This paper presents a computationally efficient variant of gradient boosting for multi-class classification and multi-output regression tasks. Standard gradient boosting uses a 1-vs-all strategy for classification tasks with more than two classes. This strategy translates in that one tree per class and iteration has to be trained. In this work, we propose the use of multi-output regressors as base models to handle the multi-class problem as a single task. In addition, the proposed modification allows the model to learn multi-output regression problems. An extensive comparison with other multi-output based gradient boosting methods is carried out in terms of generalization and computational efficiency. The proposed method showed the best trade-off between generalization ability and training and predictions speeds.

Keywords Gradient Boosting Machine · Multi-output regression · Multi-class classification

1 Introduction

We are in the thriving age of machine learning and in the midst of a revolution driven by machine learning programs. Machine learning has long been part of our daily lives. It helps to improve industrial and professional processes. There are many examples of novel machine learning applications, such as applications in business processes [1] to group customers and similar documents or to analyze quantities of customer data to improve customer service; Implementations to predict machine failures [2] and to recognize the health states of machines automatically; Prediction of risk in lung cancer patients [3]; and many more.

From the myriad of machine learning models developed, ensemble learning methods are among the best performing methods in terms of robustness and accuracy [4][5][6][7]. The idea behind ensembles is the combination multiple base learners, generally weak, into a strong learner. This combination produces a generalization ability in general superior to that of any of its members. These methods have been applied to many fields of applications in recent years and are among the best methods for tabular data classification tasks [8][9].

One of the most well-known ensemble models is Gradient Boosting (GB), also know as Gradient Boosted Decision Trees (GBDT) [10]. In GBDT, the learning method works by sequentially creating new base models that learn the portion of the concept not captured by previous learners. The problem is posed as an optimization problem in which the output of each new model is built to be correlated with the negative gradient of the loss function of previous iterations. The current implementation of GBDT has some advantages and disadvantages, and many improvements in this area have been achieved in the recent years. For instance, in [11] a fast variant of gradient booting was presented called XGBoost. This method drew much attention for achieving the best performance in many Kaggle competitions [11]. In [12], CatBoost is proposed, a Gradient Boosting method specially designed for datasets with categorical and numerical features.

One of the drawbacks of the current GBDT approaches is that, for multi-class classification, it requires to train one classifier per class and iteration. That is, the model optimizes each class in a separate process. Moreover, for multi-output regression problems, it requires to build one isolated ensemble for each output in which the correlations between
the dependent variables are ignored. As the correlations between multiple-outputs exist, and [13] shows that those correlations between outputs can improve the multi-output Support Vector Regression performance. More importantly, using one tree per class creates more complex (and slower) ensembles. There are some proposals to use a single multi-output tree for all classes at each boosting iteration to produce faster models. In [14, 15], these works are built on top of the gradient boosting based XGBoost [11] and LightGBM [16]. In both studies, the second-order Taylor expansion is used for loss function approximation, and the derivations are modified to handle vector forms of the expansion.

The objective of this study is two-fold. On the one hand a novel Gradient Boosting model that treats in the same manner different problems, such as binary/multi-class classification and single/multi-output regression is proposed. This is done by using a single, possibly multi-output, model at each step. In contrast to [14, 15], the optimization of the proposed method is based on a two-step procedure, first fitting the base learner by least-squares to the pseudo-residuals and then approximating the solution with the Newton-Raphson step following the original gradient boosting strategy [10]. The second objective of this paper is to perform an exhaustive comparison of multi-output gradient boosting methods in terms of generalization accuracy and computational efficiency.

The paper is organized as follows: In section 2, the Gradient Boosting construction and the proposed loss function and algorithm for both multi-class classification and multi-output regression problems are described, and section 3 reviews the related works. In section 4, the experiments and results of several empirical analyses are shown. Finally, the conclusions are summarized in the last section.

2 Methodology

In this section, Gradient Boosting (GB) algorithm [10] is reviewed. In addition, the proposed modifications in order to consider simultaneously at each step all classes for multi-class classification and outputs for multi-output regression is described.

2.1 Gradient Boosted Decision Trees

Considering a dataset \( D = \{ (x_i, y_i) \}_{i=1}^N \) where \( x \) and \( y \) refer to the input variables and response variable respectively. The main idea is to build the functional relationship between these two variables, \( F(X) \), that minimizes a given loss function

\[
\hat{F}(x) = \arg\min_{F(x)} \mathbb{E}_{p_x} L(y, F(x)). \tag{1}
\]

The optimization procedure followed by Gradient Boosting consists in estimating the objective function as an additive expansion

\[
\hat{F}(x) = \sum_{m=0}^{M} \gamma_m h_m(x)
\]

where \( M \) is the number of iterations and \( h(x) \) is a base regressor model. The model, \( \hat{F}(x) \), is created in a stagewise greedy process as

\[
(\gamma_m, h_m) = \arg\min_{\gamma, h} \sum_{i=1}^{N} L(y_i, F_{m-1}(x_i) + \gamma h_m(x_i)), \tag{2}
\]

where

\[
F_m(x) = F_{m-1}(x) + \gamma_m h_m(x), \tag{3}
\]

In order to optimize Eq. [2] first the model \( h \) is trained an then the value of \( \gamma \) is optimized. First, at each step a gradient descent step is performed by computing the negative gradient, or pseudo-residuals, for each data point

\[
r_{im} = -\left[ \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x_i)=F_{m-1}(x)}. \tag{4}
\]

and the \( m \)-th decision tree regressor model, \( h_m(x) \), is trained to adjust to the pseudo-residuals or gradients. Note that the gradients are optimized using a constrained function \( h \), usually a decision tree, that is built using the square loss independently of the loss function we are trying to optimize

\[
h_m = \arg\min_h \sum_{i=1}^{N} (r_{im} - h(x_i))^2. \tag{5}
\]
Hence, $\gamma$ is subsequently optimized on the original loss function using a Newton-Raphson step

$$
\gamma_m = \arg\min_{\gamma} \sum_{i=1}^{N} L(r_{im}, F_{m-1}(x_i) + \gamma h_m(x_i)) \quad (6)
$$

For the case in which the model $h$ is a decision tree, this line search optimization can be done independently for each terminal leaf. This is so because a decision tree can be seen as an additive model of the outputs of the terminal regions: $h_m(x) = \sum_{j=1}^{J} b_{mj} \mathbb{1}(x \in \mathbb{R}_j)$, where $J$ is the number of terminal nodes of the tree, $\mathbb{R}_j$ is the region covered by leaf $j$ and $b_j$ is its output. The terminal regions are disjoint and cover the whole data space. In consequence, a different $\gamma$ value can be computed for each terminal node $j$. We can integrate the general $\gamma$ constant in each node as $\gamma_{mj} = \gamma_m b_{mj}$.

With this, for the cases of binary classification or single-output regression in which one decision tree is built at each $m$ iteration, the leaf nodes output are updated as

$$
\gamma_{mj} = \arg\min_{\gamma} \sum_{x_i \in \mathbb{R}_{mj}} L(y_i, F_{m-1}(x_i) + \gamma), \quad (7)
$$

Note that for regression problems in which the square loss is optimized, this last step is not necessary as the leaf nodes already have the correct output.

### 2.2 Condensed Gradient Boosting

For the case of multi-class classification, since the base decision tree regressors supply scalar values, gradient boosting ensemble needs to build one tree per class and iteration. In this section, we derive the extension needed for GB [10] to work with a single decision tree regressor with vector size outputs for multi-class classification and multi-output regression. One of these trees could substitute the single output trees used in standard gradient boosting.

Assuming $D = \{x_i, y_i\}_{i=1}^{N}$ is the training classification data with $N$ instances where $x_i \in \mathbb{R}^D$. The $y_i \in [1, K]$ is the class label of the $i$-th instance, with $K$ the number of classes. A one-hot encoding method is applied to convert the multi-class labels to a logical matrix, in which row $i$ and column $k$ of the logical matrix $D$ is 1 if the $i$-th instance belongs to class $k$ and 0 otherwise. The objective is to find $K$ functions $\tilde{F} = \{\tilde{F}_k\}_{k=1}^{K}$ that minimize a given loss function in an additive manner using multi-output models

$$
\tilde{F}_m(x) = \tilde{F}_{m-1}(x) + \tilde{h}_m(x) \quad (8)
$$

where $\tilde{h}_m(x) = \{\gamma_{km} h_{km}(x)\}_{k=1}^{K}$ is the multi-output model with $K$ outputs. Using the one-hot encoded data set, at each iteration a single multi-output tree is trained to fit the data as $\mathbb{R}^D \rightarrow \mathbb{R}^K$ in which the values to learn is a matrix of size $N \times K$ with the residuals of the previous predictions

$$
r_{ikm} = \left[ \frac{\partial L(y_{ik}, F_{k}(x_i))}{\partial F_{k}(x_i)} \right]_{F_{k}(x)=F_{k,m-1}(x)}. \quad (9)
$$

For node $j$ with a vector of $K$ outputs of the decision tree regressor, the criteria to minimize forthcoming splits is the average of Mean Squared Error (MSE) over the $K$ outputs,

$$
Q(j) = \frac{1}{N_j K} \sum_{k=1}^{K} \sum_{x_i \in \mathbb{R}_j} (y_{ik} - \bar{y}_k)^2, \quad (10)
$$

where $\bar{y}_k$ is the mean value of target $k$ in the region $j$ and $N_j$ is the number of samples of node $j$.

As previously described, when the loss function is different to the one used when fitting the model to the matrix of residuals (given by eq. [11]) a second optimization step has to be carried out as in Eq [1]. In this second step, the $K$-dimensional vector of outputs of the leaf nodes has to be updated as

$$
\gamma_{mjk} = \arg\min_{\gamma} \sum_{x_i \in \mathbb{R}_j} L(y_{ik}, F_{mk}(x_i) + \gamma) \quad (11)
$$

For multi-class classification, if log-loss is used

$$
L(y, F(x)) = \sum_{k=1}^{K} y_k \ln \left( \frac{\exp(F_k(x))}{\sum_{k=1}^{K} \exp(F_k(x))} \right), \quad (12)
$$
the Newton-Raphson update for tree terminal leaves would be
\[
\gamma_{mjk} = \frac{\sum_{x_i \in R_j} r_{ikm}}{\sum_{x_i \in R_j} (y_{ikm} - r_{ikm}) \times (1 - (y_{ikm} + r_{ikm}))},
\] (13)
For multi-output regression, if the square loss is used, no update of the terminal vector values is needed since the trees are already optimizing the desired loss function.

2.3 Illustrative examples

Below, we include various examples to demonstrate the working modalities of the proposed condensed method and standard gradient boosting in multi-class classification. In a first experiment, the boundaries of GB and C-GB were analyzed to compare if creating single multi-output regression trees instead of one tree per class could pose difficulties learning the concepts. For this experiment a synthetic multi-class classification dataset with three classes, 1200 instances, two features, and one cluster per class was used. The generated dataset is based on the Madelon random data experiment [17]. The distribution of the training data points is shown in Fig. 1 with each class in a different color. The same hyper-parameter configuration was used for both methods (max depth=3, subsample=0.75, learning rate=0.1, decision trees=100). In Fig. 1 the decision boundaries of the two methods are shown using the same colors as the corresponding training data points. As it can be observed from the plots, both C-GB and GB perform very similarly and adjust rather good to the training instances. This shows that the proposed method is able to adapt to the problem at hand even though only one tree per iteration is trained.

In Fig. 2 the decision trees of the first iteration are shown as an example for the classification task shown in Fig. 1. The figure shows, for iteration 1, one tree per class for GB and the one tree of C-GB. The nodes of the trees show the following values: the split information for internal nodes, the MSE error of the node, the number of instances and the node output. For multi-output decision trees the MSE is the average MSE error for all outputs (Eq. 10) and the output value is a vector of size $K$-classes.

Fig. 2(a) illustrates how a single tree can manage to capture the information of the three classes. The split of the root node and the left branch is equivalent to that of the class 0 tree of GB and basically isolates the class 0 (purple dots in fig. 1) from the rest. After the root node, the first two right nodes of the C-GB tree have the same splits than the first nodes of the class 2 GB tree. This illustrates how a single tree is able to capture the information of all classes of the problem in a more compact way. Also, using a single tree would produce more coherent outputs as the same splits are used for all classes.

In order to show the performance of C-GB and GB in more detail, the convergence with respect to the number of trees of both methods on the Waveform dataset for each of its three classes was measured. The experiments were repeated 10 times and the average values reported. The hyper-parameters used are: learning rate is set to 0.1 and subsampling to 0.75. The convergence for each class is measured using average precision (i.e. true positives divided by detected positives) for each class. The results in average precision are shown in Figure 3 for different maximum depths for C-GB (blue curve) and GB (red curve). From Figure 3 it can be observed that both methods achieve equivalent
The multi-class problem into a set of binary tasks. These multi-class versions could have theoretical and practical con-
sequences. Several studies have proposed different extensions to boosting-like methods to better handle multi-class classification. These extensions are based in one of the two main families of boosting methods: AdaBoost \[18\] \[19\] \[20\] and Gradient Boosting \[10\] \[21\] \[11\]. The original AdaBoost \[18\] algorithm proposes two boosting variants to handle multi-class classification (called AdaBoost M1 and M2). AdaBoost.M1 is based on using multi-class weak base learners, while AdaBoost.M2 converts the multi-class problem into a set of binary tasks. These multi-class versions could have theoretical and practical convergence problems \[18\] \[22\]. The work proposed in \[22\] tackles these problems by defining an exponential bound on a test measure called pseudo-loss error in which each base learner (decision stumps in this work) minimizes its upper bound with gradient descent. Their method proved a better convergence than AdaBoost.M2.

For multi-class tasks, the approach followed by gradient boosting \[23\] is to optimize a multi-class loss function separately for each class by training one tree per class. The main drawback of this approach is the complexity of the solution as it generates a set of $K$ trees at each iteration.

In \[24\] an adaptive base class boosting (ABC-MART) is presented. The proposal derive the multi-class logistic regression loss function \[10\] given sum-to-zero constraint, such that the sum of the outputs of the models add up to zero. This allows them to choose at each epoch the base class that obtains the highest reduction of the training loss in a greedy manner. However, this greedy approach introduces a higher training complexity in the algorithm.

The most similar studies to the present work are \[14\] \[15\]. The idea of those studies is the same as the one of this work, that is to train a single tree for all classes at each boosting iteration. Although they are based on a different optimization procedure. The work of \[14\] is based in XGBoost \[11\]. Their implementation is, introduced as an open-source based on TensorFlow, named TFBT (stands for TensorFlow Boosted Trees) model. They showed how the use of a single multi-output regressor at each step produced less complex ensembles, which size is approximately reduced by a factor of the number of classes. They introduced two strategies in terms of loss function calculation. One of them considers the full-hessian loss, and the other assumes that the hessian matrix is diagonal, which leads to a faster
algorithm. Furthermore, they included a layer-by-layer approach that considers one tree as a whole boosting process that builds one tree layer at each gradient boosting step instead of the whole decision tree.

In a similar approach, [15] introduced a Gradient-boosted decision trees for multiple outputs (GBDT-MO) by training a single tree per iteration. The use of the loss function and its derivatives is the same as in [14]. Although GBDT-MO was implemented on top of LightGBM [16] and extended the histogram approximation of LightGBM for the multiple-outputs. They also adapted the algorithm to multi-output regression and to multi-label classification. These studies consider the vector form of Taylor expansion to approximate the loss function following the optimization procedure of XGBoost and LightGBM. In contrast, the proposed method is a two-step optimization procedure that applies gradient descent and a Newton-Raphson step approximation to find the solution, following the original gradient boosting approach.

Another recent gradient boosting study regarding the multi-output regression has been published [25]. The case study of this paper is predicting multi-step-ahead traffic speeds at the same time. Their state of the art is the Gradient Boosting Regression tree of Friedman [10] with the differentiable loss function, including the squared error and absolute error. They introduced the Multivariate Gradient-Boosting-Regression-Tree of Multivariate GBRT by considering the decision tree as the weak learner. Instead of the current approach, they also use the predicted values as an input during the model training and train each tree considering all outputs.

There are several implementations of multi-output decision trees such as [26, 27]. The work presented in [26] was designed in the context of clustering. It uses a generic prototype distance function to maximize the inter-cluster distance in a standard top-down decision tree approach [28]. Depending on the chosen prototype function the decision tree can work for classification and regression. In [26], a constrained multi-output decision tree is presented as an
instance of the algorithm presented in [27]. The proposed method trains a large multi-output decision tree. In a second step, the tree is pruned in order to satisfy the user size and accuracy constrains.

These multi-output decision trees can be combined into ensembles [29]. In this work, the multi-output decision trees of [27] are combined with bagging [30] and random forests [31]. The proposed ensembles [29] are tested on various classification and regression tasks showing a performance better than the single base models. Moreover, in the experiments carried out proposed multi-objective ensemble performed better on regression tasks than the single-objective ensembles. In classification, the performance of the multiple and single output models was equivalent.

### 4 Experiments

In this section, we carry out an exhaustive comparison of the proposed Condensed Gradient Boosting (C-GB) with respect to other similar algorithms such as TensorFlow Boosted Tree (TFBT) [14] and Gradient Boosted Decision Tree for multiple outputs (GBDT-MO) [15]. In addition, the comparison is extended to single output gradient boosting. The analyses are performed on 12 multi-class classification and three multi-output regression tasks from diverse areas of application and with different number of instances, classes and attributes. The details of the datasets are shown in Table 1. We selected these datasets in order to have a significant variation with respect to the different dimensions (samples and features) and number of classes and targets.

The code of the proposed method is implemented on top of the scikit-learn library and it is available at GitHub repository [1]. For the single output gradient boosting (GB), the scikit-learn implementation was used. For GBDT-MO, we used the implementation of the authors from the GBDTMO package [2]. The implementation of TFBT is based on TensorFlow [3]. Note, however, that in the last update of TensorFlow, the TFBT package was marked as deprecated (version 2.8.0 and older). Hence, we used a previous version of TensorFlow (version 2.4.1).

#### 4.1 Experimental setup

The validation procedure was carried out using random splits with the proportion of 20 percent for the test and the rest for the training sample, except for the CIFAR-10, Poker Hand, MNIST and Sensit for which the partition determined by the datasets was used. In order to have stable results, all experiments were repeated five times with different seed values except for the largest datasets: CIFAR-10, MNIST, Sensit, Poker Hand, and Cover Type in which only one experiment was performed. The reported generalization performance is computed as the average value of the different

---

[1] https://github.com/GAA-UAM/C-GB/
[2] https://github.com/zzd1992/GBDTMO
[3] git.kot.tools/tensorflow
Realizations. The size of the training and test for each dataset is indicated in the last column of Table 1. In an effort to achieve the highest possible accuracy performance for each model, the hyper-parameters of each model were tuned with grid-search method. The grid-search was done within train using 2-fold cross-validation for all the models and datasets. The combination of hyper-parameters that produced the best validation results was then used to train the final model of each algorithm using the whole training dataset. In Table 2 the hyper-parameter grids for each model are shown.

In addition to the generalization performance, the training and prediction times were also measured. In training, only the time necessary to train the models was logged without considering the time required to load the data in memory. The prediction time was computed as the average time each model needs to predict 10 instances.

Since the training time depends on the hyper-parameter settings, we considered a single set of hyper-parameters for all models, which was: subsample = 1, learning rate = 0.1, tree depth = 10, trees = 100. The experiments were carried out on an Intel(R) Xeon(R) CPU with six cores and a 2.40GHz base clock rate.

4.2 Evaluation

The generalization ability of the different algorithms in the classification tasks was using the accuracy of the models. For the multi-output regression problems, the root mean square error (RMSE) was used for each individual output,

$$RMSE_k = \sqrt{\frac{\sum_{i=1}^{N} (y_{ik} - \hat{y}_{ik})^2}{N}},$$

where $y_{ik}$ and $\hat{y}_{ik}$ are the target true and predicted values respectively for instance $i$ and target $k$. Furthermore, to have a unique performance criterion for each model in the multi-output regression tasks, we considered the average coefficient of determination $\alpha R^2$ over $K$ outputs

$$\alpha R^2(y_{ik}, \hat{y}_{ik}) = \frac{\sum_{k=1}^{K} \left(1 - \frac{\sum_{i=1}^{N} (y_{ik} - \hat{y}_{ik})^2}{\sum_{i=1}^{N} (y_{ik} - \bar{y}_k)^2}\right)}{K},$$

where $\bar{y}$ is the average of true target value for instance $i$. The highest possible value for $\alpha R^2$ is 1.0. Negative values indicate a poor performance, worse than predicting the average of the test real target values for all instances. We did not consider the average RMSE over all the targets as it would be an average of values on different units and in consequence difficult to interpret.

Finally, in order to compare the performance across datasets and methods, the statistical ranking methodology proposed by Demsár [37] was applied. This methodology, compute the average rank for each method across the tested datasets. The difference in average rank is considered significant using a Nemenyi test. The result of this test can be plotted using a Demsár [37] as the ones shown Figure 4. The ranking of the methods in each dataset was done using the average accuracy in the classification tasks. For the regression problems, the methods were ranked by target using the RMSE metric.

4.3 Results

The average results for the different experiments is shown in Tables 3, 4 and 5. In Table 3 the average accuracy for the multi-class tasks is shown. Tables 4 and 5 show the average RMSE and average $R^2$-score for the multi-output regression problems. In the tables, the best value for each dataset or target is highlighted in bold face.

From Table 3 it can be observed that the accuracy of GB is in general better than that of the rest of the models. GB obtained the highest accuracy in eight out of 12 datasets. The C-GB method followed with four best results. Finally,
Table 3: Average generalization accuracy for Condensed-Gradient Boosting (C-GB), Gradient Boosting (GB), Tensor-Flow Boosted Tree (TFBT), and Gradient-Boosted Decision Trees for Multiple Outputs (GBDT-MO). The best results for each dataset highlighted in bold.

| Dataset   | C-GB  | GB    | TFBT  | GBDT-MO |
|-----------|-------|-------|-------|---------|
| CIFAR-10  | 51.31 | 51.98 | 36.15 | 48.67   |
| Cover Type| 97.23 | 97.25 | 73.94 | 84.60   |
| Digits    | 97.17 | 97.39 | 95.94 | 96.39   |
| Iris      | 94.00 | 95.33 | 93.33 | 92.67   |
| Letter-26 | 96.80 | 96.57 | 76.44 | 94.74   |
| MNIST     | 97.48 | 97.63 | 80.48 | 96.71   |
| Poker Hand| 74.87 | 76.81 | 57.63 | 78.15   |
| Sensit    | 84.83 | 85.07 | 75.47 | 82.95   |
| Vehicle   | 75.06 | 75.06 | 64.24 | 72.12   |
| Vowel     | 96.16 | 95.76 | 70.91 | 83.54   |
| Waveform  | 85.12 | 85.24 | 80.00 | 84.40   |
| Wine      | 98.89 | 97.78 | 92.78 | 86.67   |

Table 4: Average generalization RMSE for C-GB, GB, and GBDT-MO.

GBDT-MO obtained one best performance and TFBT none. The difference in performance of GB and its extension C-GB is rather small in most datasets. For instance, the difference in Waveform between these two models is about 0.12, and 0.02 for Cover Type. The most favorable outcome for GB is obtained in Poker Hand with 1.94 points difference. Precisely in the dataset in which GBDT-MO got the best result. The lowest scores were obtained by TFBT in all datasets.

The results of the multi-output regression experiments are shown in Tables 4 and 5. In this experiment, as GB does not support multi-output regression, we trained one different ensemble for each output separately. Results are not reported for TFBT as this method does not handle regression tasks.

From Table 4, it can be observed that the performance of the C-GB on each target is similar to the performance of GB and superior to that of GBDT-MO. GB obtained the best result in nine targets and C-GB in five. With respect to GBDT-MO, the model could not perform as well as the other two methods. In relation to the average $R^2$ score shown in Table 5, the results show a similar behaviour: GB achieved the highest score in all datasets followed by C-GB. In addition, the average performance of GBDT-MO in the ATP1D dataset is clearly lower than that of the other two methods. To investigate more on this specific dataset, a scatter plot of the predicted and actual values for each target is shown in Fig. 5. The poor performance of GBDT-MO in this dataset can be explained as it predicts similar values for most instances.

Table 5: Average generalization coefficient of determination C-GB, GB, GBDT-MO.

Figure 4 shows the overall comparison of the tested methods using a Demsˇar diagram. The plots show the average rank of the methods for the analyzed datasets. The difference between the two methods is statistically significant if they are not connected with a horizontal solid line. The critical distance (CD) are 1.64 and 0.88 for 12 multi-class classification tasks and 14 regression targets respectively with p-value = 0.05.

Similar conclusions can be drawn from these diagrams. For the multi-class classification problems (Figure 4 subplot a), the worse performance is produced by TFBT followed by GBDT-MO. The best average rank is achieved by GB followed by the proposed condensed model. The performance of the C-GB in multi-class classification is statistically significantly better than that of TFBT. As for the regression tasks (Figure 4 subplot b), we ranked the models over...
Figure 4: Comparison of different gradient boosting models (higher rank is better) using the Nemenyi test ($p = 0.05$). The average rank for multi-class classification (a) and multi-output regression considering targets (b).

14 regression targets for three models. The best rank was achieved by the GB and C-GB with statistical significant difference in relation to GBDT-MO.

An important aspect of these methods is its computational complexity. To evaluate it, the training time and test time was measured for all datasets. The time performances are summarized in Table 6. The reported test times indicate the time needed by the methods to evaluate $10^5$ instances. The best (lowest) training and test times in the table are highlighted in bold face.

As it can be observed in Table 6, the results are generally more favorable to two methods based in single multi-output trees: C-GB and GBDT-MO. The C-GB trained faster in eight datasets, and the GBDT-MO trained faster in seven. In addition, the training times are generally favorable to C-GB in the largest datasets: for instance in CIFAR-10 and MNIST, GBDT-MO is respectively 2528.42 and 861.12 seconds slower than the C-GB. The training times for GB are clearly slower than those of C-GB. With respect to the test time needed to evaluate $10^5$ instances, the GBDT-MO model was the fastest in nine datasets and C-GB in four. The results of GB, in this regard, are somewhat more competitive in small datasets, even though one tree per class and iteration has to be evaluated. The reason for this is that in general, the size of the decision trees generated by GB is smaller.

| Models  | CIFAR-10 | Cover Type | Digits | iris | Letter-26 | MNIST | Poker Hand | Sensit | Vehicle | Vowel | Waveform | Wine | ATP1d | ATP1d | Energy |
|---------|----------|------------|--------|------|-----------|-------|------------|--------|---------|-------|----------|------|-------|-------|--------|
| C-GB    | 332.69   | 249.86     | 2.72   | 0.18 | 15.30     | 90.89 | 12.29      | 132.23 | 1.21    | 2.06  | 3.68     | 0.21 | 0.34  | 0.30  | 0.14   |
| GB      | 48.29    | 1.55       | 5.51   | 32.38| 2.16      | 15.93 | 2.33       | 2.17   | 7.95    | 7.94  | 2.31     | 32.19| 18.22 | 19.82 | 6.97   |
| TFBT    | 2274.58  | 1092.56    | 14.07  | 0.35 | 157.23    | 687.03| 71.59      | 325.21 | 3.29    | 3.29  | 7.49     | 0.39 | 1.21  | 1.07  | 0.16   |
| GBDT-MO | 42.60    | 4.78       | 19.16  | 21.92| 23.67     | 33.00 | 9.31       | 2.64   | 10.27   | 25.26 | 3.14     | 16.99| 21.23 | 21.46 | 4.16   |

Table 6: Training and prediction time comparison (in seconds) for C-GB, GB, TFBT, and GBDT-MO

5 Conclusion

In this paper, condensed gradient boosting (C-GB) is presented. C-GB is a variant of gradient boosting for multi-class classification and multi-output regression problems. In multi-class problems (i.e. tasks with more than 2 classes), gradient boosting has to train one regressor model per class and iteration. In this work, we propose the use of decision trees with vector-valued leaves in such a way that only one decision tree per iteration has to be trained. We have shown
that these multi-output regression trees are able to capture the information of all classes at once. In addition, the use of these trees allowed us to adapt the model to multi-output regression. The proposed method is implemented as an open-source package for further investigations.

An extensive experimental comparison has been carried out. The proposed model has been compared with respect to standard gradient boosting. In addition, the comparison is extended to other two similar multi-output models that use different optimization strategies. Specifically, TFBT based on XGBoost and GBDT-MO based on LightGBM. The experiments show that the proposed method accomplished a generalization performance very close to that of standard gradient boosting with a reduced use of computational resources. The ensembles generated with C-GB are faster to train and provide faster predictions than standard gradient boosting in general. Furthermore, the proposed model demonstrated superior generalization performance with respect to TFBT and GBDT-MO. In terms of computational complexity TFBT is the slowest of all methods, while GBDT-MO and C-GB are the fastest of all tested methods.
Acknowledgment

The authors acknowledge financial support from PID2019-106827GB-I00/AEI/10.13039/501100011033. And also acknowledge the Centro de Computación Científica — UAM, for the computational resource and time.
References

[1] In Lee and Yong Jae Shin. Machine learning for enterprises: Applications, algorithm selection, and challenges. *Business Horizons*, 63(2):157–170, 2020.

[2] Yaguo Lei, Bin Yang, Xinwei Jiang, Feng Jia, Naipeng Li, and Asoke K Nandi. Applications of machine learning to machine fault diagnosis: A review and roadmap. *Mechanical Systems and Signal Processing*, 138:106587, 2020.

[3] Negar Maleki, Yasser Zeinali, and Seyed Taghi Akhavan Niaki. A k-nn method for lung cancer prognosis with the use of a genetic algorithm for feature selection. *Expert Systems with Applications*, 164:113981, 2021.

[4] Zhi-Hua Zhou. *Ensemble methods: foundations and algorithms*. CRC press, 2012.

[5] Candice Bentéjac, Anna Csörgő, and Gonzalo Martínez-Muñoz. A comparative analysis of gradient boosting algorithms. *Artificial Intelligence Review*, 54:1937–1967, 2021.

[6] Manuel Fernández-Delgado, Eva Cernadas, Senén Barro, and Dinani Amorim. Do we need hundreds of classifiers to solve real world classification problems? *Journal of Machine Learning Research*, 15:3133–3181, 2014.

[7] Chongsheng Zhang, Changchang Liu, Xiangliang Zhang, and George Alpanidis. An up-to-date comparison of state-of-the-art classification algorithms. *Expert Systems with Applications*, 82:128–150, 2017.

[8] Zhiwen Yu, Yidong Zhang, CL Philip Chen, Jane You, Hau-San Wong, Dan Dai, Si Wu, and Jun Zhang. Multi-objective semisupervised classifier ensemble. *IEEE transactions on cybernetics*, 49(6):2280–2293, 2018.

[9] Josip Rudar, Teresita M Porter, Michael Wright, G Brian Golding, and Mehrdad Hajibabaei. Landmark: an ensemble approach to the supervised selection of biomarkers in high-throughput sequencing data. *BMC bioinformatics*, 23(1):1–34, 2022.

[10] Jerome H Friedman. Greedy function approximation: a gradient boosting machine. *Annals of statistics*, pages 1189–1232, 2001.

[11] Tianqi Chen and Carlos Guestrin. Xgboost: A scalable tree boosting system. In *Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining*, pages 785–794, 2016.

[12] Liudmila Prokhorenkova, Gleb Gusev, Aleksandr Vorobev, Anna Veronika Dorogush, and Andrey Gulin. Catboost: unbiased boosting with categorical features. *arXiv preprint arXiv:1706.09516*, 2017.

[13] Wei Zhang, Xianhui Liu, Yi Ding, and Deming Shi. Multi-output ls-svr machine in extended feature space. In *2012 IEEE International conference on computational intelligence for measurement systems and applications (CIMSA) proceedings*, pages 130–134. IEEE, 2012.

[14] Natalia Ponomareva, Thomas Colthurst, Gilbert Hendry, Salem Haykal, and Soroush Radpour. Compact multiclass boosted trees. In *2017 IEEE International Conference on Big Data (Big Data)*, pages 47–56. IEEE, 2017.

[15] Zhendong Zhang and Cheolkon Jung. Gbdt-mo: Gradient-boosted decision trees for multiple outputs. *IEEE transactions on neural networks and learning systems*, 32(7):3156–3167, 2020.

[16] Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. Lightgbm: A highly efficient gradient boosting decision tree. *Advances in neural information processing systems*, 30, 2017.

[17] Isabelle Guyon. Design of experiments of the nips 2003 variable selection benchmark. In *NIPS 2003 workshop on feature extraction and feature selection*, volume 253, page 40, 2003.

[18] Yoav Freund and Robert E Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of computer and system sciences*, 55(1):119–139, 1997.

[19] Llew Mason, Peter Bartlett, and Jonathan Baxter. Direct optimization of margins improves generalization in combined classifiers. *Advances in neural information processing systems*, 11, 1998.

[20] Llew Mason, Jonathan Baxter, Peter L Bartlett, Marcus Frean, et al. Functional gradient techniques for combining hypotheses. *Advances in Neural Information Processing Systems*, pages 221–246, 1999.

[21] Jerome H Friedman and Jacqueline J Meulman. Multiple additive regression trees with application in epidemiology. *Statistics in medicine*, 22(9):1365–1381, 2003.

[22] Günther Eibl and Karl-Peter Pfeiffer. Multiclass boosting for weak classifiers. *Journal of Machine Learning Research*, 6(2), 2005.

[23] Jerome Friedman, Trevor Hastie, Robert Tibshirani, et al. Additive logistic regression: a statistical view of boosting (with discussion and a rejoinder by the authors). *Annals of statistics*, 28(2):337–407, 2000.
[24] Ping Li. Abc-boost: Adaptive base class boost for multi-class classification. In Proceedings of the 26th Annual international conference on Machine Learning, pages 625–632, 2009.

[25] Xingbin Zhan, Shuaichao Zhang, Wai Yuen Szeto, and Xiquan Chen. Multi-step-ahead traffic speed forecasting using multi-output gradient boosting regression tree. Journal of Intelligent Transportation Systems, 24(2):125–141, 2020.

[26] Hendrik Blockeel, Luc De Raedt, and Jan Ramon. Top-down induction of clustering trees. In Icml, pages 55–63, 1998.

[27] Jan Struyf and Sašo Džeroski. Constraint based induction of multi-objective regression trees. In International workshop on knowledge discovery in inductive databases, pages 222–233. Springer, 2005.

[28] Leo Breiman, Jerome Friedman, Charles J Stone, and Richard A Olshen. Classification and regression trees. CRC press, 1984.

[29] Dragi Kocev, Celine Vens, Jan Struyf, and Sašo Džeroski. Ensembles of multi-objective decision trees. In European conference on machine learning, pages 624–631. Springer, 2007.

[30] Leo Breiman. Bagging predictors. Machine learning, 24(2):123–140, 1996.

[31] Leo Breiman. Random forests. Machine learning, 45(1):5–32, 2001.

[32] Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. Cifar-10 (canadian institute for advanced research). URL http://www.cs.toronto.edu/kriz/cifar.html, 5, 2010.

[33] M. Lichman. UCI machine learning repository, 2013.

[34] Li Deng. The mnist database of handwritten digit images for machine learning research [best of the web]. IEEE Signal Processing Magazine, 29(6):141–142, 2012.

[35] Marco F Duarte and Yu Hen Hu. Vehicle classification in distributed sensor networks. Journal of Parallel and Distributed Computing, 64(7):826–838, 2004.

[36] Eleftherios Spyromitros-Xioufis, Grigorios Tsoumakas, William Groves, and Ioannis Vlahavas. Multi-target regression via input space expansion: treating targets as inputs. Machine Learning, 104(1):55–98, 2016.

[37] Janez Demšar. Statistical comparisons of classifiers over multiple data sets. The Journal of Machine Learning Research, 7:1–30, 2006.