GATE: Gated Additive Tree Ensemble for Tabular Classification and Regression

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Abstract

We propose a novel high-performance, parameter and computationally efficient deep learning architecture for tabular data, Gated Additive Tree Ensemble (GATE). GATE uses a gating mechanism, inspired from GRU, as a feature representation learning unit with an in-built feature selection mechanism. We combine it with an ensemble of differentiable, non-linear decision trees, re-weighted with simple self-attention to predict our desired output. We demonstrate that GATE is a competitive alternative to SOTA approaches like GBDTs, NODE, FT Transformers, etc. by experiments on several public datasets (both classification and regression). We have made available the code at https://github.com/manujosephv/GATE under MIT License.

1. Introduction

Deep Learning (Goodfellow et al., 2016) has taken the world of machine learning by storm overthrowing state-of-the-art systems across a number of tasks in computer vision (Krizhevsky et al., 2017), natural language processing (Devlin et al., 2019), reinforcement learning (Silver et al., 2016). Gradient-based optimization using backpropagation and hierarchical representation learning seems to be the cornerstones on which the deep learning success story has been built.

Although deep learning performs outstandingly well in homogeneous data domains like images, audio, or text, tabular data is still an "unconquered castle" (Kadra et al., 2021) for deep learning. State-of-the-art in tabular data are usually "shallow" models like the gradient boosted decision trees (GBDT) (Friedman, 2001; Chen & Guestrin, 2016; Ke et al., 2017; Prokhorenkova et al., 2018). The ML community has recognized the importance of deep learning and many works (Arik & Pfister, 2021; Popov et al., 2020) have tried to address this problem. Joseph (2021) has proposed a deep learning library based on PyTorch to unify and accelerate the research in the area. Shwartz-Ziv & Armon (2022); Borisov et al. (2021) have surveyed the current state of research in the field and concluded that there is still a gap between the proposed deep learning models and the GBDT state-of-the-art. The gap is in the performance of the models as well as the training and inference times. This is further evidenced by the large number of Kaggle ML competitions with tabular data are still won using shallow GBDT models. We aim to reduce this gap by our paper.

We introduce Gated Additive Tree Ensembles (GATE), a new deep learning architecture designed to work with tabular data.

In the following sections we will explain the design choices which make GATE a competitive model choice for tabular data. Through a large number of experiments, we compare the proposed approach to leading GBDT implementations and other deep learning models and show that our model is competitive with the GBDTs and outscore other deep learning approaches in being more parameter efficient and having less computational cost.

Overall, our main contributions can be summarized as follows:

1. A novel gating mechanism, inspired from Gated Recurrent Units (Cho et al., 2014), for representation learning. To the best of our knowledge, this is the first time such an approach has been adapted to non-temporal tabular data.

2. A novel non-linear decision tree-like architecture, which is parameter efficient and scalable to large datasets with thousands of features.

3. Using a large number of datasets, we show that the GATE architecture has competitive performance along with being parameter efficient, and computation efficient.

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2. Related Work

Deep Learning approaches for tabular data: Although GBDTs are still considered state-of-the-art for tabular data, there has been considerable work from the deep learning community to make headway in tabular data domain. Tabnet(Arik & Pfister, 2021), Neural Oblivious Decision Trees(Popov et al., 2020), FT-Transformer(Gorishniy et al., 2021), and DNF-Net(Abutbul et al., 2020) all proved itself to be competitive models by performing better or as well as popular “shallow” models like the GBDT. Many of these approaches can be broadly classified into two types of models: Differentiable trees & Attention-based models. Differentiable Trees tries to capture the inductive bias of a decision tree, but still make them end-to-end differentiable to be able to train them using gradient descent. Attention based architectures are currently revolutionizing the fields of natural language processing(Devlin et al., 2019), speech recognition(Wang et al., 2020), and computer vision(Dosovitskiy et al., 2021). Several authors tried to use attention for tabular data domain as well (Huang et al., 2020; Gorishniy et al., 2021; Song et al., 2019).

Differentiable Decision Trees: Decision trees(Quinlan, 1986) have proved to have valuable inductive bias for tabular data time and again. But a vanilla decision tree has hard routing which makes it non-differentiable. This makes it impossible to include a vanilla decision tree in a neural network trained by gradient descent. One of the first soft decision tree (SDT) was introduced by (Suarez & Lutsko, 1999) where they replaced the Heaviside function with a sigmoid activation. This was still a univariate decision tree or axis-aligned decision tree. More modern approaches like (Kontschieder et al., 2015; Chen, 2020; Luo et al., 2021) used perceptrons on all the features in the gating function. This led to oblique decision trees(Murthy et al., 1994) in which the decision boundaries are “oblique” to the axes because they are constructed using a linear combination of features. Non-linear decision trees, where each split is a non-linear function of the input features, are an area that is less explored(Ittner, 1996). Our core decision tree structure is a differentiable non-linear decision tree.

Sparsity enforcing activations: Traditionally softmax was the de-facto way to map a vector of real-valued scores to a discrete probability distribution. (Martins & Astudillo, 2016) introduced a sparsity-enforcing alternative, sparsemax. And (Peters et al., 2019) proposed a generalization of softmax and sparsemax into a formulation called entmax with a parameter $\alpha$ which decides how sparse the output probability distribution should be. When $\alpha = 1$, the entmax becomes a softmax and when $\alpha = 2$ it becomes sparsemax. (Popov et al., 2020) uses entmax with $alpha = 1.5$ as the choice function in NODE and we are using the same in our architecture as well. The sparsity of entmax helps with feature selection and sparse decision trees.

Feature Representation Learning: Learning good representation of features is a fundamental problem and have been studied extensively in the literature. Since tabular features are heterogeneous and irregular, learning the right features and the interaction between features are the two fundamental problems.

Feature Selection: Unlike classical decision trees, oblique decision trees and non-linear decision trees don’t have any implicit feature selection and therefore we need an explicit feature selection in the tree structure. Tabnet(Arik & Pfister, 2021) used an attention mechanism for feature selection, but at an instance level. In contrast, in this work we use feature selection at the global level, similar to NODE(Popov et al., 2020), but we use feature selection, not only in the soft trees, but also in a separate representation learning units.

Feature Interactions: Capturing the right feature interactions is key to getting a good feature representation. Previous works have tried to learn then implicitly (Rendle, 2010; Guo et al., 2017) and explicitly (Wang et al., 2017; Lian et al., 2018; Song et al., 2019).

Gating Mechanism: Gating mechanism is widely used in deep learning to modulate the flow of information through the network. Gating mechanisms are very popular in sequence models like LSTM(Hochreiter & Schmidhuber, 1997), GRU(Cho et al., 2014), and Highway Networks(Srivastava et al., 2015) where they are used to prevent vanishing and exploding gradients. Gated Linear Units(Dauphin et al., 2017; Gehring et al., 2017) is another popular gating mechanism.

3. Gated Additive Tree Ensembles (GATE)

Ensembling of Decision Trees, Feature Selection, and Feature Engineering have proven to be the best techniques to achieve state-of-the-art performance in tabular datasets. GATE architecture has been specifically designed with these principles in mind: (i) uses a feature learning unit to select and learn new features by non-linear processing of raw features; (ii) constructs multiple multi-layered differentiable decision trees based on the learned features; (iii) ensembles and combines the outputs in a weighted ensemble where the weights are learned from data.

Suppose we have a training dataset, $\mathcal{D} = (\mathcal{X}, \mathcal{Y}) = \{(x_i, y_i)\}_{i=1}^{N}$, where each $x_i \in \mathbb{R}^d$ is a $d$-dimensional data with a corresponding label $y_i \in \mathcal{Y}$. We assume all the input features are numerical. Any categorical feature would have to be encoded using sufficient preprocessing or a learnable embedding layer. For classification problems, $\mathcal{Y} = \{1, \ldots, K\}$ and for regression $\mathcal{Y} \in \mathbb{R}$.

There are two main stages in the end-to-end GATE model.
The input features, $\mathcal{X} \in \mathbb{R}^{d}$, is first processed by a series of Gated Feature Learning Units (GFLU). The GFLUs learn the best representation of the input features by feature selection and feature interactions. This learned representation is then processed using an ensemble of Differentiable Non-Linear Decision Trees (DNDTs). Finally, the output of all the trees are re-weighted using self-attention and used for the final prediction of the model.

3.1. Gated Feature Learning Units (GFLU)

Gated Feature Learning Unit is an architecture which is directly inspired by the gating flows in Gated Recurrent Units (Cho et al., 2014), but re-purposed for sequential feature learning for tabular data. The key difference is in the way we use a learnable feature mask to softly select a subset of features as the input to the GFLU and thereby making the inputs to the different GFLUs, which are stacked on top of each other, different. Figure 3 in Appendix B shows a single Gated Feature Learning Unit. We can think of GFLUs selecting what information to use from the raw features and using its internal mechanism to learn and unlearn to create the best set of features which is required for the task. This allows the downstream modules to focus their learning capacity on only the features which are most important for the task and hence become more parameter efficient. The aim of this module is to learn a function $F : \mathbb{R}^{d} \rightarrow \mathbb{R}^{d}$. Although we can use the hidden state dimensions to increase or decrease the dimensions of the learned feature representation $\tilde{d}$, we have chosen to keep it the same in all our experiments.

3.1.1. Feature Selection:

We use a learnable mask $M_{n} \in \mathbb{R}^{d}$ for the soft selection of important features for each stage, $n$, of feature learning in hte GFLU. The mask is constructed by applying a sparse transformation on a learnable parameter vector ($W_{n} \in \mathbb{R}^{d}$). In order to encourage sparsity, we propose to use the $\alpha$-entmax transformation (Peters et al., 2019). The $\alpha$-entmax transformation is an interpolation between softmax and sparsemax (Martins et al. 2016) parametrized by a $\alpha$. The proposed masking is multiplicative. Formally this feature selection is defined by:

$$\mathcal{X}_{n} = M_{n} \odot \mathcal{X} \quad (1)$$

where $\mathcal{X}_{n} \in \mathbb{R}^{d}$ is the input features (after feature selection) and $M_{n} = \text{entmax}_{\alpha}(W_{n})$ and $\odot$ denotes an element-wise multiplication operation. In the Entmax sparsity mapping, we use the default setting of $\alpha = 1.5$ in all our experiments. In order to further encourage sparsity and diversity in the feature selection across stages, we initialize $W_{n}$ from different Beta distributions with its two parameters ($\alpha$ and $\beta$) sampled from a uniform distribution $[0.5, 10]$.

3.1.2. Gating Mechanism

The gating mechanism, which is directly inspired by Gated Recurrent Units, takes the input after applying the feature mask, $\mathcal{X}_{n} \in \mathbb{R}^{d}$, as an input and learns a feature representation, $H_{n} \in \mathbb{R}^{d}$. Instead of the hidden state that a GRU maintains to learn from a sequence, a GFLU learns a hidden feature representation. And unlike the standard GRU, weights are not shared between different GFLUs because we want the unit to apply different transformations in each stage of feature representation.

At any stage, $n$, the hidden feature representation is a linear interpolation between previous feature representation($H_{n-1}$) and current candidate feature representation($\tilde{H}_{n}$)

$$H_{n} = (1 - z_{n}) \odot H_{n-1} + z_{n} \odot \tilde{H}_{n} \quad (2)$$

where $z_{n}$ is the update gate which decides how much information to use to update its internal feature representation. The update gate is defined as

$$z_{n} = \sigma (W_{n}^{z} \cdot [H_{n-1}; \mathcal{X}_{n}]) \quad (3)$$

where $[H_{n-1}; \mathcal{X}_{n}]$ represents a concatenation operation between $H_{n-1}$ and $\mathcal{X}_{n}$, $\sigma$ is the sigmoid activation function, and $W_{n}^{z}$ is a learnable parameter.

The candidate feature representation($\tilde{H}_{n}$) is computed as

$$\tilde{H}_{n} = \tanh (W_{n}^{r} \cdot [r_{n} \odot H_{n-1}; \mathcal{X}_{n}]) \quad (4)$$

where $r_{n}$ is the reset gate which decides how much information to forget from previous feature representation, $W_{n}^{r}$ is a learnable parameter, $[\cdot]$ represents a concatenation operation, and $\odot$ represents element-wise multiplication.

The reset gate ($r_{n}$) is computed similar to the update gate

$$r_{n} = \sigma (W_{n}^{r} \cdot [H_{n-1}; \mathcal{X}_{n}]) \quad (5)$$

In practice, we can use a single matrix ($W_{n}^{i} \in \mathbb{R}^{2d \times 2d}$) to compute the reset and update gates together to save some computation. We can stack any number of such GFLUs to encourage hierarchical learning of features and the feature representation from the last GFLU stage, $\mathcal{H} \in \mathbb{R}^{d}$, is used in the subsequent stages.

3.2. Differentiable Non-Linear Decision Trees (DNDT)

This module takes in as the input the feature representation from the last GFLU stage, $\mathcal{H}$. The aim of this module is to learn a function $F : \mathbb{R}^{d} \rightarrow \mathbb{R}^{D}$, where $d$ is the dimensions of the learned feature representation from GFLUs and $D$ is the depth of the tree. Decision tree methods construct the function $F$ by recursively partitioning the feature space into
disjoint regions and assigning a label to each such region. And a Non-Linear decision tree uses all the features in a non-linear fashion for each split in the decision tree. The core building block of our model is such a non-linear decision tree.

3.2.1. SOFT BINNING FUNCTION

A binary decision tree model uses decisions made by a series of hierarchical nodes and each node can be seen as a binary classifier which routes the samples either to the left or the right leaf. It selects a single feature \( h_i \in H \subseteq \mathbb{R}^d \) and learns a cutoff \( (b_i) \) from data to form a hard routing to the left or right leaf. We can think of this as a gating function \( g(h_i, b_i) \). For the standard decision tree model, this gating function is the Heaviside function, which is not differentiable. Therefore, we need a "soft" version of this gating function. We have adopted the soft binning function (Yang et al., 2018) proposed, but with some modifications:

- Replaced the temperature controlled softmax with \( \alpha \)-entmoid to encourage sparsity in the leaf scores.
- Modified the procedure to carry out the binning for all features at once, rather than one-by-one, which decreased runtimes significantly.
- Adapted the procedure to be restricted to binary trees eliminating a few costly operations which decreased runtimes again.

Let’s assume we have a feature set, \( H \in \mathbb{R}^d \) that we want to bin into 2 bins each (binary trees). Consequently, we would need \( d \) cut points, one for each of the \( d \) features. Let’s denote these cut points as \( [\beta_1, \beta_2, \ldots, \beta_d] \). Now we construct a single layer neural network with \( \alpha \)-Entmoid, a highly optimized 2-class entmax (Peters et al., 2019; Popov et al., 2020) as the activation function. By applying the \( \alpha \)-Entmoid activation, we are relaxing the strict requirement that the probabilities that route a sample to the left and right are true probabilities. This is a conscious decision to reduce the computational complexity of the network.

\[
g = \text{entmoid}_\alpha(H \cdot W + b) \tag{6}
\]

Here, \( W \) is not a learnable parameter, rather a constant. Both \( W \) and \( b \) is set as:

\[
W \in \mathbb{R}^{d \times 2} = \begin{bmatrix} 1 & 2 \\ 1 & 2 \\ \ldots & \ldots \\ 1 & 2 \end{bmatrix}, \quad b \in \mathbb{R}^{d \times 2} = \begin{bmatrix} 0 & -\beta_1 \\ 0 & -\beta_2 \\ \ldots & \ldots \\ 0 & -\beta_d \end{bmatrix} \tag{7}
\]

\( g \in \mathbb{R}^{d \times 2} = [g_L \ g_R] \) is a tensor with two columns - the left \( (g_L) \) and right \( (g_R) \) leaf scores. While the leaf scores are the direct output from the soft binning function it is an artifact of the routing decision. Decision tree models have the routing and final output slightly different. The routing is done using the gating function but the output from the leaves are derived from all the training samples which are routed to that particular node. But this procedure is not feasible in an end-to-end differentiable model and therefore we have another set of learnable parameters as the leaf responses, \( R \in \mathbb{R}^{d \times 2} \). The final output from the decision stump is:

\[
R = [R_L \ R_R] = g \odot R \tag{8}
\]

where \( \odot \) is the element-wise multiplication.

We call this structure (Figure 1a) we just described as a decision stump because unlike a node the output is not just the routing decision, but a real valued leaf response.

3.2.2. FEATURE MASKING AND AGGREGATION

Similar to oblique decision trees, our non-linear decision trees also use all the features for a split. But instead of a linear combination of features, we use a non-linear function, or more specifically, a linear combination of non-linear functions for a split. (Yang et al., 2018) uses a Kronecker product of leaf probabilities of all the features to exhaustively calculate the final node probabilities of all nodes. This can become very large and computationally infeasible when we are looking at datasets with a large number of features. We propose a learnable feature mask, \( M \in \mathbb{R}^d \), as a way to combine the outputs, \( R \), from Equation 8. This makes sure the model can scale better to higher number of features and still use information from all the features in making split decisions.

\[
o = \left[ \sum_{i=0}^{d} M_i \times R^o_L \quad \sum_{i=0}^{d} M_i \times R^o_R \right] \tag{9}
\]

The output, \( o = [o_L \ o_R] \), of a single decision stump is a vector of two leaf values obtained by combining the leaf responses of each feature using a learned feature mask (Figure 1b). This allows the model to decide which feature to pay more attention to while making a single split decision. Similar to the feature masks in GFLU, these masks are also randomly initialized from different Beta distributions with its two parameters (\( \alpha \) and \( \beta \)) sampled from a uniform distribution \([0.5, 10]\). This encourages diversity of the nodes in the same tree and across different trees as well.

3.2.3. HIERARCHICAL STACKING OF DECISION STUMPS

A decision tree has multiple decision nodes stacked in a hierarchical structure. In standard decision trees, the Heaviside functions cleanly routes samples down the tree to the
terminal nodes. But in the context of soft decision trees the typical way to use the depth is by multiplying leaf probabilities and propagate them all the way down to the terminal nodes (Chen, 2020; Luo et al., 2021). But we found such an approach leads to unstable training, especially when using sparsity inducing activations like the entmax family of activations.

We suggest an alternative approach with which we are using information in a hierarchical way but still avoiding the unstable multiplication of probabilities. We do this by arranging the decision stumps in a structure resembling a perfect binary tree (Zou & Black, 2019; Cormen et al., 2009), and feeding any layer with the original input (residual connection) as well as all the leaf outputs from previous layer (Figure 2). For the i-th level in the decision tree of depth, \( D \), \( \{d_i\}_{i=1}^{D} \), there will be \( 2^{i-1} \) decision stumps and the outputs of each of those decision stumps are collected in a tensor, \( s_{d} \in \mathbb{R}^{2 \cdot 2^{i-1}} \). The input to the decision stumps at any level, \( d \), is the concatenation of the previous layers outputs, \( d_{l-1} \), and the learned features, \( \mathcal{H} \).

Although the number of decision stumps at each level is the same as a perfect binary tree, the connections are not. A perfect binary decision tree passes down information with a strong bias towards left and right, i.e. the left split will route information down to the set of nodes on the left side and the right split does the same towards the right side. But we use both the left and right leaf response as a feature to be used along with the original input to all the decision stumps at a level. Therefore, the input to all the decision stumps at any level is the same but we induce variety in the level by initializing the feature masks to have different Beta distributions. The concatenated outputs from the last level of the tree, \( s_{D} \), is considered the output of the tree, \( O \in \mathbb{R}^{2D} \), where \( D \) is the depth of the tree.

### 3.3. Ensembling multiple trees

Combining predictions of multiple predictors to produce a single predictor is an idea that has been a popular idea in machine learning (Wolpert, 1992; Breiman, 1996; Friedman, 2001). The resulting predictor is typically more accurate than any of the individual predictors in the set. (Popov et al., 2020) stacked many soft oblivious decision trees, feeding the output of the previous tree to the following ones and showed improvements in performance at the cost of training time. Following this principle, our architecture also has multiple DNDTs which are ensembled together in an additive manner.

Let the set of DNDTs in the ensemble be \( T = \{t_{i}\}_{i=1}^{T} \), where each \( t_{i} \) is a DNDT. The set of leaf responses from \( T \) is \( \mathcal{O} = \{O_{i}\}_{i=1}^{T} \) where each \( O_{i} \in \mathbb{R}^{2D} \).
Since all the DNDTs are trained from the same set of features the outputs from the respective trees must have some internal connections and relations. To fully exploit this inter-relation, we use a standard scaled dot product attention (Vaswani et al., 2017) to re-weight the tree outputs.

\[
\hat{O} = \text{softmax} \left( \frac{QK_T}{\sqrt{d_k}} \right) V \text{ where } Q, K, \text{ and } V \in \mathbb{R}^{T \times 2^D}
\]

The resulting output, \( \hat{O} \), is now passed through \( T \) output linear layers, one for each tree, to the desired output vector, \( Y = \{y_i\}_{i=1}^T \), where \( y_i = W_i \hat{O}_i + b_i \). \( W_i \) and \( b_i \) are learnable parameters which transforms the leaf response vector of each tree into the desired output. And the final prediction from the model is obtained by:

**Classification:** \( \hat{y} = \sigma \left( \sum_{i=1}^T \eta_i y_i \right) \) (10)

**Regression:** \( \hat{y} = T_0 + \sum_{i=1}^T \eta_i y_i \) (11)

where \( \eta \) is a learnable parameter which determines how to mix the outputs, \( Y \), and \( \sigma \) is a sigmoid in case of binary classification or a softmax in case of multi-class classification. \( T_0 \) is the average label/target value, which is initialized from training data. \( T_0 \) makes the model robust to the scale of the label, \( Y \), in case of regression.

There are two ways we can construct the additive ensemble from \( T \):

**Bagging (Parallel Trees):** All \( T \) DNDTs are executed in parallel from the same set of inputs and the outputs are combined.

\[
O_i = F_i(H) \text{ where } H \in \mathbb{R}^d
\] (12)

where \( F_i \) is function learned by the \( i \)th DNDT to map \( \mathbb{R}^d \to \mathbb{R}^{2^D} \).

**Boosting (Chained Trees):** Although technically boosting means freezing all the previous stages while training the current one, it introduces too much overhead and technical debt from an implementation point of view. Another alternative is to chain the trees in such a way that the outputs from a tree is fed as an input to tree in the next stage. (Badirli et al., 2020; Popov et al., 2020) takes this approach to good effect and we have adopted the same. Formally it can be seen as:

\[
O_i = F_i([H; O_{i-1}])
\] (13)

where where \( H \in \mathbb{R}^d; O_{i-1} \in \mathbb{R}^{2^D} \) and \([; ;] \) represents a concatenation operation.

In our experiments, we have found out that both these formulations work well, but chaining the trees introduces a bit more computation overhead because of the increase in features the DNDT has to process. Without chaining the trees, we can also leverage parallel processing of the trees to speed up inference.
Gated Additive Tree Ensemble

Table 1. Ranking under Default Hyperparameter Regime.

| Models / Datasets | Aggregate | Classification | Regression |
|-------------------|-----------|----------------|------------|
|                   | Avg Rank  | Forest | Click | A9A | Microsoft | Year |
| GATE              | 1.8       | 1      | 3     | 1   | 3         | 1    |
| LightGBM          | 1.8       | 3      | 1     | 2   | 1         | 2    |
| NODE              | 3.2       | 4      | 2     | 3   | 2         | 5    |
| FT Transformer    | 3.4       | 2      | 4     | 4   | 4         | 3    |
| TabNet            | 4.8       | 5      | 5     | 5   | 5         | 4    |

Table 2. Comparison of DL models under Parameter Matching regime

| Models          | Year | Microsoft | Parameters | MSE  | Forest | Parameters | MSE  | Click | Acc  | Parameters | MSE  | A9A | Acc  | Parameters | MSE  | Acc  |
|-----------------|------|-----------|------------|------|--------|------------|------|-------|------|------------|------|-----|------|------------|------|-----|
| GATE            | 430.51K | 76.782  | 732.50K   | 0.578| 265.02K | 0.9364   | 148.88K| 0.6612 | 636.86K | 0.8503   |
| NODE            | 442.37K | 395.619 | 758.34K   | 0.578| 223.23K | 0.7442   | 151.87K| 0.6528 | 576.13K | 0.7638   |
| FT Transformer  | 441.47K | 84.617  | 739.20K   | 0.5845| 288.00K | 0.95    | 150.80K| 0.6576 | 620.40K | 0.8501   |
| TabNet          | 453.24K | 484.091 | 754.10K   | 0.6494| 256.75K | 0.876   | 140.06K| 0.6517 | 622.96K | 0.7582   |

Table 3. Comparison of DL models under FLOPs Matching regime

| Models          | Year | Microsoft | FLOPs | MSE  | Forest | FLOPs | MSE  | Click | FLOPs | Acc  | Parameters | FLOPs | Acc  | Parameters | FLOPs | Acc  |
|-----------------|------|-----------|-------|------|--------|-------|------|-------|-------|------|------------|-------|------|------------|-------|------|
| GATE            | 18.42M | 76.782  | 35.71M| 0.578| 9.42M  | 0.9364 | 3.89M| 0.6612 | 30.17M| 0.8503 |
| NODE            | 24.73M | 3.96e+6  | 47.10M| 0.585| 13.05M | 0.7445 | 3.78M| 0.653  | 43.78M| 0.7638 |
| FT Transformer  | 25.60M | 86.441  | 51.09M| 0.585| 11.70M | 0.7487 | 4.35M| 0.6576 | 43.00M| 0.8484 |
| TabNet          | 25.11M | 179.914 | 57.58M| 0.704| 11.38M | 0.8024 | 4.11M| 0.648  | 45.39M| 0.7952 |

4. Experiments

In this section, we report the comparison of GATE with other DL models as well as leading GBDT packages. Because of a lack of standardization in the preprocessing, train test split etc. in tabular datasets, we have re-ran all experiments to make sure we are making the right comparisons. We also provide detailed ablation studies to demonstrate the importance of the architecture design decisions. Appendix A has a detailed account of the datasets, models used in the comparison, and the training process.

4.1. Comparison with SOTA

All experiments used PyTorch Tabular (Joseph, 2021) and were run on a single NVIDIA RTX 5000/RTX 4000 GPU with 8 cores and 30GB of RAM. The batch size was chosen such that it was the largest batch which could be fit in a single GPU and wherever possible tried to stick to powers of 2. Initial learning rate was fixed as 1e-3 with a standard Adam optimizer. And Cosine Annealing with Warm Restarts with \( T_0 \) of 50 was used as the learning rate decay for all experiments. The only regularization which was used through out was a weight decay of 1e-5 and early stopping.

We perform our experiments in three regimes:

**Default Hyperparameters**: We compare all the methods using the default hyperparameters. In case of GBDTs, the default hyperparameters have been battle tested to give good performance on a wide variety of datasets. The authors of the other DL models we have considered have also suggested default hyperparameters. The details regarding the default hyperparameters can be found in Appendix A.

**Parameter Matching**: Instead of tuning each model on each dataset, we chose to align the models on something as fundamental as the number of learnable parameters or FLOPs and compare them across different datasets. For this exercise, we use the Lite version of our model for both faster experimentation as well as to put the parameter efficiency to test. The hyperparameters for the Lite version of GATE can be found in Appendix A. In this regime, we matched the learnable parameters as close as possible and evaluate the different DL models on different datasets.

**FLOP Count Matching**: To make the models comparable in computation, we matched the floating point operations (FLOP) across different DL models and evaluated them on different datasets. We used \( \text{fvcore}^1 \) for all the FLOP

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1. https://github.com/facebookresearch/fvcore
calculations. Keeping in mind that the library does not
cover all the operations used in all the models, we have
kept a healthy margin between GATE and the other models
(with GATE being much lower FLOPs) when doing the
comparison. More details can be found in Appendix A.

The results and comparison are summarized in Table 1,
Table 2, Table 3, and Table 5 in Appendix B. For the default
hyperparameter regime we report the ranking of the mean
performance computed over 3 runs with different random
seeds. The actual results with the accuracy’s and MSE’s of
each dataset are included in Appendix B: Table 5.

Key Observations from the results:

- As expected, the performance of all the models vary
  with different datasets. But GATE performance seems
to be varying less wildly than the other DL models
which is apparent in the higher average rank. GATE
performs better than current SOTA (LightGBM) in 3
out of 5 datasets. GATE may not be performing the
best in all the datasets, but it consistently acquires a
position close to the top showing its robustness.

- GATE, when compared to competing DL approaches,
is very stable in achieving errors which are close to
the best, which is very much evident in YEAR dataset.
(Appendix B: Table 5).

- In the parameter matching and FLOP count matching
  regimes (Table 2 and Table 3), GATE dominates the
other competing DL models showing the parameter
and computational efficiencies of GATE architecture.

4.2. Ablation Study

We carried out ablation study to investigate the effect of
different hyperparameters and design choices. We chose the
GATE(Lite) version for these experiments and changed one
parameter at a time to evaluate the results on two datasets -
Forest (Classification) and Year (Regression). We calculated
the accuracy for classification and the mean squared error
for regression tasks. Here are our main findings (Figure 4 in
Appendix B):

- Gated Feature Learning Units (GFLU) seems to be
  the most influential hyperparameter. The accuracy for
  Forest was 0.8 with no GFLUs and 0.91 by using just
  2 GFLUs. But like any other component, without any
  other regularization, increasing the GFLUs will eventu-
  ally hurt test performance.

- Depth of the Trees also seems to have an good ef-
  fect, but not as pronounced as GFLUs. The effect of
  increasing depth also has different effect on different
datasets and has a similar problem with having too
much capacity when it begins to overfit.

- Increasing the number of trees seems to have much
  less of an effect and it’s more about finding that sweet
  spot which is just right for the dataset at hand.

- Self Attention between the tree outputs always seems
to have a positive impact on the test performance.

- Choosing between chaining the trees or using parallel
trees is not apparent and has to be evaluated for
each dataset separately.

- Sparse Activations like entmax or sparsemax always
  leads to better test performance. We have chosen ent-
max because it is a generalization of the sparsemax and
using the parameter $\alpha$ we can move between softmax
and sparsemax. So tuning this parameter to find the
right $\alpha$ value for the dataset seems to be the best bet.

5. Conclusion

We have proposed Gated Additive Tree Ensemble (GATE),
a novel deep learning architecture for tabular data. GATE
uses a gating mechanism, inspired from GRU, as a feature
representation learning unit with an in-built feature selec-
tion mechanism. We combine it with a differentiable, non-
linear decision tree, re-weighted with simple self-attention
to model our desired output. Experiments on several pub-
lic datasets (both classification and regression) verified
that GATE is not only competitive to SOTA approaches
like GBDTs, but also much more parameter and computa-
tionally efficient to competing DL alternatives. Even
though GATE handles more number of features than com-
peting soft tree based models, datasets with huge num-
ber of features would still increase computational require-
ments by many folds. We have made available the code
at https://github.com/manujosephv/GATE un-
der MIT License.

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A. Appendix A: Experiment Details

A.1. Datasets

We have used 5 datasets with varying number of features, training samples, and domain to test the performance of the models:

- **Click** - KDD cup 2012 task 2 (KDD (2012))
- **A9A** - Enhanced Adult Dataset from LibSVM (LIBSVM (1999), Platt (1999))
- **Forest** - Forest Covertype Prediction (Blackard & Dean (2000))
- **Microsoft** - Web 10k dataset from LEarning TO Rank (LETOR) by Microsoft (Qin & Liu (2013))
- **Year** - The Million song Dataset from UCI ML (Bertin-Mahieux (2012))

|             | A9A  | Click | Forest | Microsoft | Year  |
|-------------|------|-------|--------|-----------|-------|
| Training    | 26M  | 800M  | 481M   | 580.5M    | 371M  |
| Validation  | 6.5M | 100M  | 50M    | 142.9M    | 92.7M |
| Test        | 16.3M| 100M  | 50M    | 241.5M    | 51.6M |
| Features    | 123  | 11    | 54     | 136       | 90    |
| Problem     | Classification | Classification | Classification | Regression | Regression |

For datasets under Learning-to-Rank, we have considered them as regression problems. For the datasets which do not have pre-defined test split, we have made the split using stratified sampling. The train, validation and test sizes of all the datasets are available in Table 4. All the test and validation splits of the data are provided as text files in the associated github repository.

A.2. Models

We compare the canonical Accuracy for classification task and Mean Squared Error (MSE) for regression task with the following models. We have used PyTorch Tabular’s (Joseph (2021))\(^2\) implementation of different deep learning models for all the experiments.

- **LightGBM** (Ke et al. (2017)): A fast, distributed, high performance gradient boosting framework.\(^3\) We found that all the GBDT implementations give very comparable scores and picked LightGBM because it gives us good performance with faster training times.
- **TabNet** (Arik & Pfister (2021)): A high-performance and interpretable canonical deep tabular data learning architecture.
- **NODE** (Popov et al. (2020)): An ensemble of oblivious decision trees with end-to-end gradient based learning and hierarchical representation learning.
- **FTTransformer** (Gorishniy et al. (2021)): Feature Tokenizer + Transformer is a simple but effective adaptation of the Transformer architecture for the tabular domain.

A.3. Hyperparameters

These are the default hyperparameters that were used for the experiments:

\(^2\)https://github.com/manujosephv/pytorch_tabular
\(^3\)https://github.com/microsoft/LightGBM
A.3.1. LIGHTGBM:

The default parameters for LightGBM is very well documented here https://lightgbm.readthedocs.io/en/latest/Parameters.html. We have used the same without any changes.

A.3.2. GATE (Default):

- Number of GFLU stages: 6
- Number of Trees: 20
- Depth of a Tree: 5
- Chain Trees: True
- All Dropouts: 0.0

A.3.3. GATE (Lite):

- Number of GFLU stages: 4
- Number of Trees: 30^4
- Depth of a Tree: 5
- Chain Trees: False
- All Dropouts: 0.0

A.3.4. NODE:

- Number of Layers: 1
- Number of Trees: 2048
- Depth of a Tree: 6
- Additional Tree Dimension: 3
- Beta for Threshold Initialization: 1.0
- Beta for Threshold Cutoff: 1.0
- All Dropouts: 0.0

A.3.5. FT TRANSFORMER:

- Input Embedding Dimension: 192
- Number of Attention Heads: 8
- Number of blocks of attention: 3
- Attention Dropout: 0.2
- Feed Forward Dropout: 0.1
- Out Feed Forward Layers: 32
- Out Feed Forward Dropout: 0.0

^4Even though Lite has more number of trees than Default because of not chaining and having lesser depth, it has much lesser capacity than the default model
A.3.6. **TABNET**:

- Prediction Layer Dimension: 8
- Attention Layer Dimension: 8
- Number of successive steps in the network: 3
- Number of independent GLU layer in each GLU block: 2
- Number of shared GLU layer in each GLU block: 2
- Gamma - scaling factor for attention updates: 1.3
- Virtual Batch size for GhostNorm: 128

A.4. **Supported operations for FLOP count**

*fvcore* is a light-weight core library that provides the most common and essential functionality shared in various computer vision frameworks developed in FAIR. Counting the number of floating point operations is a utility that the library provides. Although the library was designed for computer vision models, it still supports quite a bit of basic components. Let’s see the components it supports:

- **nn.Linear**
- **torch.bmm**
- **torch.einsum**
- **torch.matmul**
- and some others specific to computer vision.

Since most of the root components that all the tabular DL models use are also covered here, we decided we can use this to calculate (approximately) the FLOPs for each model. And to be fair and pessimistic in our evaluations, we decided to disadvantage the GATE model by a margin when matching FLOPS with other DL models.

**B. Appendix B: Additional Figures and Results**

**B.0.1. Default Parameter Regime**

We evaluated all the models using the suggested default parameters 3 times using different random seeds and report the mean and standard deviation of Accuracy (classification) or Mean Squared Error (regression). We have chosen Accuracy for the classification problems because all the datasets do not suffer from imbalance and the F1 and Accuracy were painting the same picture.

| Models / Datasets   | Classification | Regression |
|---------------------|----------------|------------|
|                     | Forest         | Click      | A9A        | Microsoft | Year       |
| GATE                | 0.9453±3.7E-3  | 0.6550±3.4E-3 | 0.8505±1.1E-3 | 0.5791±1.8E-3 | 77.8380±1.1E+0 |
| LightGBM            | 0.8562±1.0E-4  | 0.6687±1.3E-4 | 0.8501±0.0E+0  | 0.5638±4.3E-4  | 82.8134±2.1E-2  |
| NODE                | 0.8429±4.1E-2  | 0.6553±1.2E-4 | 0.8501±9.5E-4 | 0.5727±1.8E-3  | 3.65E+6±3.8E+5  |
| FT Transformer      | 0.9263±4.4E-2  | 0.6496±1.1E-2 | 0.8478±4.6E-4 | 0.5995±6.5E-3  | 97.6020±1.9E+1  |
| TabNet              | 0.7514±1.6E-2  | 0.6450±4.0E-3 | 0.7724±1.4E-2 | 0.6391±1.9E-2  | 1.75E+6±4.7E+5  |
Figure 3. Gated Feature Learning Unit. $\otimes$ represents element wise multiplication and $\oplus$ addition

### Table 6. Parameter Matching regime Hyperparameters - NODE

| Hyperparameters / Datasets | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|---------------------------|------|------------|--------|-------|-----|
| Number of Layers          | 1    | 1          | 1      | 1     | 1   |
| Number of Trees           | 1024 | 1200       | 1000   | 1300  | 1100|
| Depth of a Tree           | 4    | 4          | 4      | 4     | 4   |
| Additional Tree Dimension | 3    | 3          | 3      | 3     | 3   |
| Beta for Threshold Initialization | 1.0  | 1.0        | 1.0    | 1.0   | 1.0 |
| Beta for Threshold Cutoff | 1.0  | 1.0        | 1.0    | 1.0   | 1.0 |
| All Dropouts              | 0.0  | 0.0        | 0.0    | 0.0   | 0.0 |

### Table 7. Parameter Matching regime Hyperparameters - FTTransformer

| Hyperparameters / Datasets | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|---------------------------|------|------------|--------|-------|-----|
| Input Embedding Dimension | 64   | 64         | 64     | 64    | 64  |
| Number of Attention Heads | 2    | 8          | 1      | 1     | 8   |
| Number of blocks of attention | 5    | 4          | 3      | 2     | 3   |
| Attention Dropout         | 0.1  | 0.1        | 0.1    | 0.1   | 0.1 |
| Feed Forward Dropout      | 0.1  | 0.1        | 0.1    | 0.1   | 0.1 |
| Out Feed Forward Layers   | 32   | 32         | 32     | 32    | 32  |
| Out Feed Forward Dropout  | 0.0  | 0.0        | 0.0    | 0.0   | 0.0 |

**B.0.2. PARAMETER MATCHING REGIME**

We tweaked the hyperparameters of the competing DL models such that they have the same number of parameters as the GATE(Lite) model. The hyperparameters for the competing DL models which was used under this regime can be found in Tables 6, 7 and 8. Each dataset has a different configuration because the parameters depend on the number of features.

**B.0.3. FLOP COUNT MATCHING REGIME**

We tweaked the hyperparameters of the competing DL models such that they have the same FLOP count as the GATE(Lite) model. The hyperparameters for the competing DL models which was used under this regime can be found in Tables 9, 10 and 11.
Table 8. Parameter Matching regime Hyperparameters - TabNet

| Hyperparameters / Datasets               | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|-----------------------------------------|------|-----------|--------|-------|-----|
| Prediction Layer Dimension              | 64   | 64        | 64     | 64    | 64  |
| Attention Layer Dimension               | 64   | 64        | 64     | 64    | 64  |
| Number of successive steps in the network | 4    | 5         | 2      | 2     | 6   |
| Number of independent GLU layer in each GLU block | 2    | 3         | 2      | 1     | 2   |
| Number of shared GLU layer in each GLU block | 3    | 3         | 2      | 2     | 3   |
| Gamma - scaling factor for attention updates | 1.3  | 1.3       | 1.3    | 1.3   | 1.3 |
| Virtual Batch size for GhostNorm        | 128  | 128       | 128    | 128   | 128 |

Table 9. FLOP count Matching regime Hyperparameters - NODE

| Hyperparameters / Datasets               | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|-----------------------------------------|------|-----------|--------|-------|-----|
| Number of Layers                        | 1    | 1         | 1      | 1     | 1   |
| Number of Trees                         | 700  | 1000      | 500    | 250   | 1000|
| Depth of a Tree                         | 4    | 4         | 4      | 4     | 4   |
| Additional Tree Dimension               | 3    | 3         | 3      | 3     | 3   |
| Beta for Threshold Initialization       | 1.0  | 1.0       | 1.0    | 1.0   | 1.0 |
| Beta for Threshold Cutoff               | 1.0  | 1.0       | 1.0    | 1.0   | 1.0 |
| All Dropouts                            | 0.0  | 0.0       | 0.0    | 0.0   | 0.0 |

Table 10. FLOP Count Matching regime Hyperparameters - FTTransformer

| Hyperparameters / Datasets               | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|-----------------------------------------|------|-----------|--------|-------|-----|
| Input Embedding Dimension               | 8    | 8         | 8      | 16    | 8   |
| Number of Attention Heads               | 2    | 2         | 2      | 1     | 2   |
| Number of blocks of attention           | 1    | 1         | 1      | 1     | 1   |
| Attention Dropout                       | 0.1  | 0.1       | 0.1    | 0.1   | 0.1 |
| Feed Forward Dropout                    | 0.1  | 0.1       | 0.1    | 0.1   | 0.1 |
| Out Feed Forward Layers                 | 32   | 32        | 32     | 32    | 32  |
| Out Feed Forward Dropout                | 0.0  | 0.0       | 0.0    | 0.0   | 0.0 |

Table 11. FLOP Count Matching regime Hyperparameters - TabNet

| Hyperparameters / Datasets               | YEAR | MICROSOFT | FOREST | CLICK | A9A |
|-----------------------------------------|------|-----------|--------|-------|-----|
| Prediction Layer Dimension              | 64   | 64        | 32     | 16    | 64  |
| Attention Layer Dimension               | 64   | 64        | 32     | 16    | 64  |
| Number of successive steps in the network | 2    | 4         | 3      | 5     | 4   |
| Number of independent GLU layer in each GLU block | 2    | 2         | 2      | 2     | 2   |
| Number of shared GLU layer in each GLU block | 2    | 3         | 3      | 3     | 2   |
| Gamma - scaling factor for attention updates | 1.3  | 1.3       | 1.3    | 1.3   | 1.3 |
| Virtual Batch size for GhostNorm        | 128  | 128       | 128    | 128   | 128 |

B.1. Ablation Study

We carried out ablation study to investigate the effect of different hyperparameters and design choices. We chose the GATE(Lite) version for these experiments and changed one parameter at a time to evaluate the results on two datasets - Forest (Classification) and Year (Regression). We calculated the accuracy for classification and the mean squared error for regression tasks. While plotting, we used the primary axis for accuracy and secondary axis for negative MSE so that the directions of improvement remains the same visually. Here are the ranges of different parameters we included in the study.
Gated Additive Tree Ensemble

- # of GFLU stages: $[0, 2, 4, 6]$
- Depth of Trees: $[0, 2, 4, 6]$
- # of Trees in the ensemble: $[5, 10, 15]$
- Self Attention between tree outputs: $[\text{True, False}]$
- Chained or Parallel Trees: $[\text{True, False}]$
- Sparse Activations: $[\text{Softmax-Sigmoid, Entmax1.5-Entmoid1.5, Sparsemax-Sparsemoid}]$

Figure 4. Ablation Study for two datasets - Forest & Year