A Generalized Stacking for Implementing Ensembles of Gradient Boosting Machines *

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Abstract. The gradient boosting machine is one of the powerful tools for solving regression problems. In order to cope with its shortcomings, an approach for constructing ensembles of gradient boosting models is proposed. The main idea behind the approach is to use the stacking algorithm in order to learn a second-level meta-model which can be regarded as a model for implementing various ensembles of gradient boosting models. First, the linear regression of the gradient boosting models is considered as a simplest realization of the meta-model under condition that the linear model is differentiable with respect to its coefficients (weights). Then it is shown that the proposed approach can be simply extended on arbitrary differentiable combination models, for example, on neural networks which are differentiable and can implement arbitrary functions of gradient boosting models. Various numerical examples illustrate the proposed approach.

Keywords: Regression · Gradient Boosting · Stacking · Ensemble · Neural network · Machine learning.

1 Introduction

One of the ways to enhance the machine learning models and to produce improved results is to apply ensemble-based techniques which are based on combining a set of the so-called base or weak models (classifiers, regressors) [18,21,24,25,34]. All approaches to combining models can be conditionally divided into three main groups: bagging, stacking and boosting. The first group consists of bagging methods [5], which are based on using bootstrapped samples. One of the most well-known bagging models is the random forest [7] using a large number of randomly built classification or regression decision trees whose predictions are combined to get the overall random forest prediction. Random forests often use the combination of the bagging and the random subspace method [10] for building trees. In contrast to bagging methods, the boosting assigns weights to elements of a training set in accordance with special rules. One of the first efficient boosting algorithms is AdaBoost [13]. Among boosting methods, we have to highlight the gradient boosting machines (GBMs) [14,15]. In accordance with

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these methods, the training of each base model depends on models that have already been trained. The interpretation of GBMs in terms of regression is the following. By using the first guess as a prediction, the residuals are computed as differences between guessed predictions and target variables. These residuals are used instead of target variables to build the next base model, for example, a regression tree which is used in turn to predict new residuals. The boosting regression model is constructed by means of iterative computing the sum of all previous regression trees and updating residuals to reflect changes in the boosting regression model. In other words, a set of regression trees is computed in the GBM such that each successive tree predicts the residuals of the preceding trees given an arbitrary differentiable loss function \[25\]. The gradient boosting has a lot of modifications. One of the most popular modifications is the XGBoost \[8\] which is much faster than other models. An efficient gradient boosting method is the CatBoost \[9\].

Another interesting ensemble-based technique is stacking \[6,31\]. This technique is used to combine different base models by means of a meta-learner that takes into account which base model are reliable and which are not. One of the combination stacking models is when outputs of the base models are used as training data for the meta-learner to approximate the same target function. A detailed review of stacking algorithms can be found in \[26\].

It should be noted that the above division of the ensemble-based approaches is rather rough because there are models which do not belong to these groups. Moreover, there are a lot of models which can be viewed as a combination of the above approaches, for example, the deep forest or gcForest which was proposed by Zhou and Feng \[35\]. Due to many outperforming properties of the deep forest and due to its architecture which is similar to the multi-layer architecture of neural networks (NNs), several modifications of the deep forest have been developed, for example, \[28,29\]. We have to point out also very interesting combination of ideas of the gradient boosting and the deep forest, which is called as the multi-layered gradient boosting decision tree forest \[11\]. It learns hierarchical distributed representations by stacking several layers of regression gradient boosting decision trees as its building blocks.

A lot of surveys have been published due to remarkable properties of ensemble-based models \[10,12,17,18,21,22,23,32,33\]. Most ensemble-based models are thoroughly studied in Zhou’s book \[34\].

By returning to the GBMs, it should be pointed out that there are some shortcomings of the technique, which are explicitly described by Natekin and Knoll \[19\]. One of the important shortcomings is that there is currently no a fast and efficient model and the corresponding implementation of the smooth continuous base learner that capture interactions between variables which may play a crucial role in the particular predictive model design. Moreover, the GBM can be regarded as a linear combination of base models with some weights, and errors of the base models are correlated for some examples of the training set such that the GBM overfits. In order to overcome this shortcoming, we propose to extend the standard GBM towards constructing ensembles of the models, i.e.,
ensembles of ensembles, to reduce the impact of errors caused by overfitting. The ensemble is organized by using the generalized stacking algorithm where inputs of the meta-model are predictions of the ensemble of GBMs, and the meta-model can be implemented as any differentiable machine learning model, i.e., the ensemble of ensembles of GBMs is constructed by using arbitrary differentiable models, for example, NNs. Moreover, the proposed approach allows us to reduce the number of tuning parameters, that is many parameters become to be trainable. It is important to note that the idea of combination of NNs and GBMs has been considered in literature. In particular, Bilal [4] proposed the so-called deep gradient boosting where the GBM was incorporated into the NN backpropagation algorithm at every layer of the NN for updating the NN weights. Another combination of the GBM and the NN was proposed by Badirli at al. [1] where the authors use shallow NNs as base learners in the GBM. The same combination of the NN and XGBoost was proposed by Weldegebriel et al. [30]. Ideas of the NN and GBM combination have been also studied by other authors, for example, [2,20]. However, our approach differs from the available ones. We apply the NN as a possible tool for implementing the stacking algorithm and the second-level ensemble of GBMs.

The peculiarities of the proposed approach open a door to develop a large class of efficient ensembles of regression gradient boosting models. Various numerical examples illustrate efficiency of the proposed ensembles of GBMs.

The paper is organized as follows. Sections 2 and 3 provide descriptions of the standard regression problem statement and the GBM. An idea of using the stacking algorithm for implementing the linear combination of GBMs is considered in Section 4. An extension of the linear combination of GBMs towards generalization of the proposed approach is given in Section 5. Numerical examples with real data are provided in Section 6. Concluding remarks can be found in Section 7.

2 Regression problem statement

Let us formally state the standard regression problem. Given $N$ training data (examples, instances, patterns) $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, in which $x_i$ may belong to an arbitrary set $\mathcal{X} \subset \mathbb{R}^m$ and represents a feature vector involving $m$ features, and $y_i \in \mathbb{R}$ represents the observed output or target value such that $y_i = f(x_i) + \varepsilon$. Here $\varepsilon$ is the random noise with expectation 0 and unknown finite variance. Machine learning aims to construct a regression model or an approximation $g$ of the function $f$ that minimizes the expected risk or the expected loss function

$$L(f) = \mathbb{E}_{(x,y)\sim P} l(y, g(x)) = \int_{\mathcal{X} \times \mathbb{R}} l(y, g(x)) dP(x,y),$$

with respect to the function parameters. Here $P(x, y)$ is a joint probability distribution of $x$ and $y$; the loss function $l(\cdot, \cdot)$ may be represented, for example, as follows:

$$l(y, g(x)) = (y - g(x))^2.$$
There are many powerful machine learning methods for solving the regression problem, including regression random forests \cite{3,7}, the support vector regression \cite{27}, etc. One of the powerful methods is the gradient boosting \cite{15}, which will be considered below.

3 The gradient boosting algorithm

Let us consider the gradient boosting decision tree algorithm \cite{15}. The algorithm is an iterative construction of a model as an ensemble of base (weak) prediction models built in a stage-wise fashion where each base model is constructed, based on data obtained using an ensemble of models already built on previous iterations, as an approximation of the loss function derivative. A model of the size $M$ is a linear combination of $M$ base models:

$$g_M(x) = \sum_{i=0}^{M} \gamma_i h_i(x), \quad (3)$$

where $h_i$ is the $i$-th base model; $\gamma_i$ is the $i$-th coefficient or the $i$-th base model weight.

The gradient boosting algorithm can be represented as the following steps:

1. Initialize the zero base model $h_0(x)$, for example, with the constant value.
2. Calculate the residual $r_i^{(t)}$ as a partial derivative of the expected loss function $L(x_i, y_i)$ at every points of the training set, $i = 1, ..., N$.
3. Build the base model $h_t(x)$ as regression on residuals $\{(x_i, r_i^{(t)})\}$;
4. Find the optimal coefficient $\gamma_t$ at $h_t(x)$ regarding the initial expected loss function \cite{5};
5. Update the whole model $g_t(x) = g_{t-1}(x) + \gamma_t h_t(x)$;
6. If the stop condition is not fulfilled, go to step 2.

Here the loss function depends on the machine learning problem solved (classification or regression). Let us consider all the above in detail. Suppose that $(M - 1)$ steps produce the model $g_{M-1}(x)$. For constructing the model $g_M(x)$, the model $h_M(x)$ has to be constructed, i.e., there holds

$$g_M(x) = \sum_{t=1}^{M} \gamma_t h_t(x) = g_{M-1}(x) + \gamma_M h_M(x). \quad (4)$$

The dataset for constructing the model $h_M(x)$ is chosen in such a way as to approximate the expected loss function partial derivatives with respect to the function of the already constructed model $g_{M-1}(x)$. Let us denote residuals $r_i^{(M)}$ defined as the values of the loss function partial derivative at point $g_{M-1}(x_i)$ in the current iteration $M$,

$$r_i^{(M)} = - \frac{\partial L(z, y_i)}{\partial z} \bigg|_{z = g_{M-1}(x_i)}. \quad (5)$$
By using the residuals, a new training set \( D_M \) can be formed as follows:

\[
D_M = \left\{ \left( x_i, r_i^{(M)} \right) \right\}_{i=1}^{N}.
\]  

and the model \( h_M \) can be constructed on \( D_M \) by solving the following optimization problem

\[
\min_N \sum_{i=1}^{N} \left\| h_M(x_i) - r_i^{(M)} \right\|^2.
\]  

Hence, an optimal coefficient \( \gamma_M \) of the gradient descent can be obtained as:

\[
\gamma_M = \arg \min_{\gamma} \sum_{i=1}^{N} L \left[ g_{M-1}(x_i) + \gamma h_M(x_i), y_i \right].
\]  

Then we get the following model at every point \( x_i \) of the training set

\[
g_M(x) = g_{M-1}(x) + \gamma_M h_M(x) \approx g_{M-1}(x) - \gamma_M \frac{\partial L(z, y_i)}{\partial z} \bigg|_{z=g_{M-1}(x)}.
\]  

If the loss function is the squared difference, then minimizing (7) corresponds to minimizing the loss function. This implies that choice of the optimal step \( \gamma_M \) is not required, and its value is 1. In order to reduce overfitting, the step \( \gamma_M \) is reduced by its multiplying by a constant called the learning rate. By introducing the learning rate, it is possible to reduce the impact of model \( h_M \) errors on the ensemble error.

The above algorithm allows us to minimize the expected loss function by using decision trees as base models. However, it requires to select the decision tree parameters, for example, depths of trees, as well as the learning rate, in order to simultaneously provide a high generalization and accuracy depending on an specific task.

The gradient boosting algorithm is a powerful and efficient tool for solving regression problems, which can cope with complex non-linear function dependencies \[19\]. However, it has a number of shortcomings. One of them is caused by the “greedy” concept used in the model implementation. The GBM \( g_M(x) \) constructed using the above algorithm is itself an ensemble of base models, i.e., a linear combination of base models with given weights \( \gamma_i \). However, each model is regarded as the “greedy” one, which means that errors of base models are correlated in the worst case when the base models are poorly approximating residuals for a set of points. As a result, the loss function can be minimized in the vicinity of such points only by overfitting. Therefore, it makes sense to construct ensembles of GBMs in order to reduce the variance of the error caused by overfitting.

4 An ensemble of GBMs

The main idea behind the construction of a more accurate ensemble of GBMs is to apply the stacking algorithm \[31\] which trains the first-level learners using
the original training dataset. The stacking algorithm generates a new dataset for training the second-level learner (meta-model) such that the outputs of the first-level learners are regarded as input features for the second-level learner while the original labels are still regarded as labels of new training data.

Let us compose an ensemble $E^K_M(x)$ of $K$ GBMs of the size $M$. It can be represented as follows:

$$E^K_M(x) = \left( g^{(j)}_M(x) \right)_{j=1}^K. \quad (10)$$

First, we consider a linear regression model for implementing the meta-model of the stacking algorithm, which is of the form:

$$S_w(t) = t \cdot w + b = \sum_{j=1}^K t_j w_j + b, \quad (11)$$

where $w = (w_1, ..., w_K) \in \mathbb{R}^K$ is a vector of weights; $t = (t_1, ..., t_K) \in \mathbb{R}^K$ is a vector of the ensemble model predictions; $b$ is the bias.

We will assume for simplicity purposes that the bias $b$ is zero. Weights of the linear regression model can be computed by means of the standard well-known approaches depending on the regularization method used (the $L_1$ or $L_2$ norms). Suppose that a differentiable expected loss function $L(\hat{y}, y)$ is given, where $y$ is a true class label, $\hat{y}$ is the model prediction. Let us set the initial approximation of the weights $w^{(0)}$. We are searching for the optimal vector of weights using the gradient descent:

$$w^{(q)} = w^{(q-1)} - \alpha \frac{1}{N} \sum_{i=1}^N \nabla_w L \left( S_w \left( E^K_M(x_i) \right), y_i \right) \bigg|_{w=w^{(q-1)}}. \quad (12)$$

Here $S_w \left( E^K_M(x_i) \right)$ is the prediction of the ensemble for the input feature vector $x_i$.

Note that the model $S_w(t)$ is differentiable both by the vector of weights and by the vector $t$ of the ensemble predictions. It has been shown that the use of the gradient boosting algorithm allows us to minimize the differentiable loss functions by constructing new models approximating values proportional to their derivatives. We will use this peculiarity to optimize not only linear regression weights, but also the ensemble of GBMs.

Let us define a new differentiable loss function as follows:

$$\mathcal{L}(t, y) = L \left( S_w(t), y \right). \quad (13)$$

Intuitively, such a loss functional “hides” the linear regression block $S_w$. Since the gradient boosting algorithm allows iteratively minimizing an arbitrary differentiable loss function, we apply it to minimize $\mathcal{L}$. Each GBM in the ensemble minimizes the corresponding loss function:

$$\mathcal{L}_i(t_i, y) = L \left( S_w(t_i), y \right). \quad (14)$$
By using gradient boosting for each fixed set of weights of the linear model, we can construct such an ensemble of GBMs, which minimizes the loss function \( \mathcal{L}(z, y_i) \) and can be determined for a fixed ensemble of GBMs. We combine these two steps into one step, i.e., we simultaneously optimize weights of the linear model and construct the ensemble of GBMs.

Suppose that an ensemble of \( K \) GBMs is composed such that every its GBM is initialized by a constant value, for example, by the mean value of the corresponding target variable. Initial weights of the linear model are set as:

\[
  w^{(0)} = \frac{1}{K}.
\]

(15)

Denote the residual of the \( j \)-th GBM for point \( x_i \) at step \( q \) as \( r_{i,j}^q \), and differentiate the loss function \( \mathcal{L} \) as:

\[
r_{i,j}^q = -\frac{\partial \mathcal{L}(t, y_i)}{\partial t_j} \bigg|_{t = E_{q-1}^K(x_i)} - \frac{\partial L(z, y_i)}{\partial z} \bigg|_{z = S_w(t)} \cdot \frac{\partial S_w(t)}{\partial t_j} \bigg|_{t = E_{q-1}^K(x_i)}.
\]

(16)

The partial derivative with respect to the \( j \)-th component of the linear regression model is nothing else but the weight \( w_j\) in (11) corresponding to this component. Hence, there holds:

\[
r_{i,j}^q = -\frac{\partial L(z, y_i)}{\partial z} \bigg|_{z = S_w(t)} \cdot w_j^{(q-1)}.
\]

(17)

Let us construct a function which approximates residuals as:

\[
h_j^q(x) = \arg \min_{h \in \mathcal{F}} \sum_{i=1}^{N} \left\| h(x_i) - r_{i,j}^q \right\|^2,
\]

(18)

where \( \mathcal{F} \) is a set of admissible functions.

We simultaneously optimize weights of the linear model and each GBM in the ensemble as follows:

\[
\begin{align*}
  w^{(q)} &= w^{(q-1)} - \alpha \frac{1}{N} \sum_{i=0}^{N} \nabla_w L \left( S_w \left( E_{q-1}^K(x_i) \right), y_i \right) \bigg|_{w = w^{(q-1)}} ,
  
  g_{(j)}^{(q)} &= g_{(j)}^{(q-1)} + \gamma_q h_j^q(x).
\end{align*}
\]

(19)

For simplicity, \( \gamma_q \) will be taken identical for all models and iterations. In sum, the learning algorithm consists of the following steps:

1. Initialize an ensemble of \( K \) GBMs.
2. Initialize model weights \( S_w \).
3. Until the stop condition is fulfilled, at step \( q \):
   
   (a) calculate the partial derivative of the loss function by weights of the linear model;
(b) calculate the residuals $r_{i,j}^q$;
(c) construct base models $h_{q}^j(x)$ approximating the corresponding residues $r_{i,j}^q$.

The resulting model will be called as an adaptive ensemble of GBMs because each member of the GBM ensemble adapts to a new loss function corresponding to each iteration.

It should be noted that results of the traditional gradient boosting algorithm are strongly influenced by the choice of parameters of base models (decision trees). For every specific problem, the most appropriate parameters exist. However, it is necessary to construct the GBM many times to find the parameters and to apply one of the evaluation methods, for example, the cross-validation method. In the adaptive ensemble of GBMs, many different parameters of the base models can be immediately included as follows. In each GBM of the ensemble, we use a unique set of parameters corresponding to the GBM throughout the entire training of the ensemble. As a result of training, the largest weights are assigned to models with the most appropriate parameters.

As a rule, decision trees in traditional gradient boosting algorithms are used as base models. In order to construct a model $h_{q}^j(x)$ approximating the residuals $r_{i,j}^q$, a tree is built that minimizes the quadratic norm of the difference between the model predictions and the residual (18). The decision tree model approximating residuals implements a piecewise constant function with a small number of unique values. That is, at each iteration of the ensemble training, accuracy of a prediction of the partial derivative of the loss function (17) is not high. Moreover, it is difficult to control the accuracy of the approximation under condition of a fixed tree depth for each specific GBM. Hence, ensembles of GBMs with a larger depth of trees will learn “faster” than GBM with a smaller depth, although trees of a smaller depth may be more preferable for a specific task. The basic idea behind the problem solution is to use more complex base models, namely, GBMs. Such models allow us to approximate the residuals with a higher accuracy by using trees of a fixed depth. It is important to note that the ensemble of GBMs, which uses GBMs as base models, is also a linear combination of decision trees, however, the algorithm at each step more accurately approximates the partial derivative of the loss function (14).

Let us consider various ways for initializing an ensemble of deep GBMs:

1. An exact initialization using the training set: each GBM is constructed by optimizing the loss function $L$ directly over a certain number of iterations $M_{init}$. The larger the number of iterations, the greater the correlation between the model predictions.
2. A random initialization: each GBM includes only a single base model built on the basis of the training set where values of free variables repeat those of $D$, and reference values of the target variable are selected as observations of a random variable from the normal distribution whose parameters, the mean and the variance, coincide with the sample mean and the sample variance of the reference target variable.
3. An exact initialization using subsets of the training set: in order to get the most diverse GBMs in the ensemble (the diversity reduces the correlation of the model prediction errors), the GBMs can be constructed on pairwise disjoint subsets of the training set.

4. An initialization with the average value of the target variable.

Weights of the linear model can be initialized with optimal values under condition that the ensemble of GBMs is fixed.

5 Generalization of the GBM ensemble

Note that only a few conditions have to be fulfilled for training the aggregate model by means of the proposed algorithm:

– the loss function $L$ has to be differentiable;
– the model $S_w(t)$ has to be differentiable with respect to the parameter $w$ and the argument $t$.

This implies that the obtained approach can be generalized by replacing the linear regression model with an arbitrary differentiable model $S^K_w(t)$, whose input is a vector of size $K$. The learning procedure for the model $S^K_w(t)$ can be carried out not only by gradient descent, but also by another algorithm, for example, by means of the support vector method. However, the model in this case has to be rebuilt after each update of the ensemble of GBMs. Therefore, we will consider only differentiable models $S^K_w(t)$ from the class of NNs of forward propagation $F$:

$$F = \{ f : \mathbb{R}^I \times \Theta \rightarrow \mathbb{R}^T \} , \quad (20)$$

where $I$ is the dimensionality of the NN input space; $\Theta$ is the set of admissible parameters of the NN; $T$ is the dimensionality of the target variable.

Any method of initializing the GBM ensemble among the considered above can be used for the case $T = 1$, and the dimension of the input space is equal to the number of models: $I = K$. If $T > 1$, then it is possible to exactly initialize every GBM in the ensemble using the training set only by constructing models with several outputs such that every GBM is a function whose values are in a space of dimension $T$. In this case, there holds $I = T \cdot K$, and the prediction of the GBM ensemble is the concatenation of predictions of every GBM. In the case of large values of $T$, construction of the GBM ensemble with several outputs may be computationally expensive. For example, if the target variable corresponds to images of sizes $100 \times 100$, and the ensemble contains 100 GBMs, then the dimension of the input space of the NN will be $10^6$. When the size of the training set is equal to 1000 in this case, the number of values that should be fed to the NN input is one billion. Therefore, it makes sense in such cases to use the random initialization which allows us to directly control the value of $I$ by setting the number of models $K$.

We can construct a model on the basis of the proposed algorithm using both the advantages of learning algorithms for base models, for example, for
decision trees, and the advantages of differentiable models, including the NN. The GBM ensemble is actually a mapping from the original feature space into a new intermediate space of dimension $I$, which is more informative in the context of a specific problem. Moreover, such the GBM ensemble has the following advantages of traditional ensembles based on decision trees:

- possibility of training the ensemble of trees on a sample of small dimension;
- interpretability of models, in particular, an assessment of the effects of specific features of input data on predictions;
- availability of deterministic algorithms for constructing decision trees;
- lack of assumptions about the existence of a linear relationship between features.

Note that the aggregate model inherits a part of the above properties, namely the interpretability and the lack of assumptions about the existence of a linear relationship between features, while the useful properties of the NN are potentially preserved, including generating high-dimensional outputs (for example, images), simultaneous solving several types of tasks (multi-task learning), parameterizing the loss function of a neural network, and so on. But it is very important that the number of NN parameters can be reduced, and, as a result, the NN can be trained on small samples because processing of the initial features is carried out to the NN.

6 Numerical experiments

In order to illustrate the proposed approach, we investigate the model for real data sets from the R Package “datamicroarray” which contains DNA microarrays. Table 1 is a brief introduction about the investigated datasets, while more detailed information can be found from, respectively, the data resources. Table 1 shows the number of features $m$ for the corresponding data set, the number of examples $n$ and the number of classes $C$. All these datasets are for solving the classification task. It can be seen from Table 1 that the number of features of every dataset is much more than the number of training examples. Accuracy measure $A$ used in numerical experiments is the proportion of correctly classified cases on a sample of data. To evaluate the average accuracy, we perform a cross-validation with 100 repetitions, where in each run, we randomly select $n_{\text{tr}} = 3n/4$ training data and $n_{\text{test}} = n/4$ testing data.

Numerical results of the DNA microarray classification are shown in Table 2. Four models are compared: the linear ensemble of GBMs (Linear GBM) in accordance with (11); combination of the NN and ensemble of GBMs (NN+GBM), the standard GBM and the random forest with the numbers of decision trees equal to 100 or 1000. The learning rates $0.1$ or $0.01$ are taken for training GBMs. Ensembles of GBMs consist of 20 machines with depths of trees from 2 to 21. The epoch number is 10, and the learning rate of every ensemble is 0.05. The fully connected NN having 3 layers of size 10 with tanh as an activation functions. The best performance for each dataset is shown in bold. It can be seen from
Table 1. A brief introduction about the DNA microarray data sets

| Data set     | Type                | m   | n   | C  |
|--------------|---------------------|-----|-----|----|
| Alon         | Colon Cancer        | 2000| 62  | 2  |
| Borovecki    | Huntington’s Disease| 22283| 31 | 2  |
| Chin         | Breast Cancer       | 22215| 118| 2  |
| Chowdary     | Breast Cancer       | 22283| 104| 2  |
| Golub        | Leukemia            | 7129| 72  | 3  |
| Gravier      | Breast Cancer       | 2905| 168| 2  |
| Pomeroy      | CNS Disorders       | 7128| 60  | 2  |
| Nakayama     | Sarcoma             | 22283| 105| 10 |
| Sorile       | Breast Cancer       | 456 | 85  | 5  |
| Singh        | Prostate Cancer     | 12600| 102| 2  |

Table 2. Comparison of four models on the DNA microarray datasets

| Data set     | Linear GBM | NN + GBM | GBM     | Random Forest |
|--------------|------------|----------|---------|---------------|
| Alon         | 0.708      | 0.833    | 0.771   | 0.762         |
| Borovecki    | 0.979      | 1.000    | 0.958   | 0.929         |
| Chin         | 0.978      | 0.894    | 0.900   | 0.933         |
| Chowdary     | 0.987      | 1.000    | 0.962   | 0.992         |
| Golub        | 0.861      | 0.991    | 0.889   | 0.911         |
| Gravier      | 0.730      | 0.766    | 0.778   | 0.748         |
| Pomeroy      | 0.511      | 0.422    | 0.556   | 0.453         |
| Nakayama     | 0.577      | 0.590    | 0.526   | 0.585         |
| Sorile       | 0.627      | 0.714    | 0.683   | 0.857         |
| Singh        | 0.929      | 0.897    | 0.897   | 0.862         |

Table 2 that the combinations of the NN and ensemble of GBMs provide better results for most datasets. Moreover, 7 datasets from 10 ones show outperforming results by using the proposed approach (2 datasets by using Linear GBM and 5 datasets by using NN+GBM).

In order to study the proposed approach for solving regression problems, we apply datasets described in Table 3. The datasets are taken from open sources, in particular, Boston Diabetes, Longley can be found in the corresponding R Packages; HouseART can be found in the Kaggle platform; Friedman 1 and 2 are described at site: https://www.stat.berkeley.edu/~breiman/bagging.pdf; Regression is available in package “Scikit-Learn”.

Numerical results in the form of the mean squared errors for the regression datasets are shown in Table 4. We again use four models described above. Ensembles of GBMs consist of 100 machines now. The NN having 3 layers of size 20 are used. Other parameters of numerical experiments are the same as in the previous experiments. It can be seen from Table 4 that the combinations of the NN and ensemble of GBMs provide better results for 4 datasets from 7 ones.

We can conclude after analyzing the numerical results that the proposed approach provides outperforming results for cases of small datasets (see, for
example, most DNA microarray datasets and the Longley dataset). This implies that ensembles of GBMs partially solve the problem of overfitting, which takes place for datasets with the small number of training examples.

7 Conclusion

A new approach for combining GBMs by using the stacking algorithm has been proposed in the paper. It has many advantages in comparison with the GBM as well as with deep differentiable models such as NNs:

– the “greedy” stacking algorithm of GBMs does not guarantee an achievement of the loss function optimum because the optimization procedure is carried out in turn. The simultaneous optimization solves this problem;
– NNs consider linear combinations of input features, which lead to a serious problem of overfitting when working with tabular data consisting of features of different nature, for example, mass and length, as well as by a large number of features and small sizes of training samples. The proposed approach allows us to process features using decision trees and to construct arbitrarily deep models taking advantages of NNs.

It should be noted that many important questions and studies remain outside the scope of our study in this paper. In particular, it is interesting to consider various types of regularization which could improve the models. Moreover, it is
interesting to consider a procedure which removes a training example from the gradient descent procedure when a current residual corresponding to the example is smaller than some threshold. This improvement may reduce the learning time and increase the model accuracy. The above questions can be regarded as directions for further research.

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