A CART-based Genetic Algorithm for Constructing Higher Accuracy Decision Trees

Elif Ersoy[a], Erinç Albey[b] and Enis Kayış[c]
Department of Industrial Engineering, Özyeğin University, 34794, Istanbul, Turkey

Keywords: Decision Tree, Heuristic, Genetic Algorithm, Metaheuristic.

Abstract: Decision trees are among the most popular classification methods due to ease of implementation and simple interpretation. In traditional methods like CART (classification and regression tree), ID4, C4.5; trees are constructed by myopic, greedy top-down induction strategy. In this strategy, the possible impact of future splits in the tree is not considered while determining each split in the tree. Therefore, the generated tree cannot be the optimal solution for the classification problem. In this paper, to improve the accuracy of the decision trees, we propose a genetic algorithm with a genuine chromosome structure. We also address the selection of the initial population by considering a blend of randomly generated solutions and solutions from traditional, greedy tree generation algorithms which is constructed for reduced problem instances. The performance of the proposed genetic algorithm is tested using different datasets, varying bounds on the depth of the resulting trees and using different initial population blends within the mentioned varieties. Results reveal that the performance of the proposed genetic algorithm is superior to that of CART in almost all datasets used in the analysis.

1 INTRODUCTION

Classification is a technique that identifies the categories/labels of unknown observations/data points, and models are constructed with the help of a training dataset whose categories/labels are known. There are many different types of classification techniques such as Logistic Regression, Naive Bayes Classifier, Nearest Neighbor, Support Vector Machines, Decision Trees, Random Forest, Stochastic Gradient Descent, Neural Networks, etc. Classification techniques are divided into two groups: (1) binary classifiers that classify two distinct classes or two possible outcomes and (2) multi-class classifiers that classify more than two distinct classes. Also, many of these methods are constructed with a greedy approach. Hence, these approaches always make the choice that seems to be the best at each step. However, these greedy approaches may not result in an optimal solution.

Decision trees (DT) are one of the most widely-used techniques in classification problems. They are guided by the training data (x_i, y_i), $i = 1, . . . , n$. (Bertsimas and Dunn, 2017). DTs recursively partition the training data's feature space through splits and assign a label(class) to each partition. Then created tree is used to classify future points according to these splits and labels. Since, conventional decision tree methods are creating each split in each node with greedy approaches and top-down induction methods, which may not capture well the underlying characteristics of the entire dataset. The possible impact of future splits is not considered while determining each split in the tree. Thus, attempts to construct near-optimal decision trees have been discussed for a long time (Safavian and Landgrebe, 1991).

The use of heuristics in creating decision trees with the greedy approach is discussed widely in the literature. Heuristic algorithms will be applied to construct decision trees from scratch or to improve the performance of constructed trees. Kolçe and Frasheri (2014) study on the greedy decision trees and focus on four of the most popular heuristic search

[a] https://orcid.org/0000-0003-1126-213X
[b] https://orcid.org/0000-0001-5004-0578
[c] https://orcid.org/0000-0001-8282-5572

Ersoy, E., Albey, E. and Kayış, E.
A CART-based Genetic Algorithm for Constructing Higher Accuracy Decision Trees.
DOI: 10.5220/0009893903280338
In *Proceedings of the 9th International Conference on Data Science, Technology and Applications (DATA 2020)*, pages 328-338
ISBN: 978-989-758-440-4

algorithms, such as hill-climbing, simulated annealing, tabu search, and genetic algorithms (Kolçe and Frasheri, 2014). For continuous feature data, evolutionary design is suggested in Zhao and Shirasaka (1999) and an extreme point tabu search algorithm is proposed in Bennett and Blue (1996).

There are some examples for optimal decision trees. For example, Blue and Bennett (1997) use a Tabu Search Algorithm for global tree optimization. In their paper, they mention that “Typically, greedy methods are constructed one decision at a time starting at the root. However, locally good but globally poor choices of the decisions at each node can result in excessively large trees that do not reflect the underlying structure of the data”. Gehrke et al. (1999), develop a bootstrapped optimistic algorithm for decision tree construction.

The genetic algorithm (GA) have been proposed to create decision trees in the literature and have been discussed in two different ways to find near-optimal decision trees. One method is for selecting features to be used to construct new decision trees in a hybrid or preprocessing manner (Bala et al., 1995) and others, applies algorithm directly to constructed decision trees to improve them (Papagelis and Kalles, 2000). Also, additionally, Chai et al. (1996) construct a linear decision binary tree with constructing piecewise linear classifiers with the GA. Therefore, we choose to use a GA to construct highly accurate decision trees to expand the search area so as not to get stuck in local optima and get close to the near-optimal tree.

In GA literature, different approaches are used to construct an initial population. Most of them use randomly generated populations (Papagelis and Kalles, 2000; Jankowski and Jackowski, 2015) and some of them use a more intelligent population with the help of greedy algorithms (Fu et al., 2003; Ryan and Rayward-Smith, 1998). In Fu et al. and Ryan et al.’s works, C4.5 is used as a greedy algorithm to construct the initial population. An intelligent population helps to start the algorithm with better fitness values. Also, in their paper, they discussed that using C4.5 is a bit computationally expensive.

In this work, we develop a GA to construct high accuracy decision trees. Also, we use greedy algorithm CART trees in the initial population to improve these trees’ performance. In GA, to implement evolutionary operations, decision trees must be represented as chromosome structures. In this work, we propose a structure to encode a decision tree to a chromosome and to generate the initial population, we divide the original dataset into subsets with reasonable size and generate trees with these subsets on CART. Then in GA full-size dataset and the initial population are used to create more accurate trees. So, we want to use the power of CART trees in our algorithm and we are trying to improve the performance of greedy CART solutions.

The rest of the paper is organized as follows. In Methodology section, you can find a more detailed explanation of our implementation of GA, chromosome structure and generated initial populations. Subsections of the Methodology section present the encoding/decoding decision trees to/from chromosomes, genetic operators like mutation and crossover, fitness functions. Experiment and Computational Result section explains the experimental details and results. Finally, Conclusion section concludes all of this work.

2 GENETIC ALGORITHM AS A SOLUTION METHOD

In this paper, we discuss GA to improve the performance of decision trees. For the GA implementation, we concentrate on the following facts: (1) new chromosome structure, (2) initial population, (3) fitness function, (4) selection algorithm, (5-6) genetic operations, (7) generation and (8) stopping condition and overall flow of GA. These are explained in detail in following subsections to understand the essentials of our GA.

2.1 Encoding the Solution Representation (Chromosome Structure)

The representation of a solution using the chromosome is critical for relevant search in solution space and tree-based representation for the candidate solution is the best one (Jankowski and Jackowski, 2015). A chromosome must contain all split decisions and rules to decode it into a feasible decision tree.

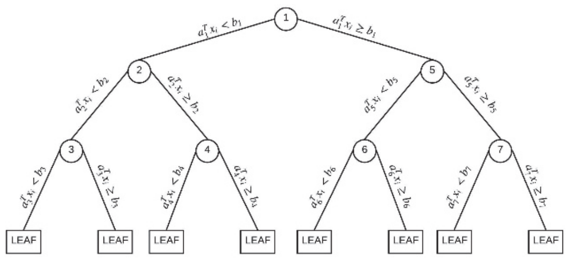


Figure 1: Tree structure and split rules at depth 3.

Decision trees are constructed based on split rules and in each node, split occurs with a rule, and data-points are following the related branch based on that rule. Also, in this paper, we concentrate on binary split trees so there are only two branches in each node splits, which means splits are bidirectional. Left branch refers less than operation and the right branch refers greater than or equal to operation (see Figure 1). So, in GA's solution representation if we encode which feature is used as a rule in which branch node, and their threshold values we will construct a tree with this linear representation. Then the fitness value will be calculated easily. To encode that representation, we use a modification of Jankowski and Jackowski (2015) as follows.

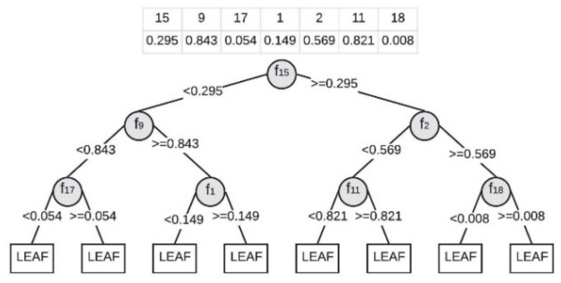
a_1	a_2	a_3	a_4	a_5	a_6	a_7
b_1	b_2	b_3	b_4	b_5	b_6	b_7

Figure 2: Chromosome structure for depth 3 tree.

Each branch node is stored in a depth-first manner as an implicit data structure in two arrays (see Figure 2). All feature IDs are maps to an integer and each feature values are maps to normalized continuous values between [0,1], so each component is numeric.

The dimension of a chromosome is $2x(2^D-1)$. We use 2 rows where first-row stores split feature information and second-row stores threshold values for the related feature. Number of columns equal to the number of total branch nodes, 2^D-1, where D is the depth of a tree. Also, in our algorithm D is used as a fixed parameter, thus chromosome dimension is also fixed. We define a tree if and only if the right branch always follows the ">=" rule and left branch follow "<" rule. Thus, if the related feature of the node's rule and the threshold for that rule is known, they are enough to construct a tree easily. So, the chromosome structure of depth 3 is presented below.

One of the decision trees at depth 3 is represented in Figure 3. To explain it in detail, split feature at the root node is 15th feature and threshold is 0.295. So, in



15	9	17	1	2	11	18
0.295	0.843	0.054	0.149	0.569	0.821	0.008

Figure 3: Example chromosome and related decision tree at depth 3.

training data, datapoints whose 15th feature is less than 0.295, follow left branch, accumulated in node 2 and points greater than or equal to 0.295, follow right branch and accumulated in node 5. Second column of the chromosome represents the rule of left node, node 2, then split feature is 9th feature and threshold is 0.843. Thus, data points accumulated in node 2 follows that rule, they are split according to their 9th feature and if the value is less than 0.843 they follow left branch, accumulated in node 3 and points greater than or equal to 0.843 follows right branch and accumulated in node 4. Then 3rd column of the chromosome is the left branch of the node 2 and split feature is 17th one, threshold is 0.149. Then if 17th features of data points in the node 2 are less than 0.149 datapoints assign to Leaf #1 and others assign to Leaf #2.

2.2 Generation of Initial Population

To generate initial solutions/populations for the GA, CART (Breiman et al., 1984) is used as a constructive algorithm. But GA needs an initial population that has more than 1 solution, so as Fu et. al (2003) used in their paper, some sub-trees are created for the initial population. In this paper, we generate sub-trees using two ways: randomly and with the CART algorithm. For random trees, we generate a tree with randomly chosen features for each node of a tree with given depth and random threshold values within the normalized values between 0 and 1. For sub-CART trees, a whole size data set is divided into some number of subsets randomly with a decided instance size (explained in Section 3.3) and CARTs are generated for these subsets. Some data points can be in multiple subsets. When subsets of this dataset are used in CART, a solution will be found for these subsets and we call them as sub-trees. Then original data will be classified using these subtrees and fitness value for each subtree is calculated for the whole dataset. Fitness is defined as the total misclassification error, which will be discussed in more detail later.

We use two different initial population mixtures (1) random trees only and (2) random trees, subtrees generated via CART, and 1 full CART solutions. Details for these population types and effects of these selections are discussed in Section 3.

2.3 Fitness Value

Fitness Value will be calculated as total number of misclassified points or total correctly classified points of each individual tree. A misclassification is number of points that are labeled incorrectly. In other words, in classification trees, leaf nodes are labeled with the majority points' class labels after split rules. Therefore, other minority points are labeled incorrectly, and the total number of that minority points is equal to the misclassification error and others are labeled correctly. Aim of our algorithm and all other classification algorithms are minimizing number of misclassification or maximizing number of correctly classified points, which are almost the same things.

In our algorithm, we choose maximizing correctly classified points as an objective. Thus, our fitness value is equal to total number of correctly classified points. We choose this one because of the working principle of our selection algorithm, we explain it in the following section in more detail.

When a new tree is reproduced after evolutionary operations, fitness value needs to be updated. Firstly, points are assigned to related leaf nodes according to new split rules. Then, each leaf is labeled with majority class, we call poin ts labeled incorrectly according to their real class labels, as misclassified points and others labeled as correctly classified points.

In the GA algorithm, we calculate the fitness function value of each individual sub-tree with the whole dataset instead of the related subset, because, in this paper, the classification tree must be generated for the whole dataset which considers all data points completely.

2.4 Parent Selection

In GA, during children production, the algorithm uses the current generation to create children that make up the next generation based on the fitness value. In GA and other evolutionary algorithms, to select parents, some well-known selection methods are tournament selection, roulette wheel selection, rank-based selection, etc. In these selection methods, each individual in the population can be selected more than once, so each individual spread its genes to possibly more than one child.

In our implementation of the GA, we use roulette wheel (RW) selection. Roulette wheel selection is under the title of Fitness Proportionate Selection Methods. In these methods, every solution has a probability of being selected according to their fitness values proportion. In roulette wheel, fitness values of each tree in the current generation take a place in the wheel according to their weighted fitness value. Thus, higher fitness takes wider proportion and it will be selected with a higher probability. Furthermore, we want to choose high accuracy trees as a parent to spread its genes to the next generations. This will help us to reproduce stronger children. If fitness value is used as a total number of correctly classified points, the roulette wheel works well and will chooses high accurate trees with higher probability. So, to select stronger parents, which has less number of misclassed points and more correctly classified ones, roulette wheel method is the proper one. That's why we choose our objective as maximize fitness function which is total number of correctly labeled points.

2.5 Crossover Operation

The algorithm creates crossover children by combining pairs of selected parents in the current population. Firstly, two individuals (parents) are chosen using the RW method. From chosen trees, a random cut point is selected according to a randomly generated number which can take values between 1 (root node) to *n* (total number of tree nodes). After identifying the random cut points in both parents, new individuals (offspring) are created by replacing sub-part form the first parent by the one from the second parent. We cut each parent from the exact same point/node and replace the remaining part with a same sized sub-parts. Figure 6 illustrates an example of the crossover operation.

Also, in this paper's algorithm, crossover is applied on linear chromosome in two ways, 1-point, and 2-point crossover. In 1-point crossover, the sub-part starting from the cutting node (and runs through the last node of the selected parent) is exchanged; whereas in 2-points crossover, we exchange interior sub-parts. In more detail, we cut sub-trees at the same level from each parent. In Figure 4, possible cut points for depth 2 trees are shown. 1-point crossover is applied when parents are cut from the 1st or 2nd cut points and crossed each other. 2-point crossover is applied when the part between the 1st and 2nd cut point

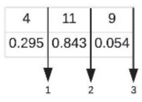


Figure 4: Possible crossover cut points in depth 2; 1 or 1-2 or 2.

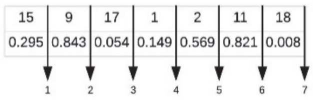


Figure 5: Possible crossover cut points in depth 3; 1 or 1-4 or 2-3 or 3-4 or 4 or 5-6 or 6.

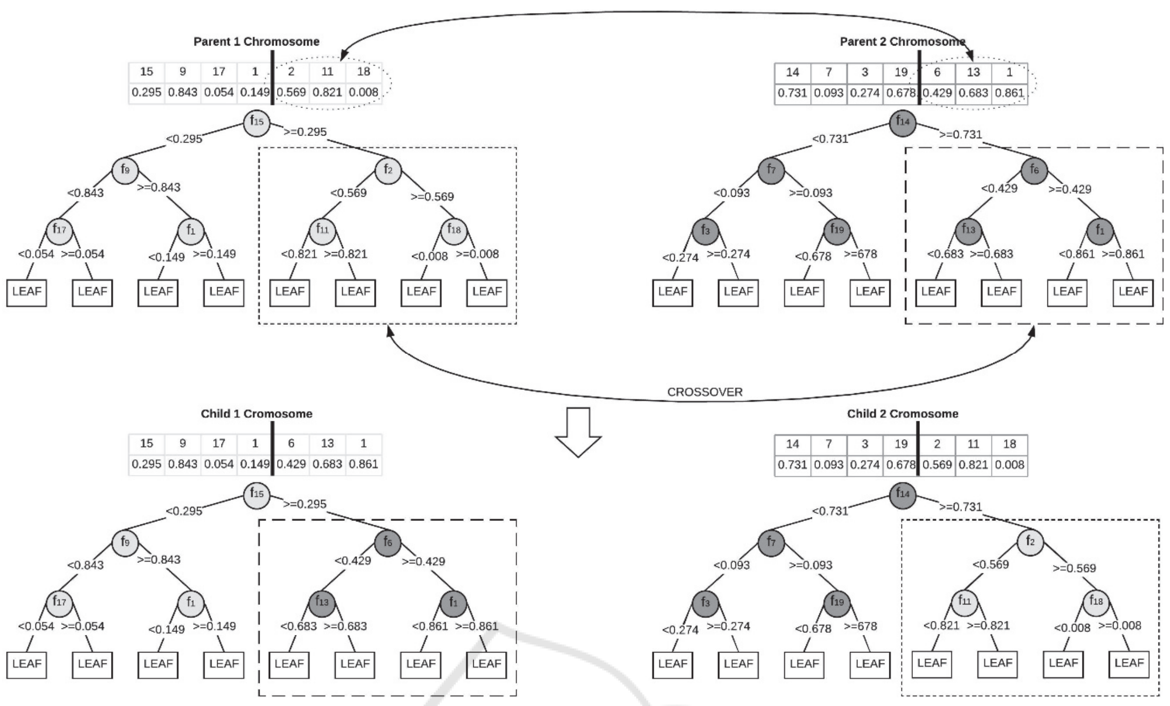


Figure 6: Crossover operation on selected parent and generated children in depth 3 trees.

is crossed. To be more precise, after the crossover operation, depth of the tree cannot change because we cut each parent from the exact same point. Figure 5 shows cut points for depth 3. For 1-point crossover at depth 3, possible cut points will be 1, 4 or 6 and for 2-point crossover, possible parts will be between 1-4, 2-3, 3-4 or 5-6. These specific cut-parts represent each meaningful sub-tree in a maximal tree. This specification also prevents depth change in the crossover.

In Figure 6, you can see the illustration of 1-point crossover on the depth 3 tree. We cut each parent from the 4th cut point, which is decided randomly in the algorithm, and cut parts crossing between each other.

2.6 Mutation Operation

Mutation operation makes changes on the individual tree in the population. In the proposed algorithm, this change is applied, based on mutation rate, on to the generated children`s randomly selected node to create a mutated child. With the help of mutation, GA enables us to search a broader space with providing genetic diversity. In our implementation, we use node base mutation similar to Jankowski and Jackowski (2015), we randomly change both feature and split threshold of a randomly selected node (see Figure 7).

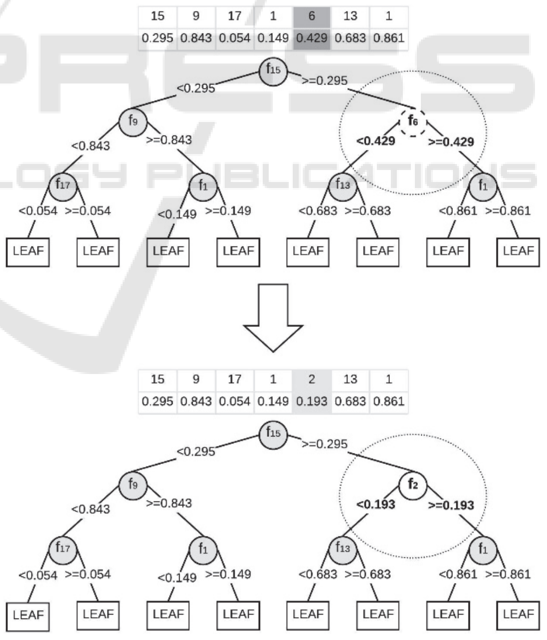


Figure 7: Tree node mutation.

Figure 7 illustrates how mutation operation applied on Child 1, which comes from the crossover. In this mutation, 5th node is selected randomly, and this node’s feature ID and threshold value are changed with randomly chosen feature ID and threshold value. With mutation, the class assignment of leaf nodes may also change based on the majority class on each node because split rule is changed. Also, there is a restriction, mutation will be applied to all branch nodes except the root node.

2.7 Replacement and New Generation

To generate a new generation of the GA, we applied the elitism procedure. Elitism keeps a proportion known as elite rate, of the fittest candidates into the next generation. For example, given a population of 100 individuals, if you have an elite rate of 5%, you choose to keep the five best individuals of the current generation to the next generations and you apply crossover and mutation to generate the rest of the new generation.

2.8 Stopping Criteria and Overall Algorithm

In the literature, there are many different applications of GA implementation. The flowchart in Figure 8 shows the general steps of our GA implementation.

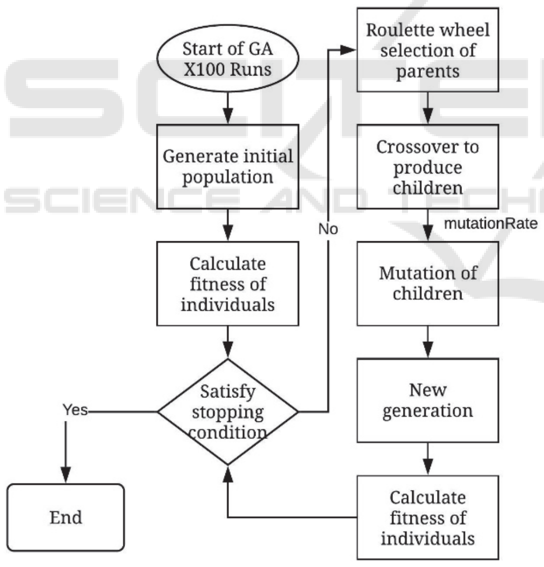

Start of GA X100 Runs
Generate initial population
Calculate fitness of individuals
Satisfy stopping condition
Yes
End
No
Roulette wheel selection of parents
Crossover to produce children
mutationRate
Mutation of children
New generation
Calculate fitness of individuals

Figure 8: Flow of GA.

To explain our algorithm in more detail, the steps of GA implementation is as follows:

Repeat below steps *TotalRun* times:

- Generate an initial population (first generation) of size *N* with the selected mixture.
- Initialize a variable, *Iter*, for keeping track of successive iterations where the best tree found in each generation has not changed.
- Repeat while *Iter* < *MaxIter*:
  - Select *eliteRate***N* best individual from the previous generation and keep them into the new generation.
  - Repeat until the new generation is fulfilled to size *N*.
    - Randomly select two members from the previous generation based on roulette wheel method.
    - Run the crossover operator: input selected two members and obtain two children.
    - Add new children to the new generation
    - Run the mutation operator: input one of the currently generated children from crossover and apply mutation if *mutationRate* is satisfied.
    - Replace mutated child in the new population.
    - If the new generation cannot provide a better tree and fitness value than the previous generation's best, increase *Iter* by 1.
- Select the best tree in the final generation and its fitness.

We repeat these steps *TotalRun* times in order to minimize the effects of randomization on overall performance. Also, we choose the final solution as the best tree found in all *TotalRun* runs.

3 COMPUTATIONAL RESULTS

In this section, we explain our datasets, parameters, initial populations, then the computational results of the proposed approach on different variations of datasets are discussed. We compare the performance of our GA to that of CART.

3.1 Datasets

To evaluate the effects of data size, number of features and class we use six different datasets with different dimensions and characteristics. These datasets are obtained from the UCI machine learning repository (Lichman, 2013). Some of these datasets are used in other classification studies as well, such as study about optimal classification tree (Bertsimas and Dunn, 2017). Details about each dataset are described below (see Table 1).

Table 1: Details of datasets used in experiments.

Data Set Name	Number of Points *(n)*	Number of Classes *(K)*	Number of Features *(p)*
Wine	173	3	13
Chess	3196	2	36
Image Segmentation	210	7	19
Avila	20867	12	10
Parkinson	756	2	754
Madelon	2600	2	500

We are given each dataset to GA in the form of (***X, Y***). To be more general, each dataset containing *n* observations, each observation is defined with *p* features and *K* possible class label. The *x* values for each feature across the data are normalized between 0 and 1, which means each $x_i \in [0, 1]^p$.

We apply 5-fold cross-validation to estimate the performance of our algorithm to minimize the overfitting problem. We split each dataset as 80% for training and 20% for testing sets. And then we take an average of 5 runs` accuracies.

3.2 Parameters

In our proposed GA, we use four parameters: (1) *maxIter* which is used for restricting the ineffective improvement moves to stop algorithm, (2) *Elite Rate* represents the proportion of best individual to keep in next generation, (3) *Mutation Rate* is the proportion for mutation operation applied on children and (4) *TotalRun* which is the total number of replications. For *maxIter*, in each ineffective generation, iteration counter increases but if the new generation improves the best solution and updates the best tree so far, iteration does not increase and iteration counter is reset. If the iteration counter reaches *maxIter,* GA terminates. We take *TotalRun* amounts of replications because, in the applied algorithm, there are lots of randomization in reproduction operators as selection, crossover and mutation. So, we apply some replications and decrease the effect of randomness over each procedure. In this work, we use the parameter values as shown in Table 2. Sensitivity analysis is applied to these parameters and final values are selected as the values that yield the best performance.

Table 2: Values of each parameter.

Parameter	Value
MaxIter	10
Elit Rate	0.2
Mutation Rate	0.1
Total Run	100

3.3 Initial Population

As mentioned before, this work aims to improve the performance of GA by using a specific initial population. We use two different population blends for initializing our algorithm. These mixtures include random trees, sub-CART trees which are generated with sub-sets of the whole datasets and 1 CART tree which is constructed with the full-size training set.

Table 3: Content of population blends.

Population	Content
MIX_V1	30 Random Trees
MIX_V2	30 Random + 30 Sub-CART + 1 full-CART Trees

We generate each random tree by assigning random rules for a given depth. Random feature ID for each node, which is integer, is assigned between [*0, p*] and threshold value, which is continuous, between [*0,1*]. For constructing CART trees, we used the *rpart* package (Therneau et al. 2019) in the R programming language version 3.5.3 (R Core Team 2019). In the rpart function, there is a control parameter called *minbucket,* which limits the minimum number of observations in any leaf node to prevent overfitting. We use this parameter as *(0.05*n).*

We add CART based decision trees into the initial population and our aim is to beat CART performances with the help of GA. We will evaluate the contributions of CART based initial population in the next subsection.

3.4 Experimental Analysis and Result

As mentioned in previous subsections, we use 6 different datasets with different sizes, and we divide them into 5 folds. We aim to find more accurate trees rather than the CART. As an initial population, we use 2 different population mixtures with different size (see Table 3).

Our first initial population includes 30 different random trees with a given depth. And second initial population type includes the same 30 random trees plus 30 sub-CART and 1 full-sized CART solution. Also, we train each dataset at 4 different depths as {2, 3, 4, 5}.

We take 100 replication runs to minimize effects of randomization. So, to compare our GA results we take best tree found in overall 100 runs as a final solution. In the below tables, "mean out-sample accuracy" is refer to average out-sample accuracy of the best tree found in 100 runs of 5 folds.

We use average out-sample accuracies across 5 folds to compare the performance of our algorithm against CART in cross-validation manner. Also, to show the exact improvement performance of our

Table 4: Full results at depth 2.

DATASET		**Mean Out-Sample Accuracy**	**Mean In-Sample Accuracy Improvement**	**Time**(sec)
Wine	CART	**88.78%**		0.112
	GA MIX_V1	88.19%	+12.22%	0.460
	GA MIX_V2	88.21%	+2.67%	0.767
Chess	CART	76.69%		0.131
	GA MIX_V1	86.64%	+17.47%	7.543
	GA MIX_V2	**86.92%**	+0.52%	7.700
Segment	CART	37.14%		0.169
	GA MIX_V1	57.14%	+8.10%	0.566
	GA MIX_V2	**58.10%**	+3.10%	0.645
Avila	CART	50.10%		0.257
	GA MIX_V1	51.14%	+3.14%	32.721
	GA MIX_V2	**51.97%**	+0.78%	41.768
Parkinson	CART	79.89%		0.349
	GA MIX_V1	79.10%	+2.71%	1.697
	GA MIX_V2	**81.88%**	+0.07%	1.872
Madelon	CART	65.19%		0.783
	GA MIX_V1	57.00%	+5.45%	7.248
	GA MIX_V2	**66.38%**	+0.77%	11.629

The best performing solutions for each dataset are highlighted in **bold**.

Table 5: Full results at depth 3.

DATASET		**Mean Out-Sample Accuracy**	**Mean In-Sample Accuracy Improvement**	**Time**(sec)
Wine	CART	91.02%		0.214
	GA MIX_V1	**96.60%**	+8.01%	0.733
	GA MIX_V2	91.57%	+2.53%	1.464
Chess	CART	90.43%		0.249
	GA MIX_V1	90.43%	+12.64%	11.192
	GA MIX_V2	**93.80%**	+3.38%	12.466
Segment	CART	52.38%		0.254
	GA MIX_V1	68.57%	+17.38%	0.984
	GA MIX_V2	**80.48%**	+10.36%	1.150
Avila	CART	52.43%		0.278
	GA MIX_V1	51.08%	+3.26%	59.846
	GA MIX_V2	**54.70%**	+1.33%	92.289
Parkinson	CART	80.95%		0.526
	GA MIX_V1	78.44%	+3.11%	3.120
	GA MIX_V2	**82.80%**	+1.03%	3.887
Madelon	CART	69.04%		1.004
	GA MIX_V1	60.00%	+6.31%	14.336
	GA MIX_V2	**69.27%**	+0.37%	16.901

The best performing solutions for each dataset are highlighted in **bold**.

algorithm over training set, we share average in-sample accuracy improvement as the difference between the accuracy of the best accurate tree out of 100 run and the initial best accurate tree in the initial generation. Table 4 presents these in-depth direct comparisons at depth 2 and Table 5 at depth 3. Result tables for depth 4 and 5 are provided in the Appendix. `Time` is the total time in seconds for population initialization plus GA execution time.

GA is codded in Java language (Java version 1.8.0) and computed on Eclipse IDE version 4.14.0. These computations are done in a PC with Intel Core i7-8550U 1.8GHz, 8GB RAM.

In Table 4, at depth 2, 5 out of 6 datasets show GA with CART based initial population (MIX_V2) is stronger than CART with an improvement over CART of about 1% to 10% nominal improvement depending on the dataset. Also, in some datasets, the performance of the GA with random initial population (MIX_V1) is also stronger than the pure CART performance but in general GA with MIX_V2 population has the best performance over CART and GA with MIX_V1.

Improvement amounts of GA with MIX_V2 increases at higher depths. Moreover, at higher depths, GA with MIX_V2 population is always the best one. Especially at depth 5 (see Appendix 2), for all the 6 datasets, GA with MIX_V2 is always the best method.

For more detail, let's analyze the results of Avila dataset at depth 2-3-4 and 5. When depths are getting deeper, out-sample accuracies are also increased. Although, in-sample accuracy improvements are almost same for all depths. But, more crucial point is difference between the MIX_V1 and MIX_V2. At all depths, MIX_V2 is always outperformed CART and MIX_V1. Only Wine dataset at depth 2 cannot outperform CART at MIX_V1 and MIX_V2. But in higher depths, we can beat CART performance as well.

These results show that our GA can outperform CART in all datasets when depth ≥3. On the other hand, in mean in-sample perspective, GA with MIX_V1 shows higher average in-sample accuracy improvement. This metric shows effect of GA over the initial population with the training set. In MIX_V1 initial population we use only random trees and their initial accuracies are very low over the training set. After the GA implementation, we can increase the accuracy of these random trees dramatically. This shows, our GA works well to increase the initial fitness of the provided problem within a reasonable execution time for small and medium size datasets.

We conclude that GA found trees with higher prediction accuracy compared to greedy CART algorithm in a reasonable time for small and medium size datasets. For large size datasets (n>20,000), the execution time increases, especially when we increase the population size along with the data size. But in all dataset sizes, we can observe at least 1% accuracy improvement, which is crucial in classification problems. Thanks to GA to improve the performance of the given initial population and find trees with better accuracies.

4 CONCLUSIONS

In this article, we describe and evaluate an evolutionary algorithm, GA, for decision tree induction. In conclusion, because of the disadvantages of greedy approaches, some heuristics will be combined to improve their performances. Genetic algorithm is chosen in this work to combine with CART. So, we use random initial population as well to compare the performance of including CART subtrees into the initial population. In GA, crossover is applied to all parents, and mutation is applied only for the given proportion of the children coming from the crossover. In mutation, the randomly chosen node is mutated.

Results show GA improves the performance of given trees in the initial population. But if the initial population contains random trees only, GA cannot outperform CART solution usually. So, when we include CART solutions to the population we can improve their performances and outperform CART. Results show MIX_V2 initial population is better than de MIX_V1 population 5 out of 6 datasets at depth 2, 3 and MIX_V2 is always the better one at depth 4 and 5.

For future work, some additional steps will be applied to this presented heuristic to observe more improvements and some other heuristic methods will be experienced to construct more accurate trees. For example, in presented GA, some additional operations and improvement moves will be tested and selected according to their contribution. Also, we will consider pruning steps in GA implementation and we will be limiting some parameters like *minbucket* and complexity parameter, which are used in constructing CART. Additionally, we will generate different initial population mixtures with the help of different decision tree induction strategies and compare their performance with the proposed ones.

REFERENCES

Bertsimas, D., & Dunn, J., 2017. Optimal classification trees. Machine Learning, 106(7), 1039-1082.

Safavian, S. R., & Landgrebe, D., 1991. A survey of decision tree classifier methodology. IEEE transactions on systems, man, and cybernetics, 21(3), 660-674.

Gehrke, J., Ganti, V., Ramakrishnan, R., & Loh, W. Y., 1999. BOAT—optimistic decision tree construction. In Proceedings of the 1999 ACM SIGMOD international conference on Management of data (pp. 169-180).

Kolçe, E., & Frasheri, N., 2014. The use of heuristics in decision tree learning optimization. International Journal of Computer Engineering in Research Trends, 1(3), 127-130.

Zhao, Q., & Shirasaka, M., 1999. A study on evolutionary design of binary decision trees. In Proceedings of the 1999 Congress on Evolutionary Computation-CEC99 (Cat. No. 99TH8406) (Vol. 3, pp. 1988-1993). IEEE.

Bennett, K. P., & Blue, J. A.,1996. Optimal decision trees. Rensselaer Polytechnic Institute Math Report, 214, 24.

Bennett, K., & Blue, J., 1997. An extreme point tabu search method for data mining. Technical Report 228, Department of Mathematical Sciences, Rensselaer Polytechnic Institute.

Bala, J., Huang, J., Vafaie, H., DeJong, K., & Wechsler, H., 1995. Hybrid learning using genetic algorithms and decision trees for pattern classification. In IJCAI (1) (pp. 719-724).

Papagelis, A., & Kalles, D., 2000. GA Tree: genetically evolved decision trees. In Proceedings 12th IEEE Internationals Conference on Tools with Artificial Intelligence. ICTAI 2000 (pp. 203-206). IEEE.

Chai, B. B., Zhuang, X., Zhao, Y., & Sklansky, J., 1996. linear decision tree with genetic algorithm. In Proceedings of 13th International Conference on Pattern Recognition (Vol. 4, pp. 530-534). IEEE.

Ryan, M. D., & Rayward-Smith, V. J., 1998. The evolution of decision trees. In Proceedings of the Third Annual Conference on Genetic Programming (pp. 350-358). San Francisco, CA.: Morgan Kaufmann.

Fu, Z., Golden, B. L., Lele, S., Raghavan, S., & Wasil, E. A., 2003. A genetic algorithm-based approach for building accurate decision trees. INFORMS Journal on Computing, 15(1), 3-22.

Jankowski, D., & Jackowski, K., 2015. Evolutionary algorithm for decision tree induction. In IFIP International Conference on Computer Information Systems and Industrial Management (pp. 23-32). Springer, Berlin, Heidelberg.

Breiman, L., Friedman, J., Stone, C. J., & Olshen, R. A., 1984. Classification and regression trees. CRC press.

Lichman, M., 2013. UCI machine learning repository. http://archive.ics.uci.edu/ml.

Therneau, T., Atkinson, B., & Ripley, B., 2019. rpart: Recursive partitioning and regression trees. http:/CRAN.R-project.org/package=rpart, R package version 4.1-15.

R Core Team., 2019. R: A language and environment for statistical computing. Vienna: R Foundation for Statistical Computing. http://www.R-project.org/.

APPENDIX

Appendix 1: Full results for depth 4.

DATASET		Mean Out-Sample Accuracy	Mean In-Sample Accuracy Improvement	Time(sec)
Wine	CART	91.02%		0.214
	GA MIX_V1	**92.11%**	10.67%	1.654
	GA MIX_V2	91.03%	3.09%	2.653
Chess	CART	89.86%		0.391
	GA MIX_V1	90.49%	15.09%	22.899
	GA MIX_V2	**94.09%**	0.23%	18.734
Segment	CART	69.05%		0.222
	GA MIX_V1	77.14%	22.02%	1.994
	GA MIX_V2	**84.29%**	7.02%	1.890
Avila	CART	55.20%		0.303
	GA MIX_V1	50.56%	2.23%	145.270
	GA MIX_V2	**57.04%**	0.86%	188.793
Parkinson	CART	80.95%		0.715
	GA MIX_V1	77.51%	3.11%	5.952
	GA MIX_V2	**83.20%**	1.49%	7.657
Madelon	CART	69.27%		1.109
	GA MIX_V1	58.73%	2.55%	25.317
	GA MIX_V2	**70.04%**	0.60%	28.863

The best performing solutions for each dataset are highlighted in **bold**.

Appendix 2: Full results for depth 5.

DATASET		**Mean Out-Sample Accuracy**	**Mean In-Sample Accuracy Improvement**	**Time**(sec)
Wine	CART	91.02%		0.237
	GA MIX_V1	91.60%	9.70%	4.140
	GA MIX_V2	**94.40%**	3.37%	3.300
Chess	CART	89.86%		0.427
	GA MIX_V1	94.15%	15.81%	55.128
	GA MIX_V2	**94.40%**	0.66%	36.076
Segment	CART	77.14%		0.253
	GA MIX_V1	77.14%	15.48%	3.150
	GA MIX_V2	**84.76%**	4.52%	3.546
Avila	CART	58.82%		0.529
	GA MIX_V1	50.32%	6.71%	139.102
	GA MIX_V2	**60.04%**	1.08%	314.508
Parkinson	CART	80.95%		0.767
	GA MIX_V1	81.08%	2.15%	6.699
	GA MIX_V2	**83.86%**	1.69%	14.384
Madelon	CART	69.27%		1.164
	GA MIX_V1	58.58%	5.30%	38.731
	GA MIX_V2	**70.85%**	1.13%	53.497

The best performing solutions for each dataset are highlighted in **bold**.