the impurity cannot be reduced in any leaf). In each step we split one of the tree’s leaves by applying an optimal split to that leaf. The inference flow of GTA is similar to the inference in CART: an input graph $G$ is given, the algorithm traverses the tree by applying split criteria on $G$ until a leaf is encountered. Similarly, in the case of a vertex-level task, each vertex traverses the tree by applying the corresponding split criteria (See Figure 1). Notice that it is possible to use GTA to form ensembles of trees using Gradient Boosted Trees [26], Random Forests [4], or any other ensembles method.
Table 1: Empirical comparison of graph classification tasks on 7 TUDatasets and one large-scale OGB dataset. Best model is highlighted in blue.

| Baseline   | PROTEINS | MUTAG | D&D | IMDB-B | NCI1 | PTC-MR | IMDB-M | HIV  |
|------------|----------|-------|-----|--------|------|--------|--------|------|
| RW         | 72.1 ± 0.6 | 82.0 ± 2.1 | 71.0 ± 1.8 | 61.2 ± 3.0 | 48.0 ± 0.9 | 55.6 ± 4.6 | 33.3 ± 1.7 | 76.7 ± 2.1 |
| WL         | 75.3 ± 1.4 | 82.8 ± 1.2 | 79.0 ± 2.0 | 70.9 ± 1.7 | 76.7 ± 0.4 | 56.3 ± 0.0 | 42.1 ± 3.8 | 72.1 ± 0.8 |
| GK         | 71.0 ± 1.2 | 81.8 ± 2.1 | 78.7 ± 2.4 | 62.5 ± 4.9 | 62.2 ± 0.2 | 57.0 ± 1.3 | 42.4 ± 3.7 | 67.2 ± 0.2 |
| GAT        | 73.7 ± 1.3 | 89.2 ± 5.0 | 76.9 ± 4.1 | 71.6 ± 1.2 | 74.2 ± 2.4 | 66.8 ± 6.7 | 46.7 ± 4.6 | 82.4 ± 3.6 |
| GCN        | 75.0 ± 3.7 | 81.9 ± 6.7 | 71.5 ± 3.7 | 71.8 ± 2.5 | 50.8 ± 6.1 | 76.4 ± 0.0 | 50.8 ± 6.1 | 76.6 ± 0.0 |
| GraphSage  | 72.3 ± 4.1 | 85.3 ± 7.6 | 72.8 ± 4.3 | 73.2 ± 5.3 | 73.5 ± 2.3 | 63.9 ± 6.2 | 49.0 ± 2.6 | 79.2 ± 1.2 |
| DGCNN      | 73.9 ± 1.4 | 85.0 ± 3.5 | 77.8 ± 0.8 | 71.0 ± 0.4 | 73.2 ± 5.1 | 65.8 ± 2.8 | 47.9 ± 0.0 | 78.9 ± 0.8 |
| GIN        | 74.4 ± 3.5 | 89.1 ± 0.5 | 78.7 ± 1.4 | 72.2 ± 4.2 | 82.1 ± 2.8 | 62.1 ± 3.2 | 49.0 ± 2.6 | 82.4 ± 0.0 |
| GTA (d=0,a=0) + LapFeatures | 75.1 ± 2.4 | 85.4 ± 0.1 | 73.5 ± 1.8 | 72.5 ± 0.8 | 68.2 ± 1.3 | 45.3 ± 1.6 | 77.9 ± 0.7 |
| GTA (d=0,a=0) | 73.2 ± 1.1 | 82.6 ± 1.2 | 64.2 ± 3.5 | 71.4 ± 0.3 | 70.2 ± 2.7 | 65.2 ± 2.3 | 48.2 ± 1.2 | 77.1 ± 0.0 |
| GTA (a=0)  | 71.3 ± 2.1 | 81.2 ± 4.7 | 75.7 ± 2.7 | 70.3 ± 3.7 | 71.8 ± 7.2 | 71.4 ± 3.8 | 47.1 ± 3.5 | 77.7 ± 1.7 |
| GTA        | 78.0 ± 1.2 | 89.9 ± 5.1 | 79.1 ± 1.2 | 75.3 ± 3.2 | 79.3 ± 0.1 | 72.7 ± 0.2 | 49.2 ± 0.6 | 82.3 ± 0.0 |

4 Empirical Evaluation

In what follows we report experiments comparing GTA to other graph learning baselines, on graph and node labeling benchmarks. We applied GTA to multiple standard and large-scale graph and node labeling benchmarks and compared the results to popular GNNs and graph kernels baselines. 

4.1 Datasets

Graph Classification To evaluate GTA on graph classification tasks, we used seven graph classification benchmarks from TUDatasets[51], and one large-scale dataset from OGB [52]. MUTAG [53] is a dataset of 188 chemical compounds divided into two classes according to their mutagenic effect on bacterium. IMDB-B & IMDB-M [54], are movie collaboration datasets with 1000 and 1500 graphs respectively. Each graph is derived from a genre, and the task is to predict this genre from the graph. Nodes represents actors/actresses and edges connect them if they have appeared in the same movie. PROTEINS & DD [17][55] are two proteins datasets consisting of 1113 and 1178 proteins graphs, respectively, where vertices corresponds to amino acids, and an edge exists between two vertices if the amino acids are less than 6 Angstroms apart. The proteins are labeled 1 if they are enzymes and 0 otherwise. NCI1 [17] is a datasets consisting of 4110 graphs, representing chemical compounds. Vertices and edges represents atoms and chemical bonds between them. The graphs are divided into two classes according to their ability to suppress or inhibit tumor growth. PTC-MR [56] is a dataset consisting of 344 chemical compounds divided into two classes according to their car-

5 Code is available at https://github.com/TAU-MLwell/GTA---Graph-Trees-with-Attention
cinogenicity for rats. HIV is a large-scale dataset consisting of 166k molecules and the task is to predict whether a molecule inhibits HIV.

Node Classification As node classification tasks, we used the three Planetoid datasets [57], and one large-scale dataset from OGB [52]: Cora, Citeseer and Pubmed are citation graphs consisting of 2708, 3327 and 19717 nodes respectively, where nodes are documents and edges are citation links. Arxiv is a large-scale directed graph over 169343 nodes, representing the citation network between all Computer Science (CS) arXiv papers. More details on these datasets are given in the supplementary materials.

4.2 Baselines

We compare GTA to eight popular graph kernels and GNN baselines: GCN (Graph Convolution Network) [16], GAT (Graph Attention Network) [15], GraphSage [58], GIN (Graph Isomorphism Network) [29], DGCNN (Disordered Graph Convolutional Neural Network) [28], GK (Graphlet graph kernels) [18], WL (Weisfeiler-Lehman Graph Kernels) [17] and a Random-Walk (RW) approach [27]. For DGCNN, we evaluate only on graph-level tasks, since its main contribution is the global pooling method. We used GTA in a GBT framework, with 50 GTA estimators, \( \text{max\_attention} = 3, \text{max\_depth} = 3, \text{min\_examples\_in\_leaf} = 10, \text{max\_leaves} = 10 \) and without considering the attention mask \( I \). We report two GTA ablations: GTA without attention and without using topological information (i.e., \( \text{max\_depth} = 0, \text{max\_att} = 0 \)), and GTA without attention (i.e., \( \text{max\_att} = 0 \)). All tree models were applied with GBT. Finally, we also evaluate the GTA version with \( \text{max\_depth} = 0 \) and \( \text{max\_att} = 0 \), with additional features based on the graph Laplacian (LapFeatures), as common in the literature [59, 60]: the dimension of the null space, the spectral gap (the smallest non-zero eigen-value), the second smallest eigenvalue (the algebraic connectivity).

4.3 Results

Following the conventions in prior work, in all datasets except HIV and ARXIV we used 10-fold-cv, whereas in HIV and ARXIV we used the predefined splits to train and test, and followed the protocols in Hu et al. [52] (see the supplementary materials for more details). The results are summarized in Table 1 and Table 2. GTA outperformed all other TBM approaches in all 12 tasks, by a margin of 3.9 – 14.9 percentage points, and outperformed GNNs in 5 out of the 7 TUDatasets tasks. Specifically, GTA was improved upon GNN approaches by a margin of 9.8 percentage points on the PTC-MR dataset and a margin of 3.2 and 1.1 percentage points on D&D and PROTEINS datasets, respectively. Moreover, GTA outperformed all kernel-based methods. Regarding the Planetoid datasets, GTA outperformed most GNNs, and was on par with the winning GNN approach in every task. The OGB datasets show interesting results: while GTA was on par with GNNs, the specified GNNs use millions of parameters: GIN used 1885206 parameters, and GCN used 527701 parameters to achieve SOTA results, while GTA was able to achieve similar results with only \( \sim 1500 \) parameters.

In the supplementary we show that even when setting \( \text{max\_depth} = 1 \) and \( \text{max\_attention} = 1 \), we obtain competitive results. Our results demonstrate that methods that are fully based on decision trees, when specialized for graphs, are competitive with, and even outperform, popular GNNs and graph kernels.

5 Explaining GTA Outputs

In this section we show that the attention mechanism can be used to explain the predictions made by GTA. This explanations mechanism ranks the vertices and edges of the graph according to their use in the active attention-sets and split criteria, and thus highlights the parts of the graph that contribute the most to the prediction.

Let \( G \) be a graph that we want to classify using a decision tree \( T \). Following Hirsch and Gilad-Bachrach [44], the key idea in the construction of our importance weight is that if a vertex appears in many attention sets when calculating the tree output for \( G \), then it has a large effect on the decision. This is quantified as follows: consider the path in \( T \) that \( G \) traverses when it is being classified. For each vertex \( i \) in \( G \), count how many attention-sets in the path contain \( i \), and denote this number by \( n_T(i) \). In order to avoid dependence on the size of \( T \) we convert the values \( n_T(1), \ldots, n_T(|V|) \) into a
new vector $r_T(1), \ldots, r_T(|V|)$ where $r_T(i)$ specifies the rank of $n_T(i)$ in $n_T(1), \ldots, n_T(|V|)$ after sorting in decreasing order. For example, $r_T(i) = 1$ if the vertex $i$ appears most frequently in active attention-sets compared to any other vertex. We shall use $2^{-r_T(i)}$ to measure the importance of the rank, so that low ranks have high importance.

Now assume we have an ensemble of decision trees $T$ (e.g., generated by GBT). For any $T \in T$ in the ensemble let $y_T$ be the value predicted by $T$ for the graph $G$. We weight the rank importance by $|y_T|$ so that trees with larger contribution to the decision have greater effect on the importance measure. Note that boosted trees tend to have large variability in leaf values between trees in the ensemble [61]. Therefore, the importance-score of vertex $i$ in the ensemble is the weighted average:

$$\text{importance}(i) = \frac{\sum_{T \in T} |y_T| 2^{-r_T(i)}}{\sum_{j \in |V|} \sum_{T \in T} |y_T| 2^{-r_T(j)}}. \quad (6)$$

The proposed importance score is non-negative and sums to 1. Furthermore, edge importance scores can be derived in a similar way, and are presented in the supplementary materials.

To demonstrate GTA’s explanations mechanism, we present, in Figure 3, vertex explanations for two problems: Red Isolated Vertex, and Mutagenicity. These explanations demonstrate how GTA’s attention mechanism is able to capture the important properties of the graph and highlight them.

**Red-Isolated-Node Explanations:** This is a synthetic task to identify if exactly one red vertex is isolated in the graph. The data consists of 1000 graphs over 50 vertices, with two features: the constant feature 1 and a binary blue/red color.

**Mutagenicity Explanations:** This dataset consists of 4337 chemical compounds of drugs divided into two classes: mutagen and non-mutagen. A mutagen is a compound that changes genetic material such as DNA, and increases mutation frequency. It is known, for example, that existence of $NO_2$ and ring groups increases the mutagenicity of compounds [63].

For each task, we trained and tested GBT with 50 GTA estimators and hyperparameters as in Section 4 using a 80/20 split. Figure 3 presents vertex explanations for two graphs from the test sets of each dataset. The size of a vertex corresponds to its importance computed according to Eq. 6. For the Red-Isolated-Node problem, it is shown that GTA attends to isolated vertices, and even more so to red isolated vertices. For the Mutagenicity problem, it is seen that GTA attends to $NO_2$ and ring groups, which are known to have mutagenic effects [63].

6 Conclusion

Graphs appear in many important applications of machine learning. In this work we proposed a novel method, Graph Trees with Attention (GTA), to perform different prediction tasks on graphs inspired by the success of tree-based methods on tabular data [1–3]. Empirically we showed that GTA outperforms other tree-based models that were adapted to operate on graphs. Moreover, when compared to commonly used Graph Neural Networks (GNNs) and graph kernels, we found that GTA was on par in all cases and outperformed all other methods in many benchmarks. This is achieved while maintaining the relative simplicity of tree-based models, in the sense that they work well “out-of-the-box” with little parameter tuning. To support these findings, our theoretical analysis showed that the attention mechanism in GTA strictly improves their expressive power. We also showed that there are graphs that GTA can tell apart while GNNs cannot. Finally, we also proposed
a mechanism for generating explanations for GTA decisions. The encouraging results presented here suggest that tree-based models can play an important role in graph prediction tasks. There are many ways in which the current work can be extended, including scaling to larger graphs and treating graphs with different combinations of vertex and edge features. We also note that while GTA may create many benefits for the society in domains such as drug discovery, there are generally classification problems that have negative societal impact. Moreover, even though we presented an explanations mechanism, it does not provide full protection against biases in the data. We continue to make efforts to alleviate these limitations.

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A Appendix A

In the appendix we present supporting material that did not fit in the main paper due to space limitations.

A.1 Datasets Summary

Table 3 presents summary of the datasets used in the experiments. The datasets used vary in the number of graphs, the sizes of the graphs, the number of features in each vertex and the number of classes. Note that although all benchmarks are classification tasks, GTA can also perform regression tasks, ranking tasks and more.

Table 3: Statistics of datasets used in experiments.

| Dataset   | # Graphs | Avg # Vertices | Avg # Edges | # Features | # Classes |
|-----------|----------|----------------|-------------|------------|-----------|
| MUTAG     | 188      | 17.93          | 19.79       | 7          | 2         |
| PROTEINS  | 1113     | 39.06          | 72.82       | 3          | 2         |
| DD        | 1178     | 284.32         | 715.66      | 0          | 2         |
| IMDB-B    | 1000     | 19             | 96          | 0          | 2         |
| IMDB-M    | 1500     | 13             | 65          | 0          | 3         |
| NCI1      | 4110     | 29.87          | 32.3        | 37         | 2         |
| PTC       | 344      | 14             | 14          | 19         | 2         |
| HIV       | 41,127   | 25.5           | 27.5        | 9          | 2         |

| Dataset   | # Vertices | # Edges | # Features | # Classes |
|-----------|------------|---------|------------|-----------|
| CORA      | 2,708      | 10,556  | 1,433      | 7         |
| CITESEER  | 3,327      | 9,104   | 3,703      | 6         |
| PUBMED    | 19,717     | 88,648  | 500        | 3         |
| ARXIV     | 169,343    | 1,166,243| 128        | 40        |

A.2 Experiments Details

In this section we describe additional details about the experiments whose results were reported in the main paper. For the following datasets: MUTAG, PROTEINS, DD, IMDB-B, IMDB-M, NCI1, PTC, CORA, CITESEER, PUBMED, we ran all models using 10-fold cross validation and report the mean accuracy and std. The HIV and ARXIV datasets are large-scale datasets provided in the Open Graph Benchmark (OGB) paper [52] with pre-defined train and test splits and different metrics and protocols for each dataset. As common in the literature when evaluating OGB datasets, for each of these two datasets we follow its defined metric and protocol:

- In the case of the HIV dataset, the used metric is ROC-AUC. As described in Hu et al. [52], we ran the GNNs 10 times with random initialization and reported the mean ROC-AUC and std over the runs. GTA and graph kernels do not have a random component equivalent to the random parameters initialization of GNNs. To provide some assessment of performance variability, we ran GTA and the graph kernels 10 times with 90% random sampling of the training data and report the mean ROC-AUC and std over the runs. This clearly only limits the performance of GTA and graph kernels with respect to GNNs, as the sampling is done from a pre-defined training set.

- In the case of the ARXIV dataset, the metric used is accuracy. Following the protocol in Hu et al. [52], we ran the GNNs 10 times with random initialization and reported the mean accuracy and std over the runs. Similarly to the setting of the HIV datasets, in the case of GTA and graph kernels we ran the models 10 times with 90% random sampling of the training data and report the mean accuracy and std over the runs.

A.3 Default-Parameters

ML algorithms sometime require extensive parameter tuning to achieve good performance, and this could be time consuming, power consuming, and may lead to overfitting. Therefore, in this section
we investigate how well GTA works without any parameter tuning. Towards this end, we set the default parameters to \( \text{max\_attention} = 1 \) and \( \text{max\_depth} = 1 \). We evaluate performance with these, and compare to other settings in which parameter tuning is performed. Figure 4 shows the results for this experiment. It shows that even with default parameters, GTA’s performance does not degrade much. Even with no parameter tuning and with small values of \( \text{max\_attention} \) and \( \text{max\_depth} \), GTA outperforms GNNs and Kernel methods in some cases.

### A.4 Extensions to GTA

In this section we propose some possible extensions to the GTA.

#### A.4.1 Additional Attention Types

In the main paper we show the significance of the attention mechanism for achieving high accuracy. Here we propose additional attention mechanisms to the one presented in Section 3.3 of the main paper. Alternative attention forms for graph-level tasks include:

\[
\text{AGG}\left(\left(A^d f_k\right) \odot 1_S\right) \leq \theta
\]

(7)

\[
\text{AGG}\left(A^d (f_k \odot 1_S)\right) \leq \theta
\]

(8)

\[
\text{AGG}\left((A \odot M)^d f_k\right) \leq \theta,
\]

(9)

and for vertex-level tasks:

\[
\left(A^d (f_k \odot 1_S)\right)_i \leq \theta
\]

(10)

\[
\left(A^d f_k \odot 1_S\right)_i \leq \theta
\]

(11)

\[
\left((A \odot M)^d f_k\right)_i \leq \theta
\]

(12)

Each such attention form can be thought of as applying different constraints on the features propagation along the graph. In the experiments reported in the paper we used only the attention form described in the main paper. It will be interesting to perform comparisons of the different attention approaches.

Figure 4: Test accuracies of GTA, with default parameters of \( \text{max\_attention} = 1, \text{max\_depth} = 1 \) (GTA 1,1), in comparison to the best test accuracy achieved by GTA, and GNNs, and Graph Kernels, as presented in Table 1 in the main paper. GTA present high performance even default (and small) \( \text{max\_attention} \) and \( \text{max\_depth} \) parameter values.
A.4.2 Weighted Adjacencies and Multiple Graphs

We also note that the adjacency matrix used in GTA can be weighted, and the split criteria and attention extend naturally to this setting. Moreover, it is possible to extend GTA to allow multiple adjacency matrices. This allows, for example, encoding of edge features and heterogeneous graphs.

A.4.3 Edge Level Tasks

In the paper we discuss vertex and graph level tasks. Nevertheless edge-level tasks also arise in many problems. We note that the task of edge labeling can be represented as a vertex-level task by using a line graph \[64\]. The line graph \(L(G)\) of a graph \(G = (V, E)\) represents the adjacencies between the edges of \(G\). Each edge \((u, v) \in E\) corresponds to a vertex in \(L(G)\), and two vertices in \(L(G)\) are connected by an edge if their corresponding edges in \(G\) share a vertex. Then, GTA for vertex-level tasks can be used to label vertices in the line graph, which corresponds to edges in the original graph.

A.5 Edge-Level Explanations

In the paper we introduce a mechanism for explaining the predictions of GTA using a scheme for computing vertex importance. Similarly to vertex importance, edge importance can be computed. We use the attention mechanism to rank the edges of a given graph by their importance. Note that each split criterion uses a subset of the graph’s edges, according to \(d\) and the active attention-set. For example, a split criterion may consider only walks of length 2 to a specific subset of vertices, which induces the used edges by the split criterion. Let \(E_1, \ldots, E_k\) denote the used edges along the prediction walk \(w_m^\pi(G)\). We now rank each edge \((i, j) \in E\) by \(r_m^\pi(i, j) = \sum_{j \in \{i, j \in E_j\}} d_{ij}\), i.e., the rank of an edge is the number of split-nodes in the prediction walk that use this edge. The ranks \(r_m^\pi(i, j)\) are then combined with the predicted value \(y_m\), as in Eq.6 in the main paper.

A.6 Public Source Code

Complete code for reproducing the experiments including all datasets references can by found here.

B Appendix B

The proofs of several lemmas presented in the main paper were skipped due to space limitations. Here we provide the proofs for these lemmas.

B.1 Proof of Lemma 3.1

**Lemma.** GTA trees are invariant to permutations in the case of graph-level tasks, and equivariant in the case of vertex-level tasks.

We first show that every component in the split criterion of GTA is permutation-equivariant, except for the aggregation function applied in the case of graph-level tasks, which is permutation-invariant. Let \(\pi\) be a permutation over the vertices, and \(P_{\pi}\) the corresponding permutation matrix. For any permutation matrix \(P\), it holds that \(P^TP = I\), therefore:

\[
\left( P_{\pi} A P_{\pi}^T \right)^d (P_{\pi}f_k) = \left( P_{\pi} A P_{\pi}^T \right) \left( P_{\pi} A P_{\pi}^T \right) \cdots \left( P_{\pi} A P_{\pi}^T \right) (P_{\pi}f_k) = P_{\pi} \left( A^d f_k \right)
\]

and therefore \(A^d f_k\) is permutation-equivariant.

Similarly, for the attention mechanism, if one uses an attention mask \(M\), the above equivariance similarly holds because:

\[
\left( P_{\pi} A P_{\pi}^T \right)^d \odot \left( P_{\pi} M P_{\pi}^T \right) (P_{\pi}f_k) = \left( \left( P_{\pi} A P_{\pi}^T \right) \left( P_{\pi} A P_{\pi}^T \right) \cdots \left( P_{\pi} A P_{\pi}^T \right) \right) \odot \left( P_{\pi} M P_{\pi}^T \right) (P_{\pi}f_k)
\]

\[
= \left( P_{\pi} A^d P_{\pi}^T \odot P_{\pi} M P_{\pi}^T \right) (P_{\pi}f_k) = P_{\pi} \left( A^d \odot M \right) P_{\pi}^T (P_{\pi}f_k) = P_{\pi} \left( A^d \odot M \right) f_k
\]
We argue that GTA without the attention mechanism cannot distinguish between these graphs. Note that for any of the features $A^0f$ is identical for $G_1$ and $G_2$ since it ignores the edges of these graphs. For $d > 1$ note that $A^d f$ is a permutation of the vector $(1, -1, 0, 0)$ for $G_1$ and $G_2$. Since the aggregation functions are permutation invariant, applying any aggregation function to $A^d f$ will generate the same value for $G_1$ and $G_2$. Moreover, since the topology of $G_1$ and $G_2$ is isomorphic, any invariant graph-theoretic feature would have the same value of $G_1$ and $G_2$. Therefore, GTA without the attention mechanism cannot distinguish between $G_1$ and $G_2$. Nevertheless, GTA can distinguish between them when using attention. Specifically, the tree shown in Figure 7 will separate these two graphs to two different leaves. The root of the tree conditions on $f_1$ which creates an attention set of the nodes $(1, 1)$ and $(1, -1)$. At the following level, the tree propagates $f_2$ along walks of length 2 masking on the attentions set. For $G_1$, the only walk that is not masked out is the walk starting and ending in $(1, 1)$ and therefore for this vertex the value 1 is computed while 0 is computed for all other vertices. However, for $G_2$, the only walk of length 2 that is not masked out is the one starting and ending at $(1, -1)$. Therefore, in $G_2$, the value $-1$ is computed for the vertex and $(1, -1)$ and the value 0 is computed for all other vertices. See Figure 8 for a visualization of this analysis. Therefore, ($A^2 \otimes M$)$f_2$ is a permutation of the vector $(1, 0, 0, 0)$ for $G_1$ and a permutation of the vector $(-1, 0, 0, 0)$ for $G_2$ and thus GTA can distinguish between these graphs.
B.3 Proof of Lemma 3.3

Figure 6: Two 4-regular non-isomorphic graphs. The two graphs differ, for example, in their number of cycles of length 3. The figure is taken from [49].

Lemma. There exist graphs which cannot be separated by GNNs but can be separated by GTA.

Let $G_1$ and $G_2$ be the two 4-regular non-isomorphic graphs as in Figure 6. Assume that all vertices have the same fixed feature 1. Namely, we wish to distinguish these two graphs only by their topological properties. It is easy to see that a GNN will not be able to distinguish these two graphs, as after the message passing phase, all nodes will result in the same embedding [49]. In contrast, GTA is able to separate these two graphs with a single tree consisting of a single split node, by applying the split rule: $\sum (A^3 \odot I_b) f_i \leq 1$. This rule counts the number of cycles of length 3 in each graph. Notice that GNNs here refer to the class of MPGNNS [31], whose discriminative power is known to be bounded by the 1-WL test [29]. In particular, popular models such as GIN, GAT and GCN [15, 16, 29], which are also presented in the empirical evaluation sections, all belong to this class of GNNs.

Figure 7: The tree that separates the two graphs $G_1$ and $G_2$ in Figure 6.
Figure 8: The prediction path of the graphs $G_1$ (red) and $G_2$ (grey) in the tree. The path is marked with bold arrows. The available attention sets that are generated by the root are marked with a dashed line next to the root edges. The active attention set used in the inner split node is shown left of the node.