Genetic Adversarial Training of Decision Trees

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Abstract

We put forward a novel learning methodology for ensembles of decision trees based on a genetic algorithm which is able to train a decision tree for maximizing both its accuracy and its robustness to adversarial perturbations. This learning algorithm internally leverages on a complete formal verification technique for robustness properties of decision trees based on abstract interpretation, a well known static program analysis technique. We implemented this genetic adversarial training algorithm in a tool called Meta-Silvae (MS) and we experimentally evaluated it on some reference datasets used in adversarial training. The experimental results show that MS is able to train robust models which compete with and often improve on the current state-of-the-art of adversarial training of decision trees while being much more compact and therefore interpretable and efficient tree models.

1 Introduction

Adversarial machine learning [27, 34] is a hot topic studying vulnerabilities of machine learning (ML) models in adversarial scenarios. Adversarial examples have been found in diverse application fields of ML, ranging from image classification to malware detection, and the current defense techniques include adversarial model training, input validation, testing and automatic verification of learning algorithms. A ML classifier is defined to be robust for some (typically very small) perturbation of its input samples, which represents an adversarial attack, when it assigns the same class to all the samples within that perturbation, so that unnoticeable malicious alterations of input objects should not deceive a robust classifier.

This work focuses on the robustness of ML classifiers consisting of decision tree ensembles, such as random forests and gradient boosted decision trees, which are well known for being both accurate and interpretable ML models and are widely used in adversarial scenarios. It has been amply shown that decision trees can be very non-robust [30, Section 8.1.4], although it is only recently that robustness verification and adversarial training of tree models started to be an active subject of investigation [2, 12, 14, 15, 21, 44, 51, 52].
1.1 Main Contributions

Genetic algorithms (GAs) [28, 50] provide a widespread effective search technique which computes the next set of hypotheses by repeatedly mutating and then combining parts of the best currently known hypotheses. A number of successful ML methodologies for decision trees are based on GAs [4, 22, 25, 31, 40, 53]. Recently, some GAs have also been investigated for adversarial training of neural networks [17, 54]. To the best of our knowledge, the use of GAs for adversarial training of ensembles of decision trees is still an unexplored topic. In this work we design and experimentally evaluate an adversarial training algorithm for decision tree ensembles based on a genetic algorithm, that we called Meta-Silvae (MS, acronym of Magister Efficiens Temperat Arbores Silva, Latin for “the efficient master mixes the trees of the forest”). and aims at maximizing both accuracy and robustness of decision trees. MS relies on an open source verification method of the robustness of ensembles of decision trees called silva [44]. This robustness verification algorithm silva performs an abstract interpretation-based static analysis [19, 46] of a decision tree classifier which is able to abstractly compute the exact set of leaves of a decision tree which are reachable from an adversarial region. By exploiting this robustness information provided by silva, MS is designed as a genetic algorithm that maximizes an objective performance function which is a linear combination of accuracy and robustness. MS is based on some well established design choices of GAs: (1) elitist selection strategy; (2) roulette wheel selection; (3) single-point crossover; (4) offspring mutation. MS has been implemented in C and experimentally evaluated on the reference datasets for adversarial training of decision tree ensembles. MS has been compared with random forests [8] and with the current state-of-the-art of adversarially trained gradient boosted decision trees [2, 14]. Overall, the experimental results show that MS trained models significantly increase their robustness over natural random forests on average of, resp., $3.4 \times$ (with an average absolute gain of $+54.3\%$) while at the same time preserving a comparable accuracy with an expected slight drop (on average $-1.8\%$). Moreover, MS models compete with and often improve on the state-of-the-art of adversarially trained gradient boosted decision trees while being much more compact and therefore interpretable (as advocated by [38] for all ML models) and efficient (as advocated by [1, Section 3.1] for ensemble models) tree models.

1.2 Illustrative Example

Fig. 1 depicts an example of an artificial dataset consisting of 100 2-dimensional random samples $(x_1, x_2) \in [0, 1]^2$ labeled as a blue cross when $x_1^2 + x_2^2 < 0.5$ holds and as a red bullet otherwise. The left diagram represents a decision tree classifier which has been trained by scikit-learn, while the right diagram has been trained by MS using as objective performance function $\varphi(\text{accuracy, robustness}) = 90\% \text{ accuracy} + 10\% \text{ robustness}$. The two diagrams in Fig. 1 show that both classifiers achieve 100% accuracy. The scikit-learn tree introduces two blue regions cutting the red area in order to achieve an accurate classification of two
blue cross samples, thus making the classification on some samples close to the borders not robust for a 2% square perturbation surrounding each input sample. The MS training algorithm is able to avoid this lack of robustness since it searches for cut hyperplanes which preserve robustness whenever possible. As displayed by the two diagrams, robustness with respect to the 2% square perturbation turns out be, resp., 87% and 94% for the left and right decision trees, thus showing a significant increase while still preserving the same 100% accuracy.

1.3 Related Work

While adversarial training of neural networks has been widely studied, few works addressed how to train decision trees which are robust to adversarial attacks [2, 11, 12, 14]. In particular, we compared our experimental results with the robust gradient boosted decision trees of [2, 14]. Abstract interpretation [19, 46] techniques have been fruitfully applied for designing precise and scalable robustness verification algorithms and adversarial training techniques for a range of ML models [10, 26, 36, 37, 43, 44, 47, 48, 49]. In particular, to our knowledge, [36] is the only work using an abstract interpretation technique for adversarial training of ML models, notably deep neural networks.

2 Background

2.1 Classifiers and Metrics

Given an input space $X \subseteq \mathbb{R}^d$ of numerical vectors and a finite set of labels/classes $\mathcal{L} = \{y_1, \ldots, y_m\}$, a classifier is a function $C : X \to \wp_{\neq}(\mathcal{L})$, where $\wp_{\neq}(\mathcal{L})$ denotes the set of nonempty subsets of $\mathcal{L}$. $C$ associates at least one label to every input in $X$ and multiple output labels can be used to model ties in
output classification (e.g. ties in voting schemes). Training algorithms take a
ground truth dataset $D \subseteq X \times \mathcal{L}$ as input and output a classifier $C : X \to \varphi_\lambda(\mathcal{L})$
which minimizes/maximizes some criteria such as a loss function for neural
networks or information gain for decision trees.

Classifiers can be evaluated and compared on the basis of several perfor-
man ce metrics. Accuracy on a test set is a standard metric for assessing a
classification model: given a test set $T \subseteq X \times \mathcal{L}$ of correctly labeled samples,
the accuracy of a classifier $C : X \to \varphi_\lambda(\mathcal{L})$ on $T$ is $acc_T(C) \triangleq \{(x, y) \in T \mid C(x) = \{y\}\}/|T|$. One typically aims at training classifiers having a
nearly perfect accuracy on suitably crafted test sets. However, according to
a growing belief [27], accuracy is not enough in ML, because the robustness
properties of a classifier may affect its safety and generalization. Given a per-
turbation function $P : X \to \varphi(X)$ modeling a notion of closeness for input
samples, the robustness of $C$ w.r.t. $P$ for a test set $T$ is defined by $rob_{T, P}(C) \triangleq \{|(x, y) \in T \mid C(x) = \{y\}, \forall x' \in P(x) : C(x') = C(x)\}|/|T|$. Perturbation re-
regions $P(x) \subseteq X$ are used to model adversarial attacks to input samples $x$, i.e.,
negligible alterations of input vectors aimed at deceiving a classifier. Widely
studied perturbations are those induced by $\ell_p$ norms, in particular the $\ell_\infty$
maximum norm [13], which, given an alteration threshold $\epsilon > 0$, defines a per-
turbation $P_{\infty, \epsilon} : X \to \varphi(X)$ as follows: $P_{\infty, \epsilon}(x) \triangleq \{x' \in X \mid \|x - x'\|_\infty \leq \epsilon\}$, where $\|x_1, \ldots, x_d\|_\infty = \max\{|x_1|, \ldots, |x_d|\}$. We also consider a more general
definition of robustness called stability which encodes the ability of a classifier
$C$ of consistently producing the same output on perturbations of input samples,
therefore including the cases where $C$ is inaccurate on some input: this is de-
defined as $st_{T, P}(C) \triangleq \{|(x, y) \in T \mid \forall x' \in P(x) : C(x') = C(x)\}|/|T|$. We will
mostly use stability rather than robustness since we deem stability to be a more
comprehensive metric to use in adversarial training.

2.2 Decision Trees and Tree Ensembles

Decision trees are well established ML models used for both classification and
regression tasks. In this work we consider standard classification trees com-
monly known as CART (Classification and Regression Trees) [9]. A classifi-
cation decision tree $t : X \to \varphi_\lambda(\mathcal{L})$ is inductively defined as follows. (1) A
base tree $t$ is a leaf $\lambda$ storing a frequency distribution of labels for the sam-
ple of the training set which some algorithmic rule (canonically the maximum
frequency) converts to one or more predicted labels; thus, we simply consider
$\lambda \in \varphi_\lambda(\mathcal{L})$ and therefore, for all $x \in X$, $t(x) = \lambda$. (2) A composite tree
$t$ is $\gamma(\text{split}, t_l, t_r)$ where $\text{split} : X \to \{t, f\}$ is a Boolean split criterion for
the internal parent node of its left and right subtrees $t_l$ and $t_r$; thus, for all
$x \in X$, $t(x) = \text{if } \text{split}(x) \text{ then } t_l(x) \text{ else } t_r(x)$. A tree stump is of the form
$\gamma(\text{split}, \lambda_l, \lambda_r)$, i.e., it has a single internal node and two leaves. The training
of a decision tree $t$ guarantees that every leaf of $t$ is reachable from at least
one sample in the training set. Although split rules in general could be of any
type, the most common decision trees employ univariate hard splits of the form
$\text{split}(x) \triangleq x_i \leq k$ for some feature $i \in [1, d]$ and threshold $k \in \mathbb{R}$.
Tree ensembles, also known as forests, are sets of decision trees which together contribute to formulate a unique classification output. Training algorithms as well as methods for computing the final output class(es) vary among different tree ensemble models. Random forests (RF) [8] are a major instance of tree ensemble where each tree of the ensemble is trained independently from the other trees on a random subset of the features. Gradient boosted decision trees (GBDT) [24] represent a different training algorithm where an ensemble of trees is incrementally built by training each new tree on the basis of the data samples which are mis-classified by the previous trees. For RFs, the final classification output is typically obtained through a voting mechanism (e.g., majority voting), while GBDTs are usually trained for binary classification problems and use some binary reduction scheme, such as one-vs-all or one-vs-one, for multi-class classification.

Our MS trees are standard CARTs and we will use the random forest model for training an ensemble of MS trees. In our experimental evaluation, on the one hand we will compare MS models with natural RFs in order to show that MS training is able to make RFs robust, and, on the other hand, MS models will be also compared with the state-of-the-art of robust GBDTs, that is, the adversarially trained models by [2] and [14].

### 3 Training as Combinatorial Optimization

Given a training dataset \( D = \{(x_1, y_1), \ldots, (x_N, y_N)\} \subseteq X \times L \), a training algorithm explores a hypothesis space \( \mathcal{H} \subseteq X \rightarrow \wp(L) \) searching for a classification model in \( \mathcal{H} \) which maximizes some performance function \( f : (X \rightarrow \wp(L)) \rightarrow \mathbb{R} \). Training set, performance function and search strategy will determine how the output classification model is computed. In the case of CART decision trees, the training process first builds a tree stump consisting of a single internal node labeled by a univariate hard split \( S_{i,k} \equiv x_i \leq k \), where the attribute \( i \) and the threshold \( k \) are selected among all possible \( i \in [1, d] \) and \( k \in \mathbb{R} \). Each split candidate \( S_{i,k} \) yields two new leaves \( \lambda_l \) and \( \lambda_r \) which store a distribution frequency of training samples \( (\#y_1, \ldots, \#y_m) \in \mathbb{N}^m \) grouped by labels \( y_i \in L \), i.e., equivalently, a probability distribution \( (p_1, \ldots, p_m) \in \mathbb{R}^m \) for labels which is used to compute either the entropy \( h \) or Gini \( g \) indexes which encode the information gain for a leaf \( \lambda = (p_1, \ldots, p_m) \) as follows:

\[
h(\lambda) \equiv -\sum_{i=1}^m p_i \cdot \log_m(p_i) \quad g(\lambda) \equiv 1 - \sum_{i=1}^m p_i^2
\]

These indexes are used to estimate the purity of a split \( S_{i,k} \) by averaging their values on its leaves \( \lambda_l \) and \( \lambda_r \) as follows:

\[
H(S_{i,k}) \equiv (|\lambda_l| h(\lambda_l) + |\lambda_r| h(\lambda_r))/(|\lambda_l| + |\lambda_r|)
\]

\[
G(S_{i,k}) \equiv (|\lambda_l| g(\lambda_l) + |\lambda_r| g(\lambda_r))/(|\lambda_l| + |\lambda_r|)
\]

where \(|\lambda|\) denotes the number of samples reaching the leaf \( \lambda \) for the split \( S_{i,k} \).

The training algorithm selects a split candidate \( S_{i,k} \) which minimizes \( H \) or \( G \),
and the process will be repeated until no more splits are possible, i.e. every leaf contains only samples with a same label, or other custom criteria are met such as maximum tree depth, maximum number of leaves or minimum number of samples per leaf (these are tunable parameters, e.g., with scikit-learn).

This training process therefore corresponds to a greedy search algorithm which tries to find a globally optimal tree by looking at local split information only. This approach exhibits two major drawbacks:

(A) it does not take robustness (or stability) into account;

(B) it is limited by information from local splits only.

These limitations may often lead to overfitting, which is a well-known phenomenon with decision trees [7, 29]. Pruning techniques, e.g. [6, 32, 33], can be used to counteract overfitting by reducing the size of the tree in order to simplify the model, although this may often lead to a loss of accuracy and may be applied just as a post-training step.

Of course, local properties of decision trees, in general, cannot be lifted globally to the whole tree, as it is the case of stability in this simple example.

Example 3.1. Consider the tree $t_1$ in Fig. 2 and its right subtree $t_r$ rooted at the split node $x_2 \leq 0$. Consider an input region $Y = \{(x_1, x_2) \in \mathbb{R}^2 \mid -1 \leq x_1 \leq 1, -1 \leq x_2 \leq 0\}$. Then, the set of reachable leaves from $Y$ in $t_r$ is labeled as $\{b\}$, hence ensuring stability of $t_r$ in $Y$, while the set of reachable leaves from $Y$ in $t_1$ is labeled as $\{a, b\}$, thus making the classification of the tree $t_1$ not stable in $Y$.

We will design a global tree training algorithm which takes stability into account. Given a (finite) set $M$ of performance metrics of type $\mathcal{H} \to \mathbb{R}$, such as accuracy on a given test set and stability on a given test set w.r.t. a perturbation, we combine them through a comprehensive performance function $\varphi_M : \mathcal{H} \to \mathbb{R}$ that will be maximized during the training process. For example, this performance function can be a simple linear combination $\varphi_M(C) = \sum_{i=1}^{\vert M \vert} w_i m_i(C)$. If $\varphi_M$ is differentiable and, for some metric $m_k \in M$, $\frac{\partial \varphi_M}{\partial m_k} \geq 0$, then a classifier $C_{\text{opt}}$ which is computed by an ideal trainer by maximizing $\varphi_M$ will be optimal for the performance metric $m_k$, meaning that for any classifier $C \in \mathcal{H}$, if $m_j(C_{\text{opt}}) = m_j(C)$ for all $j \neq k$, then $m_k(C_{\text{opt}}) \geq m_k(C)$.
Of course, metrics such as accuracy and stability can only be estimated on a finite test subset of the input space \( X \), meaning that global optima cannot be computed precisely, so that training algorithms effectively will find classifiers which are locally optimal for a finite test subset \( T \) of \( X \). Finding a locally optimal classifier for \( T \) is not necessary in practice, as local optimality is unlikely to be an appropriate measure of global optimality and could even lead to overfitting phenomena. We argue that heuristic search strategies such as genetic algorithms may provide a viable and effective training procedure of tree classifiers which closely approximate the ideal optimal solutions and may improve the state-of-the-art in practice.

## 4 Genetic Adversarial Training by Meta-Silvae

A significant number of training procedures for decision trees based on evolutionary algorithms have been investigated, as surveyed by [4]. The underlying basic idea is that evolutionary algorithms perform a robust global, as opposed to local, search in the hypothesis space and tend to cope better with relationships between different features than greedy methods [23]. To the best of our knowledge, we put forward the first adversarial training procedure for decision tree (or tree ensemble) classifiers based on a genetic algorithm, called Meta-Silvae (MS), which targets to maximize both accuracy and stability metrics. MS crucially relies on a complete formal verification method of the stability (or robustness) of ensembles of decision trees.

### 4.1 Complete Verification of Stability

We design and implement a decision tree adversarial training method based on a genetic algorithm, that we call MS (for Meta-Silvae). This genetic learning algorithm internally relies on silva [44], an open source tool based on abstract interpretation [19, 46] for the formal verification of stability properties of decision tree ensembles. Silva performs a static analysis of ensembles of decision trees in an abstract domain \( A \subseteq \wp(\mathbb{R}^d) \) which represents some selected properties of real vectors, such as hyperrectangles of intervals providing lower and upper bounds to vector components or a domain of linear relations between vector components. Silva first approximates in the abstract domain \( A \) an adversarial region \( P(x) \in \wp(\mathbb{R}^d) \) of an input vector \( x \in \mathbb{R}^d \) and then abstractly computes a sound overapproximation of the set of leaves of a decision tree (or an ensemble of trees) which are reachable from the adversarial samples ranging in \( P(x) \). This static analysis is based on the soundness principle of abstract interpretation meaning that no leaf reachable from some sample in \( P(x) \) can be missed. When adversarial attacks are modeled by the maximum norm perturbation \( P_{\infty,\epsilon}(x) \) and the analysis is performed on the abstract domain of hyperrectangles the output returned by silva turns out to be complete, meaning that each leaf computed by silva is actually reached by some adversarial input ranging in \( P_{\infty,\epsilon}(x) \), namely, no false positive (i.e., a false reachable leaf) may happen. Silva therefore pro-
vides a complete certification algorithm for the stability (or robustness) of an input sample \( x \) under adversarial attacks in \( P_{\infty,d}(x) \) and, in turn, this verification tool allows us to derive precisely (thanks to completeness) the stability \( st_{T,P_{\infty,d}} \) and robustness \( rob_{T,P_{\infty,d}} \) metrics, as defined in Section 2, for a tree ensemble classifier on some test set \( T \).

To conclude this brief outline of silva, let us recall that the abstract domain of hyperrectangles \( HR_d \) consists of \( d \)-dimensional vectors of intervals \([l, u]\), where the bounds \( l, u \in \mathbb{R} \cup \{+\infty, -\infty\} \) are such that \( l \leq u \), for example \(([0.1, 0.9], [-\infty, 0], [0.5, +\infty]) \in HR_3 \). Therefore, a hyperrectangle \([l, u] = ([l_1, u_1], ..., [l_d, u_d]) \in HR_d \) represents all the real vectors \( x \in \mathbb{R}^d \) such that, for all \( j \in [1, d], l_j \leq x_j \leq u_j \), i.e., such that lower/upper bounds of their components are correctly approximated by \([l, u]\).

### 4.2 MS Algorithm

By exploiting the stability information provided by silva, for training on a dataset \( T \), a decision tree in a hypothesis space \( \mathcal{H} \), we consider as objective performance function \( \varphi_T : \mathcal{H} \rightarrow \mathbb{R} \) a linear combination of accuracy and stability, i.e., \( \varphi_T(t) \triangleq w_{a}acc_T(t) + w_{st}st_{T,P}(t) \) for a given perturbation \( P \) and for some nonnegative weights \( w_{a}, w_{st} \geq 0 \), \( \varphi_T \) is differentiable and such that \( \frac{\partial \varphi_T}{\partial acc_T} = w_{a} \geq 0, \frac{\partial \varphi_T}{\partial st_{T,P}} = w_{st} \geq 0 \), so that an ideal training algorithm which maximizes \( \varphi_T \) will output optimal decision trees. For instance, in the training example depicted in Fig. 1 we used as objective function \( \varphi(t) \triangleq 0.9acc(t) + 0.1st_{\pm2\%}(t) \).

Our suboptimal solution is computed by the genetic Algorithm 1 called MS. At line 1, a set of trees is generated and stored as initial population, where MS can either start with a set of base trees consisting of a single leaf only (which is our choice in the experimental evaluation) or by any set of pre-trained decision trees. Then, the while-loop at lines 3-13 generates the nextPopulation and iterates until some stop criterion, such as a timeout or a bound on the population size, is met. At each iteration, the best tree w.r.t. our performance function \( \varphi_T \) will be first selected at line 4 from the current population to carry over to the next one unchanged. This therefore implements an elitist selection strategy for GAs \([3]\) which ensures that the performance function will not decrease from the current population to the next. The new individuals will be generated by the while-loop at lines 5-11, where two trees parentA and parentB are first selected from the current population, then combined in an offspring by a crossover operation, which can finally be mutated for enhancing genetic diversity.

**Selection.** A fitness proportional selection scheme \([39]\) is employed at lines 6-7, also known as roulette wheel, which selects an individual \( t_i \) from a current population \( Y \) with a probability \( p_i \) which is proportional to its fitness as determined by the objective function \( \varphi_T \) as follows: \( p_i \triangleq \frac{\varphi_T(t_i)}{\sum_{t \in Y} \varphi_T(t)} \). It should be remarked that in this selection MS exploits crucially the stability value \( st_{T,P}(t) \) given by the verification tool silva which is used by \( \varphi_T(t) \).
Algorithm 1: MS

1. \texttt{population} = \texttt{generateInitialTrees();}
2. \texttt{nextPopulation} = \emptyset;
3. \texttt{while \neg stopCriterion() do}
   \hspace{1em} // Elitist Selection
   4. \texttt{nextPopulation.push(population.selectBest(\varphi_T));}
   5. \texttt{while \neg nextPopulation.isFull() do}
      \hspace{1em} // Roulette Wheel Selection
      6. \texttt{parentA = population.select(\varphi_T);}
      7. \texttt{parentB = population.select(\varphi_T);}
      \hspace{1em} // Single-Point Crossover
      8. \texttt{offspring = crossover(parentA, parentB);}
      \hspace{1em} // Mutation With Probability \textit{p}
      9. \texttt{if offspring.shouldMutate(\textit{p}) then}
         \hspace{1em} // Grow or Grow-Or-Prune
         10. \texttt{offspring.mutate();}
         11. \texttt{nextPopulation.push(offspring);}
      12. \texttt{population = nextPopulation;}
      13. \texttt{nextPopulation = \emptyset}
   14. \texttt{return population.selectBest(\varphi_T)}

\textbf{Crossover.} The information of the two selected trees \textit{parentA} and \textit{parentB} is combined at line 8 by the following variation of the standard single-point crossover procedure \cite{41}:

1. a subtree \textit{t}_{A} is randomly selected and pruned from \textit{parentA};
2. a subtree \textit{t}_{B} is randomly selected from \textit{parentB};
3. \textit{t}_{B} is inserted as subtree of \textit{parentA} in place of the pruned subtree \textit{t}_{A};
4. consistency of the new tree is enforced by pruning those nodes which do not contain information and then by reshaping the tree as needed.

Let us illustrate this crossover function by a simple example.

\textbf{Example 4.1.} Consider as parent trees \textit{t}_1 and \textit{t}_2 in Fig. 2, and assume that the nodes labeled with splits \(x_2 \leq 0\) and \(x_3 \leq 0\) are selected, resp., as subtrees \textit{t}_A of \textit{t}_1 and \textit{t}_B of \textit{t}_2. The tree \textit{t}_B is inserted in \textit{t}_1 in place of \textit{t}_A, as depicted by the left tree \textit{t}_3 in Fig. 3. However, after this insertion, the path \((x_1 \leq 0)_B \rightarrow \lambda_2^3\) becomes infeasible due to the parent constraint \((x_1 > 0)_A\) at the root, so that the subtree of \textit{t}_3 rooted at \((x_1 \leq 0)_B\) must be pruned of the left path \((x_1 \leq 0)_B \rightarrow \lambda_2^2\), thus yielding the output tree \textit{t}_3^{\text{pr}} on the right of Fig. 3. \hfill \Box
Mutation. After crossover, mutation of the offspring happens at lines 9-10 with probability $p$ and can either prune a randomly selected subtree or transform a leaf into a single split. In the latter case, consistency of splits must be preserved so that logically inconsistent trees are never generated. The mutation probability $p$ is specified as a tunable parameter of MS, as well as the adopted mutation strategy which can be chosen between grow only and grow-or-prune. In both cases the selection is made on a stochastic basis by considering the entropy $h$ of each node (or, alternatively, the Gini index $g$). We describe this mutation procedure more in detail through an example.

Example 4.2. Consider the decision tree $t_4$ on the left of Fig. 4 whose nodes are decorated as superscripts with their entropy values. A grow mutation starts from the root node $(x_1 \leq 0)_A$, computes the entropy $h$ of its left and right children, and move toward one of them with a probability which is proportional to their respective entropies, in our example the node $(x_3 \leq 0)_B$ is chosen. Once a leaf is reached, in our example $(x_2 \leq 2.5)$, the samples associated to that leaf are used to generate a set of features $i$ and thresholds $k$ which defines a set of split candidates $x_i \leq k$. The split candidate maximizing the objective function $\varphi_T$ is then selected by applying the split and evaluating accuracy and stability of the corresponding tree. For example, the split $x_2 \leq 2.5$ is selected for growing the leaf $(...)^{0.8}$ and this yields the tree $t_{gr}^4$ depicted on the right of Fig. 4. □

It should be remarked that while the standard learning method for CART trees is a greedy algorithm which incrementally builds a decision tree by locally computing new split nodes or new leaves [9], in MS the selection of a candidate split relies on a stability test (performed by silva) on the whole corresponding candidate tree, thus meaning that the MS learning process is inherently not incremental and consequently could be computationally burdensome. We therefore introduced in MS an optimization parameter, called “aggressiveness” in the implementation of MS, which allows us to set up a threshold on the number of split candidates which are immediately evaluated during the mutation phase, while those exceeding this threshold are delayed. It turns that this optimization is effective in reducing the computational burden without sacrificing the overall generalization, because the evaluation of split candidates which are ruled out by this threshold is delayed to later iterations of MS.
For the grow-or-prune mutation, a similar strategy is applied. Starting from the root node, the mutation algorithm iteratively moves either to the right of left children with a probability which is proportional to their entropy $h$ and, at any point, the current node has a probability of $1 - h$ of being pruned. By doing so, splits with low entropies are likely to be pruned, thus improving the tree compactness and stability at the bearable cost of losing some accuracy. If no pruning happens then the mutation proceeds as in the grow case.

Output. At the end of the whole evolutionary process, the best tree classifier of the final population, which is also the best tree encountered during the whole process due to elitism, is returned as output decision tree. As an example, the diagrams in Fig. 1 have been generated by the following two decision trees, where the first one has been trained by the standard algorithm of scikit-learn and the second one by MS. In both trees, a leaf $\lambda = (n^*, m^+)$ denotes that $\lambda$ stores $n$ red bullet samples and $m$ blue cross samples.
4.3 Ensembles of MS Trees

Multiple instances of MS can be run (also in parallel: this chance was exploited in our experimental evaluation on a cluster) in order to generate a tree ensemble, which in our experiments is a random forest. When training a random forest, we need to achieve a significant random diversification among its trees, typically obtained by a random sampling of the set of features which each tree can explore when searching for a new split. MS allows to specify the number \( N \) of features which can be inspected for training a tree. A subset of features of size \( \leq N \in [1, d] \) is randomly extracted, where each feature has the same probability of being selected. This feature selection happens only once before the training, and it is therefore applied tree-wise by MS. The resulting set of trees can be used as a single classifier by applying standard voting mechanisms (such as a simple majority vote) used for natural random forests.

5 Experimental Evaluation

We implemented MS as a self-contained C program whose source code (about 3K LOC) together with datasets, classification models and scripts is publicly available on GitHub [45]. Our experiments were run on a cluster of 15 computing nodes, each equipped with two Intel Xeon CPU E5520 at 2.27GHz with 8 cores and 32GB RAM. In our experiments we considered the collection of standard datasets with numerical features summarized in Table 1: these datasets are used in [2, 14, 52], while wine is a UCI dataset [20].

5.1 Setup

MS does not require a specific tuning of hyperparameters for training decision trees, although the choice of the objective function \( \varphi \) plays a fundamental role. As described in Section 4.2, we adopted a weighted linear combination of accuracy and stability given by

\[
\varphi_T(t) = w_{\text{acc}} \text{acc}_T(t) + w_{\text{stab}} \text{st}_{T,P}(t),
\]

for a given training dataset \( T \), perturbation \( P \) and weights \( w_{\text{acc}}, w_{\text{stab}} \in [0, 1] \) such that
Table 1: Summary of Datasets.

| Dataset          | #classes | #features | values     | #train  | #test  |
|------------------|----------|-----------|------------|---------|--------|
| breast-cancer    | 2        | 10        | [1,10]     | 546     | 137    |
| cod-rna          | 2        | 8         | [0,1]      | 59535   | 271617 |
| collision-detection | 2  | 6         | [0,1]      | 30000   | 3000   |
| diabetes         | 2        | 8         | [0,1]      | 614     | 154    |
| fashion-mnist    | 10       | 784       | [0,255]    | 60000   | 10000  |
| ionosphere       | 2        | 34        | [-1,1]     | 260     | 90     |
| mnist            | 10       | 784       | [0,255]    | 60000   | 10000  |
| mnist-1-5       | 2        | 784       | [0,255]    | 12162   | 2026   |
| mnist-2-6       | 2        | 784       | [0,255]    | 11875   | 1989   |
| sensorless       | 11       | 48        | [0,1]      | 48509   | 10000  |
| wine             | 2        | 13        | [0,1]      | 128     | 50     |

Table 1: Summary of Datasets.

$w_{acc} + w_{stab} = 1$. Fig. 5 shows the impact of selecting different weights (where $w = 0.1k$ for $k \in \{0, \ldots, 10\}$) on the final tree classifier in terms of accuracy and stability on the whole training set $T$.

As expected, higher values of $w_{acc}$ tend to yield more accurate models, where we observed a converging behaviour when accuracy exceeds 70%. On the other hand, stability increases with higher $w_{stab}$ weights, it is above 45% and often above 60% already with $w_{stab} = 0.1$, although stability generally may display a more varying behaviour than accuracy. These experiments hint that an effective and well balanced choice of weights can be obtained with $w_{acc} = 0.9$, $w_{stab} = 0.1$. It is worth remarking that by setting $w_{stab} = 1$ (and therefore $w_{acc} = 0$), as expected, MS will always produce perfectly stable models corresponding to a constant function, which is generally (but not always) inaccurate.

We analysed the rate of convergence of the fitness function $\varphi_T$ along iterations of MS training. Fig. 6 displays the fitness of the best individual of population after each iteration of MS, where the number of iterations is shown on a logarithmic scale. We observe that the best gains in fitness are achieved during the first iterations and MS tends to converge within 50-70 iterations, with the exception of the dataset diabetes which needs about 500 iterations to converge. Hence, the maximum number of iterations has been set to 500 for diabetes and to 100 for the other datasets. This same method is used to decide between grow and grow-or-prune mutations as well as their “aggressiveness” threshold, as described in Section 4.2.

5.2 Results

Table 2 summarizes the main data of our MS models together with their accuracy and stability metrics. MSs have been trained for the objective performance function $\varphi_T(t) = 0.9acc_T(t) + 0.1st_{T,P_{\infty,\epsilon}},(t)$ where stability is w.r.t. a maximum norm perturbation $P_{\infty,\epsilon}$ whose magnitudes $\epsilon$ are displayed as absolute and percentage values. These magnitudes $\epsilon$ are the same used by [2, 14] for their adversarial training on 6 common datasets: breast-cancer, cod-rna,
diabetes, fashion-mnist, mnist-1-5, mnist-2-6. It is worth remarking that some of these perturbations are quite challenging, since they peak to $\pm 30.2\%$ for mnist-1-5/2-6 and $\pm 33.3\%$ for breast-cancer. For fashion-mnist and mnist we trained a random forest of 50 MS-robust trees adopting a standard majority voting for output classification. For the remaining datasets it was enough to train a single robust decision tree since in these cases random forests do not bring practical benefits in accuracy or stability, thus making these single tree models efficient and easily interpretable. It is worth observing that MS training times are modest and acceptable even for the more demanding datasets fashion-mnist and mnist. The stability metrics w.r.t. $P_{\infty,\epsilon}$ have all been computed with no imprecision by silva on the whole test sets.

Since MS utilizes a seed provided by a random number generator, in order to analyse the impact of randomness on the output models, the MS training has been repeated 1000 times for each dataset by selecting distinct values of
the seed. The distribution of accuracy and stability of the models generated by these 1000 different runs is depicted by two box plot diagrams in Fig. 7. The box is drawn from first to third quartiles, its horizontal line denotes the median. We observe that accuracy of most models is within ±5% (and often ±2.5%) of the median, with the sole exception of wine. The results for stability are similar, where the stability of the models turns out to be within ±5% of the median, with the exception of ionosphere, where unstable (meaning stability < 30%) models can be produced, although 75% of these 1000 trees has a stability ≥ 30%, and ≥ 65% for half of them.

5.3 MS vs RF

We compared our robust models trained by MS with natural random forests trained by scikit-learn [42]. Hyperparameters for training random forests have
been selected by a randomized grid search on the number of trees ranging in the interval [5, 100], maximum depth in [5, 100], and either Gini \( G \) or entropy \( H \) for split purity. By relying on the stability verification by silva [44], we selected the hyperparameters which maximize the same objective function \( \varphi_T \) used in MS training. The first table in Figure 8 shows the accuracy and stability metrics on the whole test sets for RF as compared to MS models, where, for the sake of fair comparison, in the average of the relative stability gains of MS models we excluded the RFs with 0% stability.

It turns out that all the MS models are significantly more stable than RFs (+54.3% on average). On the other hand, the average accuracy slightly decreased (−1.8%) w.r.t. natural RFs. We also emphasize that, with respect to Fig. 7, every single MS tree outperforms the corresponding Random Forest in terms of stability on every dataset but wine whose RF model already features a significant stability ≥60%. With a very significant rise in stability at least a slight drop in accuracy is generally expected, although it is worth observing that in some notable cases the accuracy increased (mnist) or remained the same (fashion-mnist). In Fig. 9 we display two box plot diagrams which compare accuracy and stability for \( P_{\infty,1} \), given as values in \([0,1]\), of all the 50 decision trees composing the RF and MS models trained on mnist. The boxes are drawn from first to third quartiles, whose horizontal lines denote the median, and the bounds of the vertical interval denote the lowest and highest data points. Interestingly, it can be observed that each single robust decision tree trained by MS is significantly more accurate and stable than each tree of the RF. We also compare an efficiency metric of RFs and MSs, where the efficiency of a classifier \( C \) w.r.t. a metric \( m \) measures which size of \( C \) is required to achieve a given value of \( m \). Here, we define an efficiency metric for a tree ensemble \( C \) which takes into account how many leaves of \( C \) are needed to reach a given performance of accuracy and stability: if \( m(C) \in [0,1] \) is the performance of \( C \) for a metric \( m \) then the corresponding efficiency of \( C \) is defined by \( \text{Eff}_{m}(C) \triangleq m(C)/\text{leaves}(C) \), where

| Dataset        | MS training | MS metrics | Dataset        | MS training | MS metrics |
|----------------|-------------|------------|----------------|-------------|------------|
|                | # of max    | time(s)    | acc%          | st%         |            |
|                | trees depth | per tree   | P_{\infty,1} (%) |             |            |
| breast-cancer  | 1           | 0.2        | 100.0         | 89.1        |            |
| cod-rna        | 1           | 20.0       | 95.6          | 89.9        |            |
| collision-det. | 1           | 28.8       | 87.5          | 45.4        |            |
| diabetes       | 1           | 2.1        | 76.0          | 68.8        |            |
| fashion-mnist  | 50          | 3593.1     | 86.4          | 46.9        |            |
| ionosphere     | 1           | 0.2        | 97.8          | 84.4        |            |
| mnist          | 50          | 3376.4     | 95.6          | 81.7        |            |
| mnist-1-5      | 1           | 133.0      | 94.7          | 57.4        |            |
| mnist-2-6      | 1           | 11.7       | 98.1          | 88.7        |            |
| sensorless     | 1           | 133.0      | 94.7          | 57.4        |            |
| wine           | 1           | 0.1        | 92.0          | 68.0        |            |

Table 2: Performance of MS
leaves(C) = \sum_{t \in C} leaves(t) is the total number of leaves of trees in C. Thus, the higher Eff_m(C) the better is the efficiency of C for m. The second table in Figure 8 compares the number of leaves and efficiency for accuracy and stability (w.r.t. P_{\infty, e}) for RFs and MSs. It turns out that MSs are much more efficient than RFs: the average of the ratios leaves(MS) leaves(RF) is 51.4\% while the average relative efficiency gains of MSs w.r.t. RFs (i.e., the ratio Eff_m(MS)/Eff_m(RF)) are, resp., 174\% for accuracy, and 1825\% for stability (by excluding in this average 4 datasets whose Eff_{st} for RFs is close to 0).

5.4 MS vs Robust Gradient Boosted Trees

Finally, we compare our MS robust models with the adversarially trained tree models of [2], denoted by AH19, and [14], denoted by CZBH19. These are gradient boosted decision trees of the same type of XGBoost trees [16], which, to the best of our knowledge, represent the state-of-the-art of adversarially trained GBDTs. Although our MS robust training generates tree ensembles which are
random forests, and RFs and GBDTs are tree ensemble models with unrelated training principles, we nevertheless compare these different models since these robust GBDTs were the only adversarially trained decision trees found in literature. We considered 6 common datasets and, as already recalled, the perturbation $P_{\infty,\epsilon}$ is exactly the same used in [2] and [14]. Let us remark that the accuracy and robustness metrics of AH19 and CZBH19 models are taken from Table 7 of the supplemental of [2], because silica cannot be used to compute the robustness of GBDTs. We also compare the objective performance function $\varphi_T$ used for training MSs, where accuracy and robustness weigh, resp., 90% and 10%.

The results of this comparison are summarized by the tables in Figure 10. For AH19 models, we also compare their size, i.e. total number of leaves, and their efficiency with MS models. The third table in Figure 10 displays the relative efficiency gains of MS w.r.t. AH19 models, which are, resp., the ratios $\frac{\text{leaves}(\text{MS})}{\text{leaves}(\text{AH19})}$, $\frac{\text{Eff}_{\text{acc}}(\text{MS})}{\text{Eff}_{\text{acc}}(\text{AH19})}$, and $\frac{\text{Eff}_{\text{rob}}(\text{MS})}{\text{Eff}_{\text{rob}}(\text{AH19})}$.

On average, it turns out that:

(i) AH19 models are moderately more robust (+7.6%) than MSs;

(ii) MSs are slightly more robust (+2.5%) than CZBH19 models;

(iii) MS models are slightly more accurate of both AH19 (+0.6%) and CZBH19 (+0.4%) models;

(iv) all three models exhibit the same average performance according to the objective function $\varphi_T$;

(v) MS models are significantly more efficient than AH19 models both for size (average 40.9%), accuracy (average 31.4×) and robustness (average 30.1×).

Our MS models compete with and often improve on the robust GBDTs of [2, 14] while being more compact and therefore interpretable and efficient tree models.
| Dataset        | CZBH19 | MS       |
|---------------|--------|---------|
|               | acc%   | rob%    | obj. $\varphi_T$ | acc%   | rob%    | obj. $\varphi_T$ |
| breast-cancer | 99.3   | 86.9    | 0.98             | 100.0  | 89.1    | 0.99             |
| cod-rna       | 95.6   | 83.3    | 0.95             | 76.0   | 59.1    | 0.74             |
| diabetes      | 59.7   | 0.76    | 86.4             | 44.8   | 0.82    |                  |
| fashion-mnist | 99.7   | 97.1    | 0.99             | 97.9   | 93.1    | 0.97             |
| mnist-1-5     | 99.5   | 93.1    | 0.99             | 98.1   | 88.1    | 0.97             |
| Average       | 91.9   | 74.6    | 0.90             | 92.3   | 77.1    | 0.91             |

| Dataset        | AH19 | MS       |
|---------------|------|---------|
|               | acc%   | rob%    | obj. $\varphi_T$ | acc%   | rob%    | obj. $\varphi_T$ |
| breast-cancer | 99.3   | 93.4    | 0.99             | 100.0  | 89.1    | 0.99             |
| cod-rna       | 93.1   | 78.7    | 0.92             | 95.6   | 83.3    | 0.95             |
| diabetes      | 72.7   | 64.3    | 0.72             | 76.0   | 59.1    | 0.74             |
| fashion-mnist | 95.8   | 76.8    | 0.85             | 86.4   | 44.8    | 0.82             |
| mnist-1-5     | 99.8   | 98.7    | 0.99             | 97.9   | 93.1    | 0.97             |
| mnist-2-6     | 99.3   | 96.2    | 0.99             | 98.1   | 88.1    | 0.97             |
| Average       | 91.7   | 84.7    | 0.91             | 92.3   | 77.1    | 0.91             |

| Dataset        | AH19 | MS       | Efficiency Gain |
|---------------|------|---------|-----------------|
|               | # leaves | # leaves | leaves | acc | rob |
| breast-cancer | 80 | 4 | 5.0% | 20.1× | 18.9× |
| cod-rna       | 913 | 85 | 9.3% | 11.0× | 12.1× |
| diabetes      | 79 | 83 | 105.0% | 1.0× | 0.9× |
| fashion-mnist | 97279 | 119986 | 123.3% | 0.8× | 0.5× |
| mnist-1-5     | 3258 | 30 | 0.9% | 106.5× | 102.4× |
| mnist-2-6     | 3777 | 76 | 2.0% | 49.1× | 45.5× |

Figure 10: Comparison between MS and AH19, CZBH19.

6 Conclusion

We believe that this work contributes to push forward the use of formal verification methods in machine learning, in particular a very well known program analysis technique such as abstract interpretation has been proved successful for training decision tree classifiers which are both accurate and robust and compete with and often improve on the state-of-the-art of adversarial training of gradient boosted decision trees while being much more compact and therefore interpretable and efficient tree models. As future work, we plan to investigate the problem of fairness verification [18, 35] for ensembles of decision trees by leveraging abstract interpretation techniques along the lines of this paper. The final goal will be to design a fairness-aware learning algorithm for decision trees, for both notions of individual and group fairness [5].
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