evtree: Evolutionary Learning of Globally Optimal Classification and Regression Trees in R

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Abstract

Commonly used classification and regression tree methods like the CART algorithm are recursive partitioning methods that build the model in a forward stepwise search. Although this approach is known to be an efficient heuristic, the results of recursive tree methods are only locally optimal, as splits are chosen to maximize homogeneity at the next step only. An alternative way to search over the parameter space of trees is to use global optimization methods like evolutionary algorithms. This paper describes the **evtree** package, which implements an evolutionary algorithm for learning globally optimal classification and regression trees in R. Computationally intensive tasks are fully computed in C++ while the **partykit** (Hothorn and Zeileis 2011) package is leveraged for representing the resulting trees in R, providing unified infrastructure for summaries, visualizations, and predictions. `evtree` is compared to `rpart` (Therneau and Atkinson 1997), the open-source CART implementation, and conditional inference trees (`ctree`, Hothorn, Hornik, and Zeileis 2006). The usefulness of `evtree` is illustrated in a textbook customer classification task and a benchmark study of predictive accuracy in which `evtree` achieved at least similar and most of the time better results compared to the recursive algorithms `rpart` and `ctree`.

Keywords: machine learning, classification trees, regression trees, evolutionary algorithms, R.

1. Introduction

Classification and regression trees are commonly applied for exploration and modeling of complex data. They are able to handle strongly nonlinear relationships with high order interactions and different variable types. The resulting model can be interpreted as a tree structure providing a compact and intuitive representation. Commonly used classification and regression tree algorithms, including *CART* (Breiman, Friedman, Olshen, and Stone 1984) and *C4.5* (Quinlan 1993), use a greedy heuristic, where split rules are selected in a forward stepwise search for recursively partitioning the data into groups. The split rule at each internal node is selected to maximize the homogeneity of its child nodes, without consideration of nodes further down the tree, hence yielding only locally optimal trees. Nonetheless, the greedy heuristic is computationally efficient and often yields reasonably good results (Murthy and Salzberg 1995). However, for some problems, greedily induced trees can be far from the optimal solution, and a global search over the tree's parameter space can lead to much more compact and accurate models.

The main challenge in growing globally optimal trees is that the search space is typically huge rendering full-grid searches computationally infeasible. One possibility to solve this problem is to use stochastic optimization methods like evolutionary algorithms. In practice, however, such stochastic methods are rarely used in decision tree induction. One reason is probably that they are computationally much more demanding than a recursive forward search but another one is likely to be the lack of availability in major software packages. In particular, while there are several packages for R (R Development Core Team 2011) providing forward-search tree algorithms, there is only little support for globally optimal trees. The former group of packages includes (among others) **rpart** (Therneau and Atkinson 1997), the open-source implementation of the CART algorithm; **party**, containing two tree algorithms with unbiased variable selection and statistical stopping criteria (Hothorn *et al.* 2006; Zeileis, Hothorn, and Hornik 2008); and **RWeka** (Hornik, Buchta, and Zeileis 2009), the R interface to **Weka** (Witten and Frank 2011) with open-source implementations of tree algorithms such as C4.5 or *M5* (Quinlan 1992). A notable exception is the **LogicReg** package (Kooperberg and Ruczinski 2011) for logic regression, an algorithm for globally optimal trees based on binary covariates only and using simulated annealing. See Hothorn (2011) for an overview of further recursive partitioning packages for R.

To fill this gap, we introduce a new R package **evtree**, available from the Comprehensive R Archive Network at `http://CRAN.R-project.org/package=evtree`, providing evolutionary methods for learning globally optimal classification and regression trees. Generally speaking, evolutionary algorithms are inspired by natural Darwinian evolution employing concepts such as inheritance, mutation, and natural selection. They are population-based, i.e., a whole collection of candidate solutions – trees in this application – is processed simultaneously and iteratively modified by *variation operators* called *mutation* (applied to single solutions) and *crossover* (merging different solutions). Finally, a survivor selection process favors solutions that perform well according to some quality criterion, usually called *fitness function* or *evaluation function*. In this evolutionary process the mean quality of the population increases over time (Bäck 1996; Eiben and Smith 2007). In the case of learning decision trees, this means that the variation operators can be applied to modify the tree structure (e.g., number of splits, splitting variables, and corresponding splitpoints etc.) in order to optimize a fitness functions such as the misclassificaion or error rate penalized by the complexity of the tree. A notable difference to comparable algorithms is the survivor selection mechanism where it is important to avoid premature convergence. In the following, we use a simple $(1+1)$ selection strategy (i.e., one parent solution competes with one offspring for a place in the population) which can be argued to offer computational advantages for the application to classification and regression trees.

The remainder of this paper is structured as follows: Section 2 describes the problem of learning globally optimal decision trees and contrasts it to the locally optimal forward-search heuristic that is utilized by recursive partitioning algorithms. Section 3 introduces the `evtree` algorithm before Section 4 addresses implementation details along with an overview of the implemented functions. A benchmark comparison – comprising 14 benchmark datasets, 3 real-world datasets, and 3 simulated scenarios – is carried out in Section 5, showing that the predictive performance of `evtree` is often significantly better compared to the commonly used algorithms `rpart` and `ctree` (from the **party** package). Finally, Section 6 gives concluding remarks about the implementation and the performance of the new algorithm.

2. Globally and locally optimal decision trees

Classification and regression tree analysis aims at modeling a response variable Y by a vector of P predictor variables $X = (X_1, ..., X_P)$ where for classification trees Y is qualitative and for regression trees Y is quantitative. Tree-based methods first partition the input space X into a set of M rectangular regions R_m $(m = 1, ..., M)$ then fit a (typically simple) model within each region $\{Y|X \in R_m\}$, e.g., the mean, median, or variance etc. Typically, the mode is used for classification trees and the arithmetic mean is applied for regression trees.

To show why forward-search recursive partitioning algorithms typically lead to globablly suboptimal solutions, their parameter spaces and optimization problems are presented and contrasted in a unified notation. Although all arguments hold more generally, only binary tree models with some maximum number of splits $M_{\max}$ are considered. Both restrictions make the notation somewhat simpler while not really restricting the problem: (a) Multiway splits are equivalent to a sequence of binary splits in predictions and number of resulting subsamples. (b) The maximal size of the tree is always limited by the number of observations in the learning sample.

In the following, a binary tree model with M terminal nodes (which consequently has $M - 1$ internal splits) is denoted by

$$\theta \;=\; (v_{n_1}, s_{n_1}, ..., v_{n_{M-1}}, s_{n_{M-1}}), \tag{1}$$

where the $n_r \in \{1, ..., M_{\max} - 1\}$ are the positions of the internal *nodes*, $v_r \in \{1, \ldots, P\}$ the associated splitting *variables*, and s_r the associated *split* rules $(r = 1, \ldots, M - 1)$. Depending on the domain of X_{v_r}, the split rule s_r contains either a cutoff (for ordered and numeric variables) or a a nonempty subset of $\{1, \ldots, c\}$ (for a categorical variable with c levels), determining which observations are sent to the first or second subsample. In the former case, there are $u - 1$ possible split rules if X_{v_r} takes u distinct values; and in the latter case, there are $2^{c-1} - 1$ possible splits. Thus, the product of all of these combinations forms all potential elements θ from Θ_M, the space of conceivable trees with M terminal nodes. The overall parameter space is then $\Theta = \bigcup_{M=1}^{M_{\max}} \Theta_M$ (which in practice is often reduced by exluding elements θ resulting in too small subsamples etc.).

Finally, $f(X, \theta)$ denotes the prediction function based on all explanatory variables X and the chosen tree structure θ from Equation 1. As pointed out above, this is typically constructed using the means or modes in the respective partitions of the learning sample.

2.1. The parameter space of globally optimal decision trees

As done by Breiman *et al.* (1984), let the complexity of a tree be measured by a function of the number of terminal nodes, without further considering the depth or the shape of trees. The goal is then to find that classification and regression tree which optimizes some tradeoff between predicition performance and complexity:

$$\hat{\theta} \;=\; \underset{\theta \in \Theta}{\operatorname{argmin}}\; \operatorname{loss}\{Y, f(X, \theta)\} \;+\; \operatorname{comp}(\theta). \tag{2}$$

where $\operatorname{loss}(\cdot, \cdot)$ is a suitable loss function for the domain of Y; typically, the misclassification rate MC and the mean squared error MSE are employed for classification and regression, respectively. The function $\operatorname{comp}(\cdot)$ is a function that is monotonically non-decreasing in the

number of terminal nodes M of the tree θ, thus penalizing more complex models in the tree selection selection process. Note that finding $\hat{\theta}$ requires a search over all Θ_M.

The parameter space Θ becomes large for already medium sized problems and a complete search for larger problems is computationally intractable. In fact, Hyafil and Rivest (1976) showed that building optimal binary decision trees, such that the expected number of splits required to classify an unknown sample is minimized, is NP-complete. Zantema (2000) proved that finding a decision tree of minimal size that is decision-equivalent to a given decision tree is also NP-hard. As a consequence the search space is usually limited by heuristics.

2.2. The parameter space of locally optimal decision trees

Instead of searching all combinations in Θ simultaneously, recursive partitioning algorithms only consider one split at a time. At each internal node $r \in \{n_1, ..., n_{M-1}\}$, the split variable v_r and the corresponding split point s_r are selected to locally minimize the loss function. Starting with an empty tree $\theta_0 = (\emptyset)$, the tree is first grown recursively and subsequently *pruned* to satisfy the complexity tradeoff:

$$\tilde{\theta}_r = \underset{\theta=\theta_{r-1}\cup(v_r,s_r)}{\operatorname{argmin}} \operatorname{loss}\{Y, f(X,\theta)\} \qquad (r = 1, \ldots, M_{\max} - 1), \tag{3}$$

$$\tilde{\theta} = \underset{\tilde{\theta}_r}{\operatorname{argmin}} \operatorname{loss}\{Y, f(X,\tilde{\theta}_r)\} + \operatorname{comp}(\tilde{\theta}_r). \tag{4}$$

For nontrivial problems, forward-search recursive partitioning methods only search a small fraction of the global search space $(v_1, s_1, \ldots, v_{M_{\max}-1}, s_{M_{\max}-1})$. They only search each (v_r, s_r) once, and independently of the subsequent split rules, hence typically leading to a globally suboptimal solution $\tilde{\theta}$.

Note that the notation above uses an exhaustive search for the r-th split, jointly over (v_r, s_r), as is employed in CART or C4.5. So-called *unbiased* recursive partitioning techniques modify this search by first seleting the variable v_r using statistical significance tests and subsequently selecting the optimal split s_r for that particular variable. This approach is used in conditional inference trees (see Hothorn *et al.* 2006, for references to other algorithms) and avoids selecting variables with many potential splits more often than those with fewer potential splits.

2.3. An illustration of the limitations of locally optimal decision trees

A very simple example that illustrates the limitation of forward-search recursive partitioning methods is depicted in Figure 1. The example only contains two independent variables and can be solved with three splits that partition the input space into four regions. As expected the recursive partitioning methods `rpart` and `ctree` fail to find any split at all, as the loss function on the resulting subsets cannot be reduced by the first split. For methods that explore Θ in a more global fashion it is straightforward to find an optimal solution to this problem. One solution is the tree constructed by `evtree`:

```
Model formula:
Y ~ X1 + X2

Fitted party:
[1] root
```

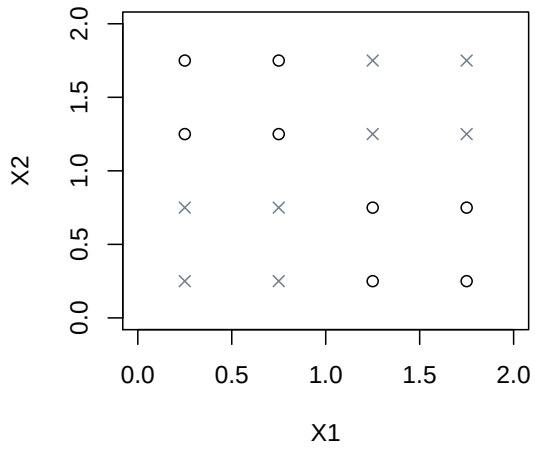


Figure 1: Class distribution of the (X_1, X_2)-plane. The two classes are indicated by black circles and gray crosses.

```
|   [2] X1 < 1.25
|   |   [3] X2 < 1.25: X (n = 4, err = 0.0%)
|   |   [4] X2 >= 1.25: O (n = 4, err = 0.0%)
|   [5] X1 >= 1.25
|   |   [6] X2 < 1.25: O (n = 4, err = 0.0%)
|   |   [7] X2 >= 1.25: X (n = 4, err = 0.0%)

Number of inner nodes:    3
Number of terminal nodes: 4
```

All instances are classified correctly. Each of the terminal nodes 3 and 7 contain four instances of the class `X`. Four instances of class `O` are assigned to each of the terminal nodes 4 and 6.

2.4. Approaches for learning globally optimal decision trees

When compared with the described forward stepwise search, a less greedy approach is to calculate the effects of the split rules deeper down in the tree. In this way optimal trees can be found for simple problems. However, split selection at a given node in Equation 3 has complexity $O(PN)$ (if all P variables are numeric/ordered with N distinct values). Through a global search up to D levels – i.e., corresponding to a full binary tree with $M = 2^D$ terminal nodes – the complexity increases to $O(P^D N^D)$ (Papagelis and Kalles 2001). One conceivable compromise between these two extremes is to look ahead d steps with $1 < d < D$ (see e.g., Esmeir and Markovitch 2007), also yielding a locally optimal tree but less constrained than that from a 1-step-ahead search.

Another class of algorithms is given by stochastic optimization methods that, given an initial tree, seek improved solutions through stochastic changes to the tree structure. Thus, these algorithms try to explore the full parameter space Θ but cannot be guaranteed to find the

globally optimal solution but only an approximation thereof. Besides evolutionary algorithms (Koza 1991), *Bayesian CART* (Denison, Mallick, and Smith 1998) and *simulated annealing* (Sutton 1991) were used successfully to solve difficult classification and regression tree problems. Koza (1991) first formulated the concept of using evolutionary algorithms as a stochastic optimization method to build classification and regression trees. Papagelis and Kalles (2001) presented a classification tree algorithm and provided results on several datasets from the UCI machine learning repository (Frank and Asuncion 2010). Another method for the construction of classification and regression trees via evolutionary algorithms was introduced by Gray and Fan (2008) and Fan and Gray (2005), respectively. Cantu-Paz and Kamath (2003) used an evolutionary algorithm to induce so-called oblique classification trees.

3. The `evtree` algorithm

The general framework of evolutionary algorithms emerged from different representatives. Holland (1992) called his method *genetic algorithms*, Rechenberg (1973) invented *evolution strategies*, and Fogel, Owens, and Walsh (1966) introduced *evolutionary programming*. More recently, Koza (1992) introduced a fourth stream and called it *genetic programming*. All four representatives only differ in the technical details, for example the encoding of the individual solutions, but follow the same general outline (Eiben and Smith 2007). Evolutionary algorithms are being increasingly widely applied to a variety of optimization and search problems. Common areas of application include data mining (Freitas 2003; Cano, Herrera, and Lozano 2003), statistics (de Mazancourt and Calcagno 2010), signal and image processing (Man, Tang, Kwong, and Halang 1997), and planning and scheduling (Jensen 2003).

The pseudocode for the general evolutionary algorithm is provided in Table 1. In the context of classification and regression trees, all *individuals* from the population (of some given size) are θs as defined in Equation 1. The details of their evolutionary selection is given below following the general outline displayed in Table 1.

As pointed out in Section 2, some elements $\theta \in \Theta$ are typically excluded in practice to satisfy minimal subsample size requirements. In the following, the term *invalid node* refers to such excluded cases, not meeting sample size restrictions.

---

1. Initialize the population.
2. Evaluate each individual.
3. While(termination condition is not satisfied) do:
    a. Select parents.
    b. Alter selected individuals via variation operators.
    c. Evaluate new solutions.
    d. Select survivors for the next generation.

Table 1: Pseudocode of the general evolutionary algorithm.

3.1. Initialization

Each tree of the population is initialized with a valid, randomly generated, split rule in the root node. First, v_1 is selected with uniform probability from $1, ..., P$. Second, a split point s_1 is selected. If X_{v_1} is numeric or ordinal with u unique values, a split point s_1 is selected with uniform probability from the $u-1$ possible spit points of X_{v_1}. If X_{v_1} is nominal and has c categories, each $k = 1, ..., c$ has a probability of 50% to be assigned to the left or the right daughter node. In cases where all k are allocated to the same terminal node, the assignment of one category is flipped to the other terminal node. If this procedure results in a non-valid split rule, the two steps of random split variable selection and split point selection are repeated. With the definition of $r = 1$ and the selection of v_1 and s_1, the initialization is complete and each individual of the population of trees is of type $\theta_1 = (v_1, s_1)$.

3.2. Parent selection

In every iteration, each tree is selected once to be modified by one of the variation operators. In cases where the crossover operator is applied, the second parent is selected randomly from the remaining population. In this way, some trees are selected more than once in each iteration.

3.3. Variation operators

Four types of mutation operators and one crossover operator are utilized by our algorithm. In each modification step, one of the variation operators is randomly selected for each tree. The mutation and crossover operators are described below.

Split

Split selects a random terminal-node and assigns a valid, randomly generated, split rule to it. As a consequence, the selected terminal node becomes an internal node r and two new terminal nodes are generated.

The search for a valid split rule is conducted as in see Section 3.1 for a maximum of P iterations. In cases where no valid split rule can be assigned to the internal node at position r, the search for a valid split rule is carried out on another randomly selected terminal node. If, after 10 attempts, no valid split rule can be found, then $\theta_{i+1} = \theta_i$. Otherwise, the set of parameters in iteration $i + 1$ are given by $\theta_{i+1} = \theta_i \cup (v_r, s_r)$.

Prune

Prune chooses a random internal node r, where $r > 1$, which has two terminal nodes as successors and prunes it into a terminal node. The tree's parameters at iteration $i + 1$ are $\theta_{i+1} = \theta_i \setminus (v_r, s_r)$. If θ_i only comprises one internal node, i.e., the root node, then $\theta_{i+1} = \theta_i$.

Major split rule mutation

Major split rule mutation selects a random internal node r and changes the split rule, defined by the corresponding split variable v_r, and the split point s_r. With a probability of 50%, a value from the range $1, ..., P$ is assigned to v_r. Otherwise v_r remains unchanged and only s_r is modified. Again, depending on the domain of X_{v_r}, either a random split point from the

range of possible values of X_{v_r} is selected, or a non-empty set of categories is assigned to each of the two terminal nodes. If the split rule at r becomes invalid, the mutation operation is reversed and the procedure, starting with the selection of r, is repeated for a maximum of 3 attempts. Subsequent nodes that become invalid are pruned.

If no pruning occurs, θ_i and θ_{i+1} contain the same set of parameters. Otherwise, the set of parameters $(v_{m_1}, s_{m_1}, ..., v_{m_f}, s_{m_f})$, corresponding to invalid nodes, is removed from θ_i. Thus, $\theta_{i+1} = \theta_i \setminus (v_{m_1}, s_{m_1}, ..., v_{m_f}, s_{m_f})$.

Minor split rule mutation

Minor split rule mutation is similar to the *major split rule mutation* operator, but it does not alter v_r and only changes the split point s_r by a minor degree. If X_{v_r} is numerical or ordinal the split point s_r is changed by a non-zero number of unique values of X_{v_r}. In cases where X_{v_r} has less then 20 unique values, the split point is change to to the next larger, or the next lower, unique value of X_{v_r}. Otherwise, s_r is randomly shifted by a number of unique values that is not larger than 10% of the range of unique values of X_{v_r}. If X_{v_r} is a nominal variable, with less than 20 categories, one of the categories is randomly modified. Otherwise, at least one and at most 10% of the variable's categories are changed. In cases where subsequent nodes become invalid, further split points are searched that preserve the tree's topology. After five non-successful attempts at finding a topology preserving split point, the non-valid nodes are pruned.

Equivalently to the *major split rule mutation* operator the subsequent solution $\theta_{i+1} = \theta_i \setminus (v_{m_1}, s_{m_1}, ..., v_{m_f}, s_{m_f})$.

Crossover

Crossover exchanges, randomly selected, subtrees between two trees. Let θ_i^1 and θ_i^2 be the two trees chosen from the population for crossover. First, two internal nodes r_1 and r_2 are selected randomly from θ_i^1 and θ_i^2, respectively. Let $\text{sub1}(\theta_i^j, r_j)$ denote the subtree of θ_j rooted by r_j $(j = 1, 2)$, i.e., the tree containing r_j and its descendant nodes. Then, the complementary part of θ_i^j can be defined as $\text{sub2}(\theta_i^j, r_j) = \theta_i^j \setminus \text{sub1}(\theta_i^j, r_j)$. The crossover operator creates two new trees $\theta_{i+1}^1 = \text{sub2}(\theta_i^1, r_1) \cup \text{sub1}(\theta_i^2, r_2)$ and $\theta_{i+1}^2 = \text{sub2}(\theta_i^2, r_2) \cup \text{sub1}(\theta_i^1, r_1)$. If the crossover creates some invalid nods in either one of the new trees θ_{i+1}^1 or θ_{i+1}^2, these are omitted.

3.4. Evaluation function

The evaluation function represents the requirements the population should adapt to. In general, these requirements are formulated by Equation 2. A suitable evaluation function for classification and regression trees minimizes the models' accuracy on the training data, and the models' complexity. This subsection describes the currently implemented choices of evaluation functions for classification and for regression.

Classification

The quality of a classification tree is most commonly measured as a function of its misclassification MC and the complexity of a tree by a function of the number of its terminal nodes M. `evtree` uses $2N \cdot \text{MC}(Y, f(X, \theta))$ as a loss function. The number of terminal nodes, weighted

by $\log N$ and a user-specified parameter α, measures the complexity of trees.

$$\begin{aligned} \text{loss}(Y, f(X, \theta)) &= 2N \cdot \text{MC}(Y, f(X, \theta)) \\ &= 2 \cdot \sum_{n=1}^{N} I(Y_n \neq f(X_{\cdot n}, \theta)), \\ \text{comp}(\theta) &= \alpha \cdot M \cdot \log N. \end{aligned} \tag{5}$$

With these particular choices, Equation 2 seeks trees $\hat{\theta}$ that minimize the misclassification loss at a BIC-type tradeoff with the number of terminal nodes.

Other, existing and commonly used choices of evaluation functions include the *Bayesian information criterion* (BIC, as in Gray and Fan 2008) and *minimum description length* (MDL, as in Quinlan and Rivest 1989). For both evaluation functions deviance is used for accuracy estimation. Deviance is usually preferred over the misclassification rate in recursive partitioning methods, as it is more sensitive to changes in the node probabilities (Hastie, Tibshirani, and Friedman 2009, pp. 308–310). However, this is not necessarily an advantage for global tree building methods like evolutionary algorithms.

Regression

For regression trees, accuracy is usually measured by the mean squared error MSE. Here, it is again coupled with a BIC-type complexity measure:

Using $N \cdot \log \text{MSE}$ as a loss function and $\alpha \cdot 4 \cdot (M + 1) \cdot \log N$ as the complexity part, the general formulation of the optimization problem in can be rewritten as:

$$\begin{aligned} \text{loss}(Y, f(X, \theta)) &= N \log \text{MSE}(Y, f(X, \theta)) \\ &= N \log \left\{ \sum_{n=1}^{N} (Y_n - f(X_{\cdot n}, \theta)^2) \right\}, \\ \text{comp}(\theta) &= \alpha \cdot 4 \cdot (M + 1) \cdot \log N. \end{aligned} \tag{6}$$

Here, $M+1$ is the effective number of estimated parameters, taking into account the estimates of a mean parameter in each of the terminal nodes and the constant error variance term. With $\alpha = 0.25$ the criteria is, up to a constant, equivalent to the BIC used by Fan and Gray (2005). However, the effective number of parameters estimated for is actually much higher than $M+1$ due to the selection of parameters in the split variable and the selection of the variable itself. It is however unclear how these should be counted (Gray and Fan 2008; Ripley 2008, p. 222). Therefore, a more conservative default value of $\alpha = 1$ is assumed.

3.5. Survivor selection

The population size stays constant during the evolution and only a fixed subset of the candidate solutions can be kept in memory. A common strategy is the $(\mu + \lambda)$ selection, where μ survivors for the next generation are selected from the union of μ parents and λ offsprings. An alternative approach is the (μ, λ) strategy where μ survivors for the next generation are selected from λ offsprings.

Our algorithm uses $(1 + 1)$ selection, where one parent solution competes with one offspring for a place in the population. In the case of a mutation operator either the solution before θ_i

or after modification θ_{i+1} is kept in memory. In the case of the crossover operator, the initial solutions of θ_i^1 competes with its subsequent solutions θ_{i+1}^1. Correspondingly, one of the two solutions θ_i^2 and θ_{i+1}^2 is rejected. The survivor selection is done deterministically. The tree with lower fitness, according to the evaluation function, is rejected. Note that, due to the definition of the crossover operator, some trees are selected more than once in an iteration. Correspondingly, these trees undergo the survival selection process more than once in an iteration.

As in classification and regression tree analysis the individual solutions are represented by trees. This design offers computational advantages over $(\mu + \lambda)$, with $\mu > 1$ and $\lambda > 1$, and (μ, λ) strategies. In particular, for the application of mutation operators no new trees have to be constructed. The tree after modification is simply accepted or reversed to the previous solution.

There are two important issues in the evolution process of an evolutionary algorithm: population diversity and selective pressure (Michalewicz 1994). These factors are related, as with increasing selective pressure the search is focused more around the currently best solutions. An overly strong selective pressure can cause the algorithm to converge early in local optima. On the other hand, an overly weak selective pressure can make the search ineffective. Using a $(\mu + \lambda)$ strategy, a strong selective pressure can occur in situations as follows. Suppose the b-th tree of the population is one of the fittest trees in iteration i, and in iteration i one split rule of the b-th tree is changed only by a minor degree. Then very few instances are classified differently and the overall misclassification might not even change. However, as they represent one of the best solutions in iteration i, they are both selected for the subsequent population. This situation can occur frequently, especially when a fine-tuning operator like the *minor split rule mutation* is used. Then, the diversity of different trees is lost quickly and the algorithm likely terminates in a local optimum. The $(1 + 1)$ selection mechanism clearly avoids these situations, as only the parent or the offspring can be part of the subsequent population.

3.6. Termination

Using the default parameters, the algorithm terminates when the quality of the best 5% of trees stabilizes for 100 iterations, but not before 1000 iterations. If the run does not converge the algorithm terminates after a user-specified number of iterations. In cases where the algorithm does not converge, a warning message is written to the command line. The tree with the highest quality according to the evaluation function is returned.

4. Implementation and application in practice

Package **evtree** provides an efficient implementation of an evolutionary algorithm that builds classification trees in R. CPU- and memory- intensive tasks are fully computed in C++, while the user interfaces and plot functions are written in R. The `.C()` interface (Chambers 2008) was used to pass arguments between the two languages. **evtree** depends on the **partykit** package (Hothorn and Zeileis 2011), which provides an infrastructure for representing, summarizing, and visualizing tree-structured models.

4.1. User interface

The principal function of the **evtree** package is the eponymous function `evtree()` taking arguments

```
evtree(formula, data = list(), weights = NULL, subset = NULL,
  control = evtree.control(...), ...)
```

where `formula`, `data`, `weights`, and `subset` specify the data in the usual way, e.g., via `formula = y ~ x1 + x2`. Additionally, `control` comprises a list of control parameters

```
evtree.control(minbucket = 7L, minsplit = 20L, maxdepth = 9L,
  niterations = 10000L, ntrees = 100L, alpha = 1,
  operatorprob = list(pmutatemajor = 0.2, pmutateminor = 0.2,
    pcrossover = 0.2, psplit = 0.2, pprune = 0.2),
  seed = NULL, ...)
```

where the parameters `minbucket`, `minsplit`, and `maxdepth` constrain the solution to a minimum number of observations in each terminal node, a minimum number of observation in each internal node and a maximum tree depth. Note that the memory requirements increase by the square of the maximum tree depth. Parameter `alpha` regulates the complexity parameter α in Equation 5 and 6, respectively. `niterations` and `ntrees` specify the maximum number of iterations and the number of trees in the population, respectively. With the argument `operatorprob`, user-specified probabilities for the variation operators can be defined. For making computations reproducible, argument `seed` is an optional integer seed for the random number generator (at C++ level). If not specified, the random number generator is initialized by `as.integer(runif(1, max = 2^16))` in order to inherit the state of `.Random.seed` (at R level). If set to `-1L`, the seed is initializied by the system time.

The trees computed by `evtree` inherit from class '`party`' supplied by the **partykit** package. The methods inherited in this way include standard `print()`, `summary()`, and `plot()` functions to display trees and a `predict()` function to compute the fitted response or node number etc.

4.2. Case study: Customer targeting

An interesting application for classification tree analysis is target marketing, where limited resources are aimed at a distinct group of potential customers. An example is provided by Lilien and Rangaswamy (2004) in the *Bookbinder's Book Club* marketing case study about a (fictitious) American book club. In this case study, a brochure of the book "The Art History of Florence" was sent to 20,000 customers, 1,806 of which bought the book. The dataset contains a subsample of 1,300 customers for building a predictive model of customer choice.

Besides predictive accuracy, model complexity is a crucial issue in this application: Smaller trees are easier to interpret and communicable to marketing experts and management professionals. Hence, we use `evtree` with a maximal depth of two levels of splits only. This is contrasted with `rpart` and `ctree` with and without such a restriction of tree depth to show that the evolutionary search of the global parameter space can be much more effective in balancing predictive accuracy and complexity compared to forward-search recursive partitioning.

All trees are constrained to have a minimum number of 10 observations per terminal node. Additionally, a significance level of 1% is employed in the construction of conditional inference trees which is more appropriate than the default 5% level for 1,300 observations. To provide uniform visualizations and predictions of the fitted models, 'party' objects are used to represent all trees. For, 'rpart' trees **partykit** provides a suitable `as.party()` method while a reimplementation of `ctree()` is provided in **partykit** (as opposed to the original in **party**) that directly leverages the 'party' infrastructure.

First, the data is loaded and the forward-search trees are grown with and without depth restriction, visualizing the unrestricted trees in Figure 2.

```
R> data("BBBClub", package = "evtree")
R> library("rpart")
R> rp  <- as.party(rpart(choice ~ ., data = BBBClub, minbucket = 10))
R> rp2 <- as.party(rpart(choice ~ ., data = BBBClub, minbucket = 10,
+    maxdepth = 2))
R> ct  <- ctree(choice ~ ., data = BBBClub, minbucket = 10, mincrit = 0.99)
R> ct2 <- ctree(choice ~ ., data = BBBClub, minbucket = 10, mincrit = 0.99,
+    maxdepth = 2)
R> plot(rp)
R> plot(ct)
```

With the objective of building a smaller, but at still accurate tree, `evtree` is constrained to a maximum tree depth of 2, see Figure 3.

```
R> set.seed(1090)
R> ev <- evtree(choice ~ ., data = BBBClub, minbucket = 10, maxdepth = 2)
```

The resulting evolutionary tree is printed below and visualized in Figure 3.

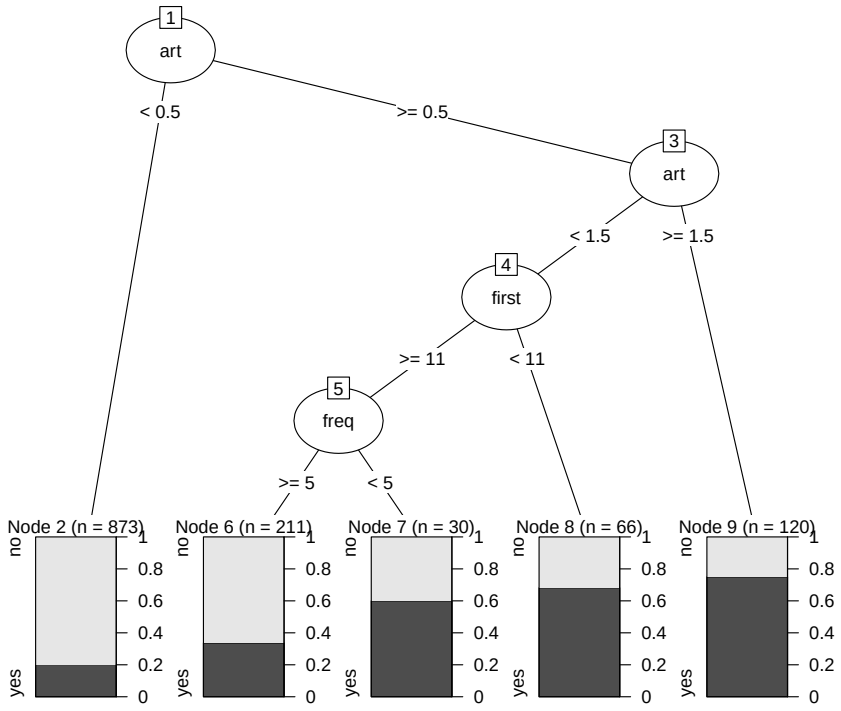
```
R> plot(ev)
R> ev

Model formula:
choice ~ gender + amount + freq + last + first + child + youth +
    cook + diy + art

Fitted party:
[1] root
|   [2] first < 12
|   |   [3] art < 1: no (n = 250, err = 30.8%)
|   |   [4] art >= 1: yes (n = 69, err = 30.4%)
|   [5] first >= 12
|   |   [6] art < 2: no (n = 864, err = 21.8%)
|   |   [7] art >= 2: yes (n = 117, err = 25.6%)

Number of inner nodes:    3
Number of terminal nodes: 4
```

`rpart`



`ctree`

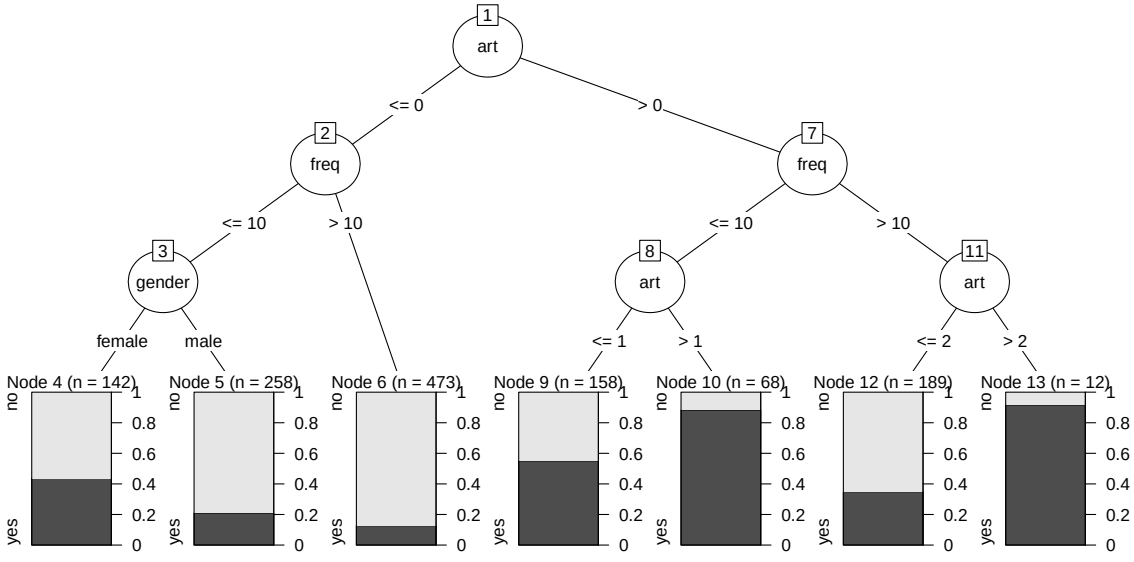


Figure 2: Trees for customer targeting constructed by `rpart` (upper panel) and `ctree` (lower panel). The target variable is the customer's choice of buying the book. The variables used for splitting are the number of art books purchased previously (`art`), the number of months since the first purchase (`first`), the frequency of previous purchases at the Bookbinder's Book Club (`freq`) and the customer's `gender`.

`evtree`

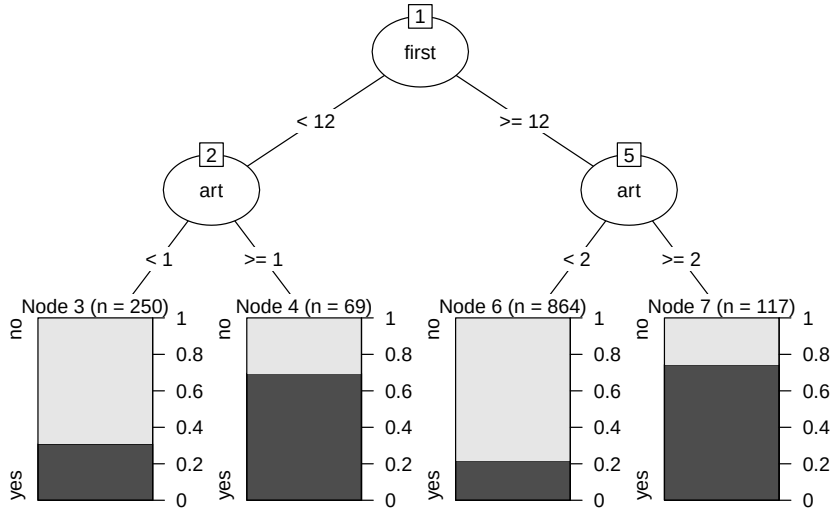


Figure 3: Tree for customer targeting constructed by `evtree` The target variable is the customer's choice of buying the book. The variables used for splitting are the number of art books purchased previously (`art`) and the number of months since the first purchase `first`.

Not surprisingly, the explanatory variable `art` – the number of art books purchased previously at the book club – plays a key role in all constructed classification trees along with the number of months since the first purchase (`first`), the frequency of previous purchases (`freq`) and the customer's `gender`. Interestingly, though, the forward-search trees select the arguably most important variable in the first split while the evolutionary tree uses `first` in the first split and `art` in both second splits. Thus, the evolutionary tree uses a different cutoff in `art` for bookclub members that joined in the last year as opposed to older customers. While the former are predicted to be buyers if they previously bought at least one art book, the latter are predicted to purchase the advertised art book only if they previously bought at least two other art books. Certainly, this classification is easy to understand and communicate (helped by Figure 3) to practitioners.

However, we still need to answer the question how well it performs in contrast to the other trees. Hence, we set up a function `mc()` the computes the misclassification rate as a measure of predictive accuracy and a function `evalfun()` that computes the evaluation function (i.e., penalized by tree complexity) from Equation 5.

```
R> mc <- function(obj) 1 - mean(predict(obj) == BBBClub$choice)
R> evalfun <- function(obj) 2 * nrow(BBBClub) * mc(obj) +
+    width(obj) * log(nrow(BBBClub))
R> trees <- list("evtree" = ev, "rpart" = rp, "ctree" = ct, "rpart2" = rp2,
+    "ctree2" = ct2)
R> round(sapply(trees, function(obj) c("misclassification" = mc(obj),
+    "evaluation function" = evalfun(obj))), digits = 3)
```

```
                      evtree   rpart   ctree  rpart2  ctree2
misclassification      0.243   0.238   0.248   0.262   0.255
evaluation function 660.680 655.851 694.191 701.510 692.680
```

Not surprisingly the evolutionary tree `ev` outperforms the depth-restricted trees `rp2` and `ct2`, both in terms of misclassification and the penalized evaluation function. However, it is interesting to see that `ev` performs even better than the unrestricted conditional inference tree `ct` and is comparable in performance to the unrestricted CART tree `rp`. Hence, the practitioner may choose the evolutionary tree `ev` as it is the easiest to communicate.

Although the constructed trees are considerably different, the code above shows that the predictive accuracy is rather similar. Moreover, below we see that the structure of the individual predictions on the dataset are rather similar as well:

```
R> ftable(tab <- table(evtree = predict(ev), rpart  = predict(rp),
+    ctree  = predict(ct), observed = BBBClub$choice))

                   observed  no yes
evtree rpart ctree
no     no    no             799 223
             yes             38  24
       yes   no               0   0
             yes             12  18
yes    no    no               0   0
             yes              0   0
       yes   no              21  19
             yes             30 116

R> sapply(c("evtree", "rpart", "ctree"), function(nam) {
+    mt <- margin.table(tab, c(match(nam, names(dimnames(tab))), 4))
+    c(abs = as.vector(rowSums(mt))[2],
+      rel = round(100 * prop.table(mt, 1)[2, 2], digits = 3))
+  })

     evtree   rpart   ctree
abs 186.000 216.000 238.000
rel  72.581  70.833  66.387
```

In this case, `evtree` classifies less customers (186) as buyers as `rpart` (216) and `ctree` (238). However, `evtree` achieves the highest proportion of correct classification among the declared buyers: 72.6% compared to 70.8% (`rpart`) and 66.4% (`ctree`).

In summary, this illustrates how `evtree` can be employed to better balance predictive accuracy and complexity by searching a larger space of potential trees. As a final note, it is worth pointing out that in this setup, several runs of `evtree()` with the same parameters typically lead to the same tree. However, this may not always be the case. Due to the stochastic nature of the search algorithm and the vast search space, trees with very different structures but similar evaluation function values may be found by subsequent runs of `evtree()`. Here, this problem is alleviated by restricting the maximal depth of the tree, yielding a clear solution.

5. Performance comparison

In this section, we compare `evtree` with `rpart` and `ctree` in a more rigorous benchmark comparison.

In the first part of the analysis (Section 5.1) the algorithms are compared on 14 benchmark datasets that are publicly available and 3 real-world datasets from the Austrian *Diagnosis Related Group (DRG)* system (Bundesministerium für Gesundheit 2010). The analysis is based on the evaluation of 250 bootstrap samples for each of the 20 datasets. The misclassification rate on the *out-of-bag* (Hothorn, Leisch, Zeileis, and Hornik 2005) samples is used as a measure of predictive accuracy. Furthermore, the complexity is estimated by the number of terminal nodes.

In the second part (Section 5.2) the algorithms' performances are assessed on an artificial chessboard problem that is simulated with different noise levels. The estimation of predictive accuracy and the number of terminal nodes is based on 250 realizations for each simulation.

All models are constrained to a minimum number of 7 observations per terminal node, 20 observations per internal node and a maximum tree depth of 9. Apart from that, the default settings of the algorithms are used. For assessment of significant differences in predictive accuracy and complexity, respectively, Dunnett's correction from R package **multcomp** (Hothorn, Bretz, and Westfall 2008) was used for calculating simultaneous 95% confidence intervals on the individual datasets.

As missing values are currently not supported by `evtree` (e.g., by surrogate splits), the 16 missing values in the *Breast Cancer Database* – the only dataset in the study with missing values – were removed before analysis.

5.1. Benchmark and real-world problems

In Table 2 the benchmark and real-world datasets from the Austrian DRG system are described. In the Austrian DRG system, resources are allocated to hospitals by simple rules mainly regarding the patients' diagnoses, procedures, and age. Regression tree analysis is performed to model patient groups with similar resource consumption. A more detailed description of the datasets and the application can be found in Grubinger, Kobel, and Pfeiffer (2010).

The relative performance of `evtree` and `rpart` is summarized in Figure 4 (upper panels). Performance differences are displayed relative to `evtree`'s performance. For example, on the *Glass* dataset, the average misclassification rate of `rpart` is 2.7% higher than the misclassification rate of `evtree`. It can be observed that on 12 out of 17 datasets `evtree` significantly outperforms `rpart` in terms of predictive accuracy. Only on the *Contraceptive Method* dataset `evtree` performs slightly worse. In terms of complexity, `evtree` models are significantly more complex on 10 and less complex on 7 datasets.

Figure 4 (lower panels) summarizes the relative performance of `evtree` and `ctree`. For 15 out of 17 datasets `evtree` shows a better predictive performance. The algorithms' performances is significantly worse on the *MEL0101* dataset, where the average misclassifiation rate of `ctree` is 5.6% lower. However, on this dataset, `ctree` models are on average 86.5% larger than `evtree` models. The relative complexity of `evtree` models is significantly smaller for 15 and larger for 1 dataset.

Disadvantages of the `evtree` algorithm are computation time and memory requirements.

Dataset	Instances	Attributes				
		Binary	Nominal	Ordered	Metric	Classes
Glass identification#	214	-	-	-	9	6
Statlog heart*	270	3	3	1	6	2
Ionosphere#	351	2	-	-	32	2
Musk+	476	-	-	-	166	2
Breast cancer database#	685	-	4	5	-	2
Pima Indians diabetes#	768	-	-	-	8	2
Vowel#	990	-	1	-	9	11
Statlog German credit*	1000	2	10	1	7	2
Contraceptive method*	1437	3	-	4	2	3
DNA#	3186	180	-	-	-	3
Spam+	4601	-	-	-	57	2
MAGIC gamma telescope*	19020	-	-	-	10	2
Servo#	167	-	4	-	-	-
Boston housing#	506	1	-	-	12	-
MEL0101◇	875	1	4	1	108	-
HDG0202◇	3933	1	7	1	46	-
HDG0502◇	8251	1	7	1	91	-

Table 2: Description of the evaluated benchmark datasets. The datasets marked with $*$ originate from the UCI machine learning repository (Frank and Asuncion 2010) and are made available in the **evtree** package. Datasets marked with # and + are from the R packages **mlbench** (Leisch and Dimitriadou 2010) and **kernlab** (Karatzoglou *et al.* 2004), respectively. The three real-world datasets from the Austrian DRG system are marked with ◇.

While the smallest of the analyzed datasets, *Glass identification*, only needed approximately 4–6 seconds to fit, larger datasets demanded several minutes. The fit of a model from the largest dataset, *MAGIC gamma telescope*, required approximately 40–50 minutes and a main memory of 400 Mbit. The required resources were measured on an Intel Core 2 Duo with 2.2 GHz and 2 GB RAM using the 64-bit version of Ubuntu 10.10.

Another important issue to be considered is the random nature of evolutionary algorithms. For larger datasets, frequently, considerable different solutions exist that yield a similar or even the same evaluation function value. Therefore, subsequent runs of `evtree` can result in very different tree structures. This is not a problem if the tree is intended only for predictive purposes, and it is also not a big issue for many decision and prognosis tasks. Typically, in such applications, the resulting model has to be accurate, compact, and meaningful in its interpretation, but the particular tree structure is of secondary importance. Examples of such applications include the presented marketing case study and the Austrian DRG system. In cases where a model is not meaningful in its interpretation, the possibility of constructing different trees can even be beneficial. However, if the primary goal is to interpret relationships in the data, based on the selected splits, the random nature of the algorithm has to be considered.

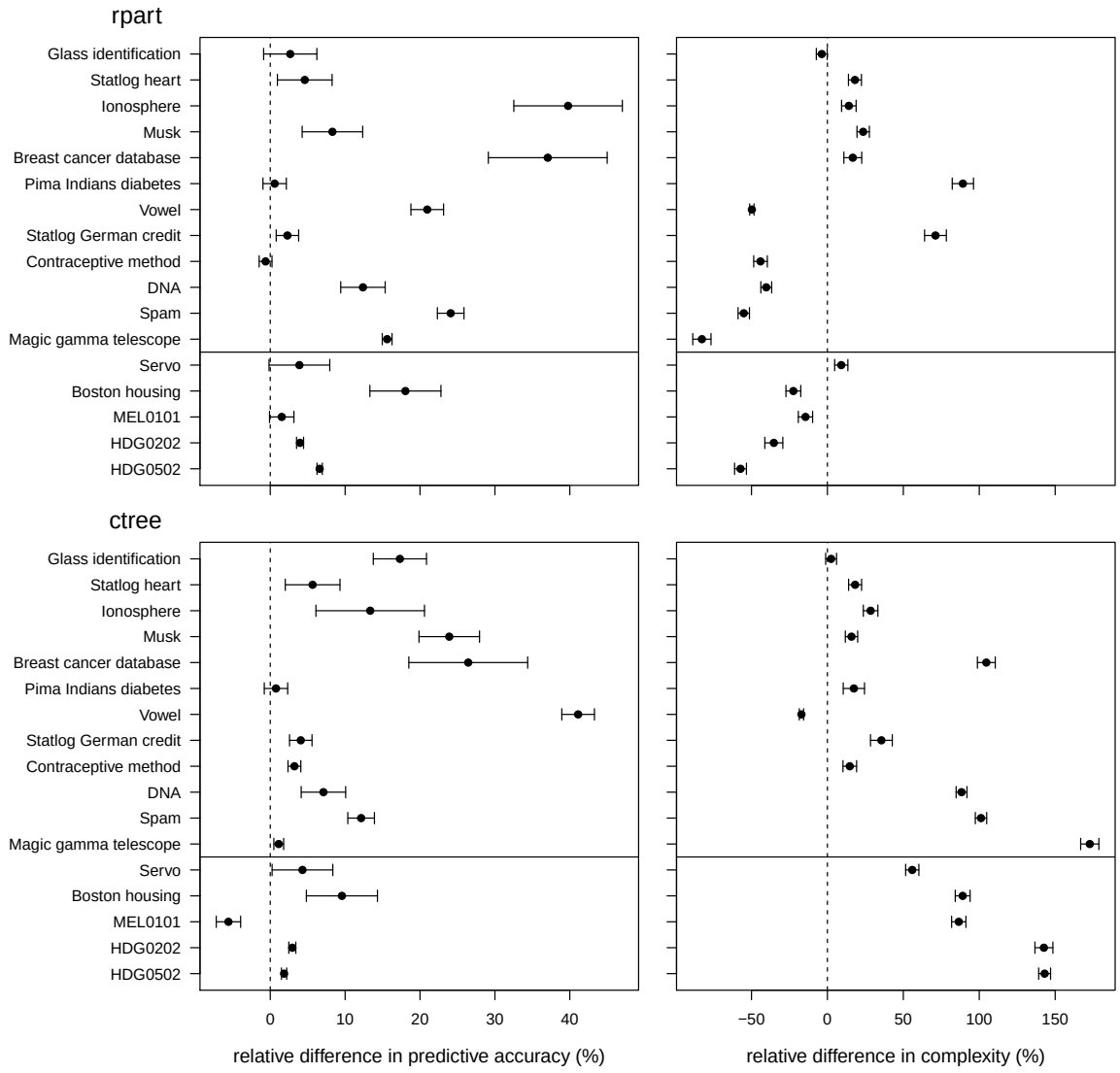


Figure 4: Performance comparison of `evtree` vs. `rpart` (upper panels) and `evtree` vs. `ctree` (lower panels). Prediction error (left panels) is compared by the relative difference of the misclassification rate or the mean-squared error. The complexity (right panels) is compared by the relative difference of the number of terminal nodes.

5.2. Artificial problem

In this section we demonstrate the ability of `evtree` to solve an artificial problem that is difficult to solve for most recursive classification tree algorithms (Loh 2009). The data was simulated with 2000 instances for both the training-set and the test-set. Predictor variables X_1 and X_2 are simulated to be uniformly distributed in the interval $[0, 4]$. The classes are distributed in alternating squares forming a 4×4 chessboard in the (X_1, X_2)-plane. One realization of the simulated data is shown in Figure 5. Furthermore, variables $X_3 - X_8$ are

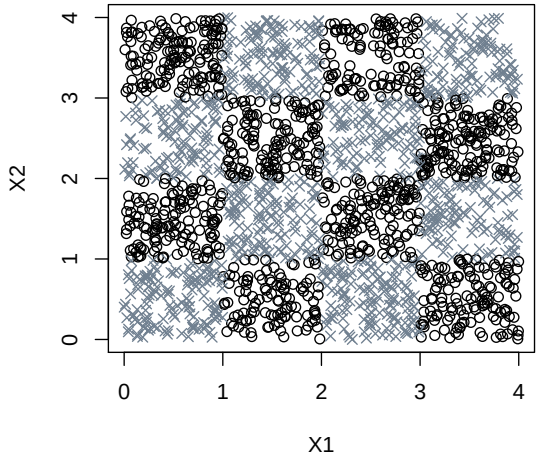


Figure 5: Class distribution of the simulated 4×4 chessboard problem with zero noise, plotted on the (X_1, X_2)-plane. The two classes are indicated by black circles and gray crosses, respectively.

noise variables that are uniformly distributed on the interval [0, 1]. The ideal model for this problem only uses variables X_1 and X_2 and has 16 terminal nodes, whereas each terminal node comprises the observations that are in the region of one square. Two further simulations are done in the same way, but 5% and 10% percent of the class labels are randomly changed to the other class.

The results are summarized in Table 3. It can be seen that, in the absence of noise, `rpart` models on average classify 69.1% of the data points correctly and had 16.6 terminal nodes. An average `ctree` model only has 1.1 terminal nodes and a classification accuracy of 49.9%. In contrast, `evtree` classifies 93.2% of the instances correctly and requires 14.4 terminal nodes. In the presence of 5% and 10% noise, `evtree` classifies 89.0% and 84.5% of the data correctly.

Noise (%)	Accuracy			Terminal nodes		
	`evtree`	`rpart`	`ctree`	`evtree`	`rpart`	`ctree`
0	93.2(7.4)	69.1(18.3)	49.9(1.1)	14.4(2.2)	16.6(8.2)	1.1(0.3)
5	89.0(6.8)	65.7(17.4)	50.1(1.6)	14.4(2.2)	14.6(8.0)	1.1(0.7)
10	84.5(5.6)	62.8(14.1)	50.1(1.3)	14.6(2.0)	14.3(7.3)	1.1(0.4)

Table 3: Mean (and standard deviation) of accuracy and number of terminal nodes for simulated 4×4 chessboard examples.

6. Conclusions

In this paper, we presented the **evtree** package, which implements classification and regression

trees that are grown by an evolutionary algorithm. The package uses standard `print()`, `summary()`, and `plot()` functions to display trees and a `predict()` function to predict the class labels of new data from the **partykit** package. As evolutionary learning of trees is computationally demanding, most calculations are conducted in C++. At the moment our algorithm does not support parallelism. However, we intend to extend **evtree** to parallel computing.

The comparisons with recursive partitioning methods `rpart` and `ctree` in Sections 4 and 5 shows that `evtree` performs very well in a wide variety of settings, often balancing predictive accuracy and complexity better than the forward-search methods.

However, the goal of `evtree` is not to replace the well-established algorithms like `rpart` and `ctree` but rather to complement the tree toolbox with an alternative method which may perform better given sufficient amounts of time and main memory. By the nature of the algorithm it is able to discover patterns which cannot be modeled by a greedy forward-search algorithm. As `evtree` models can be substantially different to recursively fitted models, it can be beneficial to use both approaches, as this may reveal additional relationships in the data.

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