Gradient Boosting Neural Networks: GrowNet
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Abstract

A novel gradient boosting framework is proposed where shallow neural networks are employed as “weak learners. General loss functions are considered under this unified framework with specific examples presented for classification, regression and learning to rank. A fully corrective step is incorporated to remedy the pitfall of greedy function approximation of classic gradient boosting decision tree. The proposed model rendered state-of-the-art results in all three tasks on multiple datasets. An ablation study is performed to shed light on the effect of each model components and model hyperparameters.

1. Introduction

AI and machine learning pervades every aspect of modern life and email spam filtering, to e-commerce and online advertising, to fraud detection, banking and financial security, to medical diagnostics (McKinney et al., 2020; Simeon et al., 2019). Deep learning in particular has been one of the key innovations that has truly pushed the boundary of science beyond what was considered feasible (He et al., 2016; Goodfellow et al., 2014).

However, in spite of its seemingly limitless possibilities, both in theory as well as demonstrated practice, developing tailor-made deep neural networks for new application areas remains notoriously difficult because of its inherent complexity. Designing architectures for any given application requires immense dexterity and often a lot of luck. The lack of an established paradigm for creating an application-specific DNN presents significant challenges to practitioners, and often results in resorting to heuristics or even hacks.

In this paper, we attempt to rectify this situation by introducing a novel paradigm that builds neural networks from the ground up layer by layer. Specifically, we use the idea of gradient boosting (Friedman, 2001) which has a formidable reputation in machine learning for its capacity to incrementally build sophisticated models out of simpler components, that can successfully be applied to the most complex learning tasks. Popular GBDT frameworks like XGBoost (Chen & Guestrin, 2016), LightGBM (Ke et al., 2017) and CatBoost (Prokhorenkova et al., 2018) use decision trees as weak learners, and combine them using a gradient boosting framework to build complex models that are widely used in both academia and industry as a reliable workhorse for common tasks in a wide variety of domains.

However, while useful in their own right, decision trees are not universally applicable, and there are many domains—especially involving structured data—where deep neural networks perform much better (Zoph et al., 2019; Yang et al., 2019; Bao et al., 2019). In this paper, we combine the power of gradient boosting with the flexibility and versatility of neural networks and introduce a new modelling paradigm called GrowNet that can build up a DNN layer by layer. Instead of decision trees, we use shallow neural networks as our weak learners in a general gradient boosting framework that can be applied to a wide variety of tasks spanning classification, regression and ranking. We introduce further innovations like adding second order methods to the training process, and also including a global corrective step that has been shown, both in theory (Zhang & Johnson, 2014) and in empirical evaluation, to provide performance lift and precise fine-tuning to the specific task at hand.

Our specific contributions are summarised below:

- We propose a novel approach to combine the power of gradient boosting to incrementally build complex deep neural networks out of shallow components. We introduce a versatile framework that can readily be adapted for a diverse range of machine learning tasks in a wide variety of domains.
- We develop an off-the-shelf optimisation algorithm that is faster and easier to train than traditional deep neural networks.
- We introduce training innovations including second order methods and global corrective steps that improve stability and allow finer-grained tuning of our models for specific tasks.
• We demonstrate the efficacy of our techniques using experimental evaluation, and show state-of-the-art results on multiple real datasets in three different ML tasks: classification, regression and learning-to-rank.

2. Preliminaries and Related Work

In this section, we briefly summarize the gradient boosting algorithms with decision trees and general boosting/ensemble methods for training neural nets.

2.1. Gradient Boosting Algorithms

Gradient Boosting Machine (GBM) (Friedman, 2001) is a function estimation method using numerical optimization in function space. Unlike parameter estimation, function approximation cannot be solved by traditional optimization methods in Euclidean space. Decision Trees are the most common functions/predictive learners that are used in Gradient Boosting framework. In his seminal paper, (Friedman, 2001) proposed GBDT where decision trees are trained in sequence and each tree is modeled by fitting negative gradients. In recent years, there have been many implementations of GBDT in machine learning literature. Among these, (Tyree et al., 2011) used GBDT to perform learning to rank, (Friedman et al., 2000) did classification and (Chen & Guestrin, 2016; Ke et al., 2017) generalized GBDT for multi-tasking purposes. In particular, scalable framework of (Chen & Guestrin, 2016) made it possible for data scientists to achieve state-of-the-art results on various industry related machine learning problems. For that reason, we took XGBoost (Chen & Guestrin, 2016) as our baseline. Unlike these GBDT methods, we propose gradient boosting neural network where we train gradient boosting with shallow neural nets. Using neural nets as base learners also gives our method an edge over GBDT models where we can correct each previous model after adding new models, referred as corrective step as well as we can propagate information from previous predictors to the next ones.

2.2. Boosted Neural Nets

Although boosting and ensemble methods are popular with weak learners like decision trees, there have been a substantial work done on combining neural nets with boosting/ensemble methods for better performance over single large/deep neural networks. The idea of seeing shallow neural nets as weak learners and combining them constructively started with (Fahlman & Lebiere, 1990). In their pioneering work, fully connected multi-layer perceptrons are trained in a layer-by-layer fashion and added to get cascade-structured neural net. Their model is not exactly a boosting as the final model is a one multi-layer neural network.

In 1990’s, ensemble of neural networks got popular as ensemble methods helped to significantly improve the generalization ability of neural nets. Nevertheless, these methods were simply either majority voting (Hansen & Salamon, 1990) for classification tasks, simple averaging (Opitz & Shavlik, 1996) or weighted averaging (Perrone & Cooper, 1993) for regression tasks. After introduction of adaptive boosting (Adaboost) algorithm (Freund, 1995), (Schwenk & Bengio, 1997) investigated boosting with multi-layer neural networks for character recognition task and achieved remarkable performance improvement. They extended the work to traditional machine learning tasks with variation of Adaboost methods where different weighting schemes are explored (Schwenk & Bengio, 2000). The adaptive boosting can be seen as a specific version of the gradient boosting algorithm where a simple exponential loss function is used (Friedman et al., 2000).

In recent years, there have been some works done to explain the success of deep residual neural networks (He et al., 2016) with hundreds of layers by showing that they can be decomposed into an collection of many short paths rather than a very long one. These short paths do not show strong dependence and they exhibits ensemble-like behavior (Veit et al., 2016). Authors of the work argue that these deeper layers might serve as a bagging mechanism in a similar spirit to random forest classifier. (Olson et al., 2018) even argues that slightly tuning deep neural networks one can get on par results on many real-world datasets from the UCI Machine Learning Repository. Furthermore, they empirically demonstrate that neural networks can be decomposed into an ensemble of sub-networks each of which achieves low training errors. These studies challenge the common belief that neural networks are too strong to serve as weak learners for boosting methods.

Perhaps the most relevant work to ours are (Moghimi et al., 2016; Zhang et al., 2016) where they proposed a framework to combine Gradient Boosting with Convolutional Neural Nets (CNN). (Zhang et al., 2016) trains gradient boosting machine with CNN as a base learner by introducing a custom multi-class softmax loss function for a specific scene classification task in remote sensing domain. (Moghimi et al., 2016), on the other hand, trains each CNN sequentially on the mistakes of the previous networks, similar to Adaboost to perform on solely image classification task. Our method is different from (Zhang et al., 2016; Moghimi et al., 2016) as we propose a more general framework to perform various machine learning tasks like classification, regression and even learning to rank in one place. Moreover, unlike those two methods, we leveraged a corrective step to update previously added predictor parameters and achieved a significant performance boost.
3. Model

In this section, we first describe the basic framework of GrowNet for general loss functions and then we show how the corrective step is incorporated.

The key idea in gradient boosting is to take simple lower-order models as weak learners, and use them as fundamental building blocks to build a powerful higher-order model by sequential boosting using first or second order gradient statistics. We use shallow neural networks (e.g., with one or two hidden layers) as weak learners in this paper. As each boosting step, we augment the original input features with the outputs from the penultimate layer of the current model complexity but it is omitted for simplicity in this work. As the objective we are optimizing is over the functions not on the parameters, traditional optimization tech-

Algorithm 1 Full GrowNet training

**Input:** $f_0(x) = \log(\frac{n_i}{n})$, $\alpha_0$, Training data $D_{tr}$

**Output:** GrowNet $E$

for $k = 1$ to $M$

# Individual model training

Initialize model $f_k(x)$

Calc. 1st order grad.: $g_i = \partial_{\tilde{y}_i}l(y_i, \tilde{y}_i^{(k-1)}) \forall x \in D_{tr}$

Calc. 2nd order grad.: $h_i = \partial^2_{\tilde{y}_i}l(y_i, \tilde{y}_i^{(k-1)}) \forall x \in D_{tr}$

Train $f_k(x)$ by least square regression on $\{x_i, -g_i/h_i\}$

Add the model $f_k(x)$ into the GrowNet $E$

# Corrective step

for epoch = 1 to $T$

Calc. GrowNet output: $\hat{y}_i = \sum_{m=0}^{K} \alpha_m f_m(x_i) \forall x \in D_{tr}$

Calculate Loss from GrowNet: $L = \frac{1}{n} \sum_{i=0}^{n} l(y_i, \hat{y}_i)$

Update model $f_i$ parameters through back-propagation $\forall i \in \{1,...,k\}$

Update step size $\alpha_k$ through back-propagation

end for

end for

3.1. Gradient Boosting Neural Network: GrowNet

Let’s assume a dataset with $n$ samples in $d$ dimensional feature space $D = \{(x_i, y_i) | x_i \in \mathbb{R}^d, y_i \in \mathbb{R}, |D| = n\}$. GrowNet uses $K$ additive functions to predict the output,$$
\hat{y}_i = \mathcal{E}(x_i) = \sum_{k=0}^{K} \alpha_k f_k(x_i), f_k \in \mathcal{F}
$$

where $\mathcal{F}$ is the space of multilayer perceptrons and $\alpha_k$ is the step size (boost rate). Each function $f_k$ represents an independent shallow neural network with a linear layer as an output layer. For a given sample $x$, model calculates the prediction as a weighted combination of scores from all these sequentially trained models.

$$
\mathcal{L}(\mathcal{E}) = \sum_{i=0}^{n} l(y_i, \hat{y}_i)
$$

We may further add regularization term to penalize the model complexity but it is omitted for simplicity in this work. As the objective we are optimizing is over the functions not on the parameters, traditional optimization tech-
niques will not work here. Analogous to GBDT (Friedman, 2001), the model is trained in an additive manner.

Let \( \hat{y}_i^{(t-1)} = \sum_{k=0}^{t-1} \alpha_k f_k(x_i) \) be the output of the GrowNet at stage \( t-1 \) for the sample \( x_i \). We greedily seek next weak learner \( f_t(x) \) that will minimize the loss at stage \( t \) which can be summarized as

\[
L^{(t)} = \sum_{i=0}^{n} l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i))
\tag{3}
\]

In addition, Taylor expansion of the loss function \( l \) was adopted to ease the computation complexity. As second-order optimization techniques are proven to be superior to first-order ones and require less steps to converge, we trained the models on Newton-Raphson steps. Consequently, regardless of the ML task, individual model parameters are optimized by running regression on second order gradients of the GrowNet’s outputs. The objective function for weak learner \( f_t \) can be simplified as below,

\[
L^{(t)} = \sum_{i=0}^{n} (\hat{y}_i - f_t(x_i))^2
\tag{4}
\]

where

\[
\hat{y}_i = -\frac{g_i}{h_i}
\tag{5}
\]

\( g_i \) and \( h_i \) are the first and second order gradients of the objective function \( l \) at \( x_i \) w.r.t. \( \hat{y}_i^{(t-1)} \). The the pseudo-code of the procedure is explained in Individual model training part of algorithm 1.

3.2. Corrective Step

In traditional boosting framework, each weak learner is greedily learned. This means that only the parameters of \( t^{th} \) weak learner are updated at boosting step \( t \) where all the parameters of previous \( t-1 \) weak learners remain unchanged. The myopic learning procedures may cause the model to stuck in a local minimal and fixed boosting rate \( \alpha_k \) aggravates the issue (Friedman, 2001). Therefore, we implemented a corrective step to address this problem. In the corrective step, instead of fixing the previous \( t-1 \) weak learners, we allow updating of the parameters of the previous \( t-1 \) weak learner through back-propagation. Moreover, we incorporated the boosting rate \( \alpha_k \) into parameters of the model and it is automatically updated whenever corrective step is executed. On top of getting better performance, this move saves us from tuning a delicate parameter. The usefulness of this step is empirically and theoretically investigated in (Zhang & Johnson, 2014) for gradient boosting decision tree models. Our experiments in ablation section further validate the necessity of corrective step in our model as well. The corrective step is summarized in the second part of algorithm 1.

4. Applications

In this section, we show how GrowNet can be adapted for regression, classification and learning to rank problems.

4.1. GrowNet for Regression

We employ mean squared error loss function for regression task. Let’s assume \( l \) is mean squared loss and we can easily obtain \( \hat{y}_i \), first order and second order statistics at stage \( t \) as following:

\[
g_i = 2(\hat{y}_i^{(t-1)} - y_i), \quad h_i = 2
\]

\[
\tilde{y}_i = y_i - \hat{y}_i^{(t-1)}
\]

Then we train next weak learner \( f_t \) by least square regression on \( \{x_i, \tilde{y}_i\} \) for \( i = 1, 2, ..., n \). In the corrective step, all model parameters in GrowNet are updated again using MSE loss.

4.2. GrowNet for Classification

For the illustration purpose, let’s take binary cross entropy loss function to start with, yet note that any differentiable loss function can be used. Choosing labels \( y_i \in \{-1, +1\} \) (this notation has an advantage of \( \bar{y}_i^2 = 1 \) which will be used in the derivation), the first and second order gradients, \( g_i, h_i \), at stage \( t \) can be written as below,

\[
g_i = \frac{-2y_i}{1 + e^{2y_i\tilde{y}_i^{(t-1)}}}, \quad h_i = \frac{4y_i^2e^{2y_i\tilde{y}_i^{(t-1)}}}{(1 + e^{2y_i\tilde{y}_i^{(t-1)}})^2}
\]

\[
\tilde{y}_i = -\frac{g_i}{h_i} = y_i(1 + e^{-2y_i\tilde{y}_i^{(t-1)}})/2
\]

The next weak learner \( f_t \) is fitted by least square regression using second order gradient statistics on \( \{x_i, \tilde{y}_i\} \). In the corrective step, parameters of all predictive functions added are updated by retraining the whole model using binary cross entropy loss. This step slightly corrects weights according to the main objective function of the task at hand, in this case classification.

4.3. GrowNet for Learning to Rank

In this part, we demonstrate how the model executes on learning to rank with a pairwise loss. In learning to rank (L2R) framework, there are queries and documents associated with each query. A document can be associated to many different queries. And for each query, the associated documents have relevance score. Assume for a given query, a pair of documents \( U_i \) and \( U_j \) is chosen. Assume further that we have a feature vector for these documents, \( x_i \) and \( x_j \). Let \( \hat{y}_i \) and \( \hat{y}_j \) denote the output of the model for samples \( x_i \) and \( x_j \) respectively. A common pairwise loss for a given
query can be formulated as below (Burges, 2010),
\[
l(\hat{y}_i, \hat{y}_j) = \frac{1}{2}(1 - S_{ij})\sigma_0(\hat{y}_i - \hat{y}_j) + \log(1 + e^{-\sigma_0(\hat{y}_i - \hat{y}_j)})
\]
where \(S_{ij} \in \{0, -1, +1\}\) denotes the documents’ relevance difference: it is 1 if the \(U_i\) has a relevance score greater than \(U_j\), \(-1\) vice-versa and 0 if both document have been labeled with the same relevance score. \(\sigma_0\) is the sigmoid function. Note that the cost function \(l\) is symmetric and gradients can be easily computed as below, (for the details reader can refer to (Burges, 2010))
\[
\begin{align*}
\partial_{\hat{y}_i} l(\hat{y}_i, \hat{y}_j) &= \sigma_0(\frac{1}{2}(1 - S_{ij}) - \frac{1}{1 + e^{\sigma_0(\hat{y}_i - \hat{y}_j)})}) \\
&= - \partial_{\hat{y}_j} l(\hat{y}_i, \hat{y}_j) \\
\partial_{\hat{y}_i}^2 l(\hat{y}_i, \hat{y}_j) &= \sigma_0^2(\frac{1}{1 + e^{\sigma_0(\hat{y}_i - \hat{y}_j)})}(1 - \frac{1}{1 + e^{\sigma_0(\hat{y}_i - \hat{y}_j)})})
\end{align*}
\]
where \(I\) denotes the set of pairs of indices \(\{i, j\}\), for which \(U_i\) is desired to be ranked differently from \(U_j\) for a given query.

Then for a particular document \(U_i\), loss function and its first and second or statistics can be derived as below,
\[
l = \sum_{j: \{i,j\} \in I} l(\hat{y}_i, \hat{y}_j) + \sum_{j: \{j,i\} \in I} l(\hat{y}_i, \hat{y}_j)
\]
\[
g_i = \sum_{j: \{i,j\} \in I} \partial_{\hat{y}_i} l(\hat{y}_i, \hat{y}_j) - \sum_{j: \{j,i\} \in I} \partial_{\hat{y}_j} l(\hat{y}_i, \hat{y}_j)
\]
\[
h_i = \sum_{j: \{i,j\} \in I} \partial_{\hat{y}_i}^2 l(\hat{y}_i, \hat{y}_j) - \sum_{j: \{j,i\} \in I} \partial_{\hat{y}_j}^2 l(\hat{y}_i, \hat{y}_j)
\]

5. Experiments

5.1. Experiment Setup

All predictive functions added to the model are multilayer perceptrons with one hidden layer. We generally set the number of hidden layer units to roughly half or less of the input feature dimension. More hidden layers degraded the performance as the model starts overfitting. The additive functions were employed in the experiments for all three tasks. Boosting rate is initially set to 1 and automatically adjusted during corrective step.

We trained each predictive function just 1 epoch and the entire model is also trained 1 epoch during corrective step by stochastic gradient descent with Adam optimizer. Epoch numbers are increased to 2 for ranking task. Increasing the epoch number more than that does not contribute to the performance and higher numbers cause overfitting. We also performed 2D batch normalization for hidden layers.

We designed 2 versions of the model: simple and stacked one. In the simple version input feature for each additive function is kept same yet in the stacked model, as the name suggests, we combined original input features with penultimate layer features from the previous predictor (see Figure 1).

We compared the model performance with XGBoost since similar results are obtain using LightGBM or CatBoost.

5.2. Datasets

We evaluate our model on 5 datasets from 3 different tasks. A brief description of these datasets are presented in Table 1.

We used Higgs Bozon dataset\(^1\) for classification. Higgs data is created using Monte Carlo simulations on high energy physics events. It is a binary event classification data with 28 attributes.

To perform regression, 2 datasets from UCI machine learning repository are randomly selected. The first one is Computed Tomography (CT) slice localization data\(^2\) where the aim is to retrieve the location of CT slices on axial axis. The data was constructed from a set of 53,500 CT images that were taken from 74 different patients (43 male, 31 female).

The second regression dataset is YearPredictionMSD\(^3\) data, subset of Million Song dataset, from UCI repository. The goal is to predict the release year of a song from audio features. Songs are mostly western, commercial tracks ranging from 1922 to 2011, with a peak in the year 2000s.

We choose Yahoo LTRC dataset\(^4\) (Chapelle & Chang, 2011) for learning to rank task to make fair comparison with XGBoost. The dataset has 20K queries each associated with approximately 22 documents. Train-test split from the original paper is preserved. The second benchmark ranking

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\(^1\)https://archive.ics.uci.edu/ml/datasets/HIGGS  
\(^2\)https://archive.ics.uci.edu/ml/datasets/Relative+location+of+CT+slices+on+axial+axis  
\(^3\)https://archive.ics.uci.edu/ml/datasets/YearPredictionMSD  
\(^4\)https://webscope.sandbox.yahoo.com/catalog.php?datatype=c
dataset we used is MSLR-WEB 10K⁵ in which there are 10K queries, each corresponding to list of 100 – 200 documents.

5.3. Regression

Table 3 reports regression performance from GrowNet and XGBoost on two UCI datasets. GrowNet outperforms XGBoost on both datasets, in particular, our model displays 17% decrease in RMSE on CT slice localization dataset.

Table 3. Regression results, in root mean square error (RMSE), on music release year and slice localization datasets from UCI ML repository. GrowNet results are average of 5 iterations and the values in the parenthesis represents the standard deviation.

|                         | Music Year Prediction | Slice Localization |
|-------------------------|-----------------------|--------------------|
| XGBoost                 | 8.9301                | 6.6744             |
| GrowNet                 | 8.8156 (0.0061)       | 5.5420 (0.2022)    |

5.4. Classification

To make a fair comparison with XGBoost, we tested our model on Higgs bozon dataset. Classification results are presented in the Table 4. GrowNet clearly outperforms XGBoost using all the data. Subsampling 10% of the data for training each weak learner also renders better performance. We used 30 weak learners (multilayer perceptrons with one hidden layer of 16 units) and the number of the weak learners to be used in test time is chosen by validation results. In all 3 experiments, this number was chosen 30 by cross validation.

Table 4. Classification results, in AUC, on Higgs bozon dataset. For our model, we preset 3 different results: using all the data, 10% of the data (1M), and 1% of the data (100K).

|                         | Higgs Bozon |
|-------------------------|-------------|
| XGBoost                 | 0.8304      |
| GrowNet (all data)      | 0.8510      |
| GrowNet (data sampling= 10%) | 0.8439     |
| GrowNet (data sampling= 1%)  | 0.8180     |

were enough.

6. Ablation study

We explored different components of GrowNet. We picked 2 datasets for these experiments: Higgs and Microsoft. For Higgs dataset, we picked randomly 1M points for training, 5% of the remaining as a validation set and original test data was used as it is. For Microsoft dataset we used Fold 1 and original split was preserved. In all upcoming experiments, only the component that is being analyzed is altered, the rest of the parameters is kept unchanged. All ablation experiments are reported in Table 5 and the third column (GrowNet) represents the results from final version of our model on these datasets.

6.1. Stacked versus simple version

As it is observed from Figure 1, every weak learner except the first one is trained on combined features from original input and penultimate layer features from previous predictive function. These features leveraged our model by propagating the information from previous model to the new one. To test the advantage of this stacked model, we compared the proposed model against its simple version in which original input features are used for all learners. The sixth row in Table 5 displays the results from simple version. In both tasks, stacked version outperforms simple version, specially, the difference is noteworthy in ranking task. Training loss from Figure 2 also validates the information gain while stacked version is utilized. Unlike tree boosting methods, our model made this architecture possible through its flexible weak learners.
Table 5. Ablation study experiment results on Higgs 1M and Microsoft (Fold 1) datasets. All models have shallow network with one hidden layer. Hidden layer dimension is 16 for classification and 64 for ranking task. The third column is the final GrowNet model that all different versions are compared against. Reported results are AUC scores for classification and NDCG for ranking.

| Datasets | Eval. metric | GrowNet | 1st order grad. | Constant α | Simple version | No corrective step | C/s in every 5 stage |
|----------|--------------|---------|----------------|------------|---------------|-------------------|-------------------|
| Higgs 1M | AUC          | 0.8385  | 0.8363         | 0.8396     | 0.8326        | 0.8093            | 0.8315            |
| MSLR Fold1 | NDCG@5     | 0.5106  | 0.5001         | 0.5005     | 0.4836        | 0.4743            | 0.4881            |
|          | NDCG@10     | 0.5195  | 0.5104         | 0.5081     | 0.4972        | 0.4872            | 0.4998            |

Figure 2. Training loss visualization. For the learning to rank part we used pairwise loss.

6.2. Analyzing corrective step

Perhaps among all components of the model, corrective step is the most vital one. In this procedure, parameters of all weak learners added to the model are updated by training the whole model on original inputs without penultimate layer features. The loss function used in this step is a task specific one. This practise allows the model to rectify the parameters to specifically better accommodate the task at hand rather than fitting negative gradients. Moreover, within this step, we incorporated the boosting rate $\alpha_t$ and it is automatically adjusted without needing any tuning. The last two rows of the Table 5 present the classification and learning to rank results from GrowNet without using any corrective step and using corrective step in every 5 stage, respectively. The performance is severely degraded in the former one and the model hardly learned any information after couple predictive functions added. Flat training loss in Figure 2 confirms this phenomenon as well. Running corrective step in every 5 step rendered much better performance yet not as good as running it in every stage. Stair-like loss curve in the Figure 2 plainly displays the influence of corrective step on model training.

6.3. First order statistics vs second order statistics

In this experiment, we explored the impact of first and second order statistics on model performance as well as on the convergence of training loss. As the forth row of Table 5 displays, using second order (third row in the table 5) renders a slight performance boost over first order in classification and almost 2% increase in learning to rank task. Figure 2 displays effects of order statistics on training loss. Final model (with second order statistics) again shows slightly better convergence on classification yet the difference is more apparent on ranking. As learning rate is decreased by a rate of 0.167 per 15 weak learners, sudden drops are observed in classification loss curve at 15th and 30th stages in Figure 2 (a).

6.4. Dynamic boost rate

Within the corrective step, we are able to dynamically update the boost rate $\alpha_t$ (at stage $t$). Taking this measure saved us from tuning one more parameter as well as yielded a mild performance increase in all tasks. Moreover, the model obtained better training loss convergence compared to constant boost rate which is set to 1 in this experiment (see Figure 2). In our setup, starting with $\alpha_0 = 1$, the boost rate is automatically updated each time the corrective step is executed. Constant boost rate result is reported in fifth row of Table 5.
6.5. Analyzing the effect of hidden layers

As the literature suggests, boosting algorithms work best with weak learners, thus we utilized very shallow neural network with one hidden layer as a weak predictor for our model. Once more hidden layers are added, it would yield stronger predictor, nevertheless, it doesn’t serve as a weak learner anymore. Figure 3 (a) demonstrates training loss with test AUC scores from GrowNet with 1, 2, 3, and 4 hidden layers. Each hidden layer has 16 units. Although more hidden layers render better training loss convergence as expected, the model starts overfitting. The worst test AUC score is from the model with 4 hidden layers shown by red arrow. With no hidden layer, model struggles to learn anything and training loss starts oscillating and never converges. Performance significantly drops as well.

Altering the number of hidden units has lesser effect on the performance. To illustrate the impact of hidden layer dimension, we tested the final model (weak learner with one hidden layer and 16 hidden units) with various hidden units. Higgs data has 28 features and we tested the model with 2, 4, 8, 16, 32, 64, 128 and 256 hidden units. The smaller hidden layer dimension is, the less information propagation weak learners gets. On the other hand, having more units also leads to overfitting after certain point. Figure 3 (b) displays test AUC scores from this experiment on Higgs 1M data. The highest AUC of 0.8478 is achieved with 128 units yet increasing the number to 256 makes the performance worse.

6.6. GrowNet versus DNN

One might ask what would happen if you just combine all these shallow networks into one deep neural network. There are couple issues with this approach: (1) it is very time-consuming to tune the parameters of DNN, like number of hidden layers, number of units in each hidden layer, overall architecture, batch normalization, dropout level, and etc., (2) DNNs require huge computational power and runs slower. We compared our model (with 30 weak learners) against DNN with 30 hidden layers. DNN produced 0.8301 on Higgs 1M data with 1000 epochs and each epoch took 15 seconds. DNN achieved this score (its best) at epoch 700. GrowNet rendered 0.8385 AUC on the same configuration with 30 weak learners. Each stage including corrective step took 35 seconds. We find that GrowNet has a clear advantage over stacked DNN on all these aspects.

7. Conclusion

In this work, we propose GrowNet, a novel approach to leverage shallow neural networks as “weak learners” in gradient boosting framework. This flexible network structure allows us to perform multiple machine learning tasks under a unified framework while incorporating second order statistics, corrective step and dynamic boost rate to remedy the pitfalls of traditional gradient boosting decision tree. Ablation study is conducted to explore the limits of neural networks as weak learners in boosting paradigm and analyze the effects of each GrowNet component on model performance and convergence. We show that the proposed model achieves better performance in regression, classification and learning to rank on multiple datasets compared to state-of-the-art method. We further demonstrate that GrowNet is a better alternative to DNN in these tasks as it yields better performance, requires less training time, and it is much easier to tune.
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