Scalable Whitebox Attacks on Tree-based Models

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Abstract

Adversarial robustness is one of the essential safety criteria for guaranteeing the reliability of machine learning models. While various adversarial robustness testing approaches were introduced in the last decade, we note that most of them are incompatible with non-differentiable models such as tree ensembles. Since tree ensembles are widely used in industry, this reveals a crucial gap between adversarial robustness research and practical applications. This paper proposes a novel whitebox adversarial robustness testing approach for tree ensemble models. Concretely, the proposed approach smooths the tree ensembles through temperature-controlled sigmoid functions, which enables gradient descent-based adversarial attacks. By leveraging sampling and the log-derivative trick, the proposed approach can scale up to testing tasks that were previously unmanageable. We compare the approach against both random perturbations and blackbox approaches on multiple public datasets (and corresponding models). Our results show that the proposed method can 1) successfully reveal the adversarial vulnerability of tree ensemble models without causing computational pressure for testing and 2) flexibly balance the search performance and time complexity to meet various testing criteria.

1 Introduction

Machine learning (ML) models are proven to be vulnerable to adversarial examples [11]; small but carefully crafted distortions of inputs created by adversaries could fool the ML models. For safety-sensitive applications (e.g. finance [10], health service [18], and autopilot systems [23]), such an issue could result in catastrophic consequences. This has attracted much attention from the research community (see [5, 9]). In particular, effectively testing the adversarial robustness before model deployment is one of the most crucial challenges [4].

In the literature, many adversarial robustness testing approaches mainly focus on deep learning models. For instance, [14] proposed Fast Gradient Sign Method (FGSM) to test the robustness of neural networks by generating adversarial examples through a one-step update. Later, the Basic Iterative Method (BIM) [20] extended FGSM by introducing multi-step gradient updates that result in a better success rate. [15] introduced a data-guided methodology to determine regions that are likely to be safe (instead of focusing on individual points).

Despite their testing effectiveness, we note that few of the existing approaches support non-differentiable models that are widely used in the industry. Indeed, many ML models used in product lines are tree ensemble models (see [11, 24, 13]) due to model computational efficiency and transparency (with readable interpretations for humans). This fact reveals a crucial gap between adversarial robustness research and practical applications. To address this research gap, [19] proposed

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a white-box attack method using Mixed Integer Linear Programming (MILP) to avoid computing
gradients. [6], alternatively, formulated the adversarial robustness test into a maximum clique enu-
meration task which shows better scalability than the MILP approach. While these approaches
are enlightening, they appear to be computationally intractable in practice, where the testing task may
involve an ensemble with hundreds of trees, thousands of features, and millions of data points to test
on. Hence, blackbox attack approaches [16, 2] become a relatively practical option for large-scale
testing, while still computationally expensive.

In this paper, we propose a scalable whitebox adversarial robustness testing approach for tree
ensemble models. In particular, we aim to unlock gradient descent-based adversarial robustness
testing on tree ensemble models by smoothing the trees. By replacing each decision node in a tree
with a temperature-controlled sigmoid function, we can approximate the original target model with a
controllable error gap. To facilitate efficient adversarial example search, we propose two approaches
by either injecting sparse noise during gradient descent or introducing a log-derivative trick and
Monte Carlo sampling to approximate the gradients. Both variants provide sufficient stochasticity
that maximize the search coverage.

To demonstrate the effectiveness of the proposed method, we compared it against multiple approaches,
such as random perturbations, and black box attack methods on multiple public datasets and corre-
sponding models. Our experimental results show the proposed method can 1) successfully reveal the
adversarial vulnerability of tree ensembles without causing computational pressure for testing, and 2)
flexibly balance the search performance and time complexity to meet various testing criteria.

2 Preliminary

In this section, to ground our main contribution, we highlight previous research in the field of
adversarial robustness testing. We then review existing work on ensembles of decision trees to
facilitate our description of the proposed attack.

2.1 Adversarial Robustness Testing

The vulnerability of deep networks to adversarial attacks was first introduced in [25], which demon-
strated that small, imperceptible perturbations to a model’s inputs were capable of dramatically
changing its outputs. Aside from the iconic adversarial attack approaches, such as FGSM [14]
and BIM [20], mentioned in the introduction section, there are many extensions to improve the
adversarial example searching efficiency. For example, Projected Gradient Descent (PGD) [21]
suggested random initialization for adversarial example search. And, DeepFool [22], on another
hand, focuses on generating adversarial examples by minimizing perturbations. These approaches all
formulate an adversarial objective, which aims to minimize classification performance while using
some norm to bound the perturbation. These perturbations are then generated using gradient descent,
which is computed by backpropagating through the target model. These approaches thus make two
assumptions: (1) the model is fully accessible, and thus these are classified as white-box attacks. (2)
the model is differentiable.

When either of these assumptions are violated, we must consider different attack algorithms. A
common strategy is to estimate gradient information through numerical approximation, as done using
finite difference methods in ZOO [7], or by drawing random samples (as in NES [16] and SPSA [26]).
Alternatively, gradient-free optimizers may be employed, such as genetic algorithms in GenAttack [2].
In addition to their effectiveness in constructing adversarial examples, these algorithms may be ranked
according to the number of queries needed to run the attack.

2.2 Decision Trees and Tree Ensemble Models

A Decision Tree makes a prediction based on the value of the leaf node to which the input observation
x gets routed, where the leaf node is determined by following the decision trajectory of the input x
from the root node in the tree. Specifically, in each internal decision node k of a tree t denoted as
\( D_{t,k} \), the input x is categorized (or directed) to one of the child nodes based on a simple statement (or
condition) such as \( x_j > v_{k} \) for certain feature j and constant \( v_{k} \). Since the entire decision-making
process can be written as a decision rule with a set of propositional statements, decision trees are
widely used in the industry for their transparency.

A Tree Ensemble makes a prediction by combining decisions from multiple decision trees by
averaging them. Formally, given \(|T|\) decision trees \( \{D_1 \cdots D_{|T|}\} \) with tree contribution weight
With the above smoothing steps, the prediction of the tree ensemble model is
\[
\hat{y} = M(x) = \sum_{t=1}^{T} w_t D_t(x) \quad \text{and} \quad \hat{y} = \arg\max_c M(x) = \arg\max_c \sum_{t=1}^{T} w_t I[D_t(x) = c],
\]
where \( I[\cdot] \) denotes the indicator function and \( c \in C \) denotes the class index. This formulation applies to most of the well-known tree ensemble models, such as Random Forest [3], Boosted Trees [12], and XGBoost [8]. In this paper, we consider adversarial robustness testing for tree ensemble models.

3 Large-scale Adversarial Robustness Testing on Tree Ensembles

Given a predictive model \( \hat{y} = M(x) \), adversarial robustness testing aims to find an adversarial example \( x' \) (for each testing sample \( x \)), which would cause the model to violate criteria tuple \( (\Phi, \Psi, \epsilon, \delta) \) by allowing
\[
\Psi(M(x'), M(x)) > \delta \quad \text{when} \quad \Phi(x', x) \leq \epsilon,
\]
where \( \Phi \) denotes distance of inputs, \( \Psi \) denotes distance of predictions, \( \epsilon \) denotes perturbation criteria, and \( \delta \) denotes the tolerance in prediction shift. In the literature, input distance \( \Phi \) is usually the \( l_\infty \) norm, whereas output distance \( \Psi \) is the \( l_1 \) norm (absolute difference). Intuitively, adversarial robustness describes how well the model can preserve its prediction when the input data point is perturbed within a pre-defined perturbation bound.

This paper proposes a large-scale adversarial robustness testing approach on tree ensemble models through iterative gradient descent. We first describe how to smooth the trees to support gradient descent. Then, we show how to conduct the adversarial example search on smoothed trees efficiently.

3.1 Tree Ensemble Smoothing through Branching Node Relaxation

Among various white-box adversarial attack methods, gradient descent-based approaches usually show a significant advantage in effectiveness and computational efficiency (with the existing toolboxes for auto-differentiation). To enable such an attack on tree ensemble models, we propose smoothing the tree ensemble to support auto-differentiation.

As reviewed in Section 2.2, the prediction of a tree ensemble is a linear combination of predictions from a set of decision trees. Since each decision tree can be factorized as a set of piece-wise branching nodes, we can smooth it by replacing the branching nodes with the softmax function. Concretely, for an intermediate node \( k \in \{1, \ldots, |K|\} \) of a tree \( D_t \) with two child nodes \((D_{t,k}^{\text{left}}, D_{t,k}^{\text{right}})\) and branching condition \( x_j > v_k \) in the form of
\[
D_{t,k}(x) = \begin{cases} 
D_{t,k}^{\text{left}}(x) & x_j > v_k \\
D_{t,k}^{\text{right}}(x) & \text{otherwise}
\end{cases}
\]
we relax each intermediate node with a probabilistic distribution such that
\[
\tilde{D}_{t,k}(x) = Q_{t,k}^{\text{left}}(x) \tilde{D}_{t,k}^{\text{left}}(x) + Q_{t,k}^{\text{right}}(x) \tilde{D}_{t,k}^{\text{right}}(x),
\]
where the distribution can be expressed through a simple sigmoid function
\[
Q_{t,k}^{\text{left}}(x) = \text{sigmoid}\left(\frac{x_j - v_k}{\sigma_j}\right) \quad \text{and} \quad Q_{t,k}^{\text{right}}(x) = 1 - Q_{t,k}^{\text{left}}(x).
\]
Here, we introduced the standard deviation \( \sigma_j \) of feature \( j \) in the training set into the sigmoid function to normalize the signals from all decision nodes.

With the above smoothing steps, the prediction of the smoothed tree ensemble \( \tilde{M} \) can be represented as
\[
\hat{y} = \arg\max_c \tilde{M}(x) = \arg\max_c \sum_{t=1}^{T} w_t \sum_{p=1}^{|P_t|} v_p \prod_{l=1}^{|L_p|} Q_{t,l}^p(x),
\]
\[
\tilde{D}_t(x)
\]

\footnote{While the smoothing operation supports multi-children branching, in practice, the internal nodes in a decision tree are usually binary branching nodes. In this paper, our description focuses on binary nodes.}
where \( P_t \) denotes the set of possible paths of a tree \( t \), \( l \in L_p \) denotes the \( l \)'th node in the decision path \( p \), and \( v_p \in C \) denotes the leaf node value of path \( p \).

While our approach on smoothing a tree ensemble appears similar to the smoothing approach introduced in Soft Decision Tree [17], the fundamental difference is that we smooth the tree ensembles as a post-processing step to facilitate adversarial robustness testing instead of doing so to train a decision tree.

3.1.1 Balancing Gradient Descent Efficiency and Decision Surface Preservation

While smoothing tree ensembles with sigmoid functions enables the usage of gradient descent, we note that the smoothed model may introduce two potential problems: 1) significant prediction gaps between the smoothed model and the original model, and 2) vanishing gradients due to the saturation of forward propagation over sigmoid functions.

To address the two potential problems, we introduce a hyper-parameter \( \tau \) to control the activation of sigmoid functions (also called tempered sigmoids in the literature) such that

\[
Q_{t,k}^\tau(x) = \text{sigmoid}(\frac{x_j - v_k}{\tau \sigma_j}).
\]

Figure 1 demonstrates the effect of controlling temperature hyper-parameter \( \tau \). A higher temperature results in a smoother decision surface while severely increasing the approximation gap between the smoothed model and the original model. Conversely, a low temperature may not support adversarial example search since the surface exhibits piece-wise behaviour. In the limit when \( \tau \to 0 \), the smoothed tree ensemble will fall back to the original model.

3.2 Gradient Descent based Adversarial Example Search on Smoothed Trees

According to the Basic Iterative Method (BIM) [20], given data point \((x, y)\), gradient descent based search aims to create a potential adversarial example \( x' \) by iteratively maximizing the prediction cost function \( J(M, x, y) \) with

\[
x^{(i+1)} = x^{(i)} + \nabla_x J(M, x^{(i)}, y) \quad \text{for} \quad i \in 1 \cdots |I|,
\]

where \( x^{(0)} = x \) as the starting point.

Using the gradient of Equation 6 directly in BIM requires traversing all the possible paths in the trees, which could be computationally intensive. Moreover, tree ensembles and their applications are different from neural networks: i) their decision surfaces are piece-wise constant, which reduces the efficiency of naïve gradient search; and ii) the inputs of the models may be not normalized and originate from very different distributions. Thus, using the same tolerance \( \epsilon \) for inputs with different distributions could be misleading. In the subsequent sections, we propose some strategies to address these problems.

3.2.1 Noise Injected Gradient Descent and Search Coverage Maximization

The travel direction of the largest gradient is not necessarily the shortest path to finding an adversarial example, as shown in Figure 2(a). Indeed, the shortest path to flip the decision could require climbing
While many other whitebox attack algorithms also introduce noise during the adversarial example search, both (b) illustrates the purpose of injecting noise into the gradient.

To mitigate this problem, we adopt Noise Injected Gradient Descent, where we add sparse noise in each step of the optimization such that

$$x^{(i+1)} = \left[ (1 + \xi) x^{(i)} + \nabla_x J(\tilde{M}, x^{(i)}), y \right] \text{ for } i \in \{1 \cdots |I|\},$$

where \(i\) denotes the iteration of the search, and we sample \(\xi_j \sim \mathcal{N}(0, \lambda)\) for a sampled feature index \(j\) to maximize the coverage of the adversarial example search. For other feature dimension \(j'\), the value of \(\xi_{j'}\) remains zero. Here, we introduce a hyper-parameter \(\lambda\) that controls the noise level. Figure 2 (b) illustrates the purpose of injecting noise into the gradient.

While many other whitebox attack algorithms also introduce noise during the adversarial example search, there are two differences between our approach and the others: 1) The noise introduced is NOT additive to the original value of \(x\) and thus keeps the scale of the feature value under consideration, which is particularly useful for applications where features are not of the same magnitude. 2) The noise is sparse and thus limits the noise injection to one dimension at a time. This helps improve the efficiency of noise injection since the movement to the closest adversarial example is always perpendicular to the decision boundary, which is near piece-wise in smoothed trees.

### 3.2.2 Tree Sampling for Fast Adversarial Example Search

Calculating the gradient of a smoothed tree ensemble \(\frac{\partial \hat{M}(x)}{\partial x}\) based on the model description shown in Equation [3] is the computationally expensive. The operation requires traversing all the nodes in each of the trees \(D_t\) and leads to computational complexity \(O(|K_t| + |L_t|)\) for a tree with \(|K_t|\) nodes and depth \(|L_t|\). In the worse case, we note \(|K_t| + |L_t| \approx 2^{|K_t|}\).

To mitigate the computational pressure, we propose sampling trajectories from each of the smoothed trees in a similar fashion to the original decision tree (only track one single path from all possible paths from root to leaves). Concretely, we aim to approximate the derivative of the smoothed tree ensemble \(\nabla_x \hat{M}(x)\) with a log-derivative trick to enable sampling:

$$\nabla_x \hat{M}(x) = \nabla_x \sum_{t=1}^{T} \sum_{p=1}^{|P_t|} \sum_{l=1}^{|L_p|} v_p \prod_{l=1}^{|L_p|} Q^p_{t,l}(x) = \sum_{t=1}^{T} \sum_{p=1}^{|P_t|} \sum_{l=1}^{|L_p|} Q^p_{t,l}(x) \nabla_x \log Q^p_{t,l}(x)$$

$$\approx \sum_{t=1}^{T} \sum_{p=1}^{|P_t|} \sum_{l=1}^{|L_p|} \nabla_x \log Q^p_{t,l}(x) v_p \text{ for } p \sim \text{Mult}(P_t, Q_t),$$

This log-derivative trick is commonly used in the reinforcement learning literature to avoid non-differentiable reward functions. E.g. policy gradient.
As the CDF is inaccessible in practice, we approximate the CDF empirically (ECDF) by 1) sorting with hyper-parameter $\epsilon$ which allows us to obtain an unbiased estimate of the derivative (controlled by $\epsilon$).

To reduce the variance of the estimate, we can also choose to sample multiple times and take the numerical expectation. However, from our experiments, we empirically show that sampling once is sufficient to achieve a reasonable approximation, as shown in Figure 3. Our conjecture of the observation is that we ensemble many trees in the tree ensemble model which smooths the noise introduced by the sampling.

### 3.2.3 Feature Dependent Perturbation Range

Many existing works use a universal $l_\infty$ norm to define the distance between the original input and adversarial example up to tolerance $\epsilon$. While using a universal distance metric and tolerance is a reasonable setup in an experimental environment, we note that the synthetic setting would result in a misleading conclusion for predictive tasks whose input are tabular data, where we expect the features of the data to have different ranges, distributions, and interpretations. This is particularly critical task to address for tree based models, since the training data for tree ensemble models is not necessarily normalized (which is different from deep learning models).

In this paper, we propose allowing the input perturbation range to be automatically adjusted for each feature based on feature statistics.

Assuming there is an unknown Cumulative Density Function (CDF) $F_j$ for each feature $j$, where any observed feature assignment $x_j$ is a sample from the CDF such that

$$x_j = F_j^{-1}(q) \quad \text{and} \quad q \sim \mathcal{U}(0, 1). \quad (11)$$

Here, $\mathcal{U}$ denotes a uniform distribution. We propose bounding the feature perturbation in the range

$$x_j^{(i+1)} \in [F^{-1}(F(x_j)^{(i)}) - \epsilon, F^{-1}(F(x_j) + \epsilon)] \quad (12)$$

with hyper-parameter $\epsilon \in \mathcal{U}(0, 1)$. Intuitively, the above operation enables a uniform perturbation (controlled by $\epsilon$) with implicit feature normalization.

As the CDF is inaccessible in practice, we approximate the CDF empirically (ECDF) by 1) sorting feature observations in the training data, 2) sampling data with their percentile scores (i.e. the indices of the sorted observation list), and 3) linearly interpolating these feature values and percentile scores.

### 4 Experiment and Evaluation

Now we proceed to evaluate the proposed adversarial robustness testing approach to answer the following questions:

- **RQ1**: How effective is the proposed approach in terms of searching for adversarial examples on tree ensembles compared to existing state-of-the-art approaches (e.g. blackbox attacks) and random perturbations?
- **RQ2**: How efficient is the proposed approach in terms of computational cost and time?
Table 1: Performance Comparison of Adversarial Robustness Testing. Here we measure the prediction accuracy after adversarial attack. Lower is better. Results are collected from 3-fold cross-validation, and error shows standard derivation.

| Ensemble | Data Name    | Original | Tolerance | STA-Exhaustive | STA-Sampling | GenAttack | NES | Random |
|----------|--------------|----------|-----------|----------------|--------------|-----------|-----|--------|
| Forest   | German Credit| 71.89% ± 1.83% | c = 0.2 | 44.80 ± 2.72 | 45.60 ± 2.73 | 42.90 ± 3.62 | 45.60 ± 2.82 | 70.54 ± 1.59 |
|          |              |          | c = 0.5 | 25.79 ± 12.22 | 26.39 ± 12.67 | 22.69 ± 13.26 | 26.59 ± 12.27 | 66.89 ± 0.86 |
|          |              |          | c = 0.8 | 22.49 ± 11.59 | 22.39 ± 11.83 | 17.69 ± 13.64 | 23.39 ± 11.83 | 64.89 ± 2.64 |
|          | Adult Salary | 77.59% ± 0.27% | c = 0.2 | 7.07 ± 0.16 | 7.11 ± 0.17 | 7.63 ± 0.22 | 7.24 ± 0.17 | 43.71 ± 1.98 |
|          |              |          | c = 0.5 | 0.54 ± 0.07 | 0.55 ± 0.05 | 0.58 ± 0.02 | 0.76 ± 0.02 | 32.81 ± 1.82 |
|          |              |          | c = 0.8 | 0.18 ± 0.12 | 0.19 ± 0.11 | 0.14 ± 0.13 | 0.43 ± 0.13 | 29.89 ± 1.87 |
|          | Breast Cancer| 95.43% ± 1.51% | c = 0.2 | 7.38 ± 2.29 | 8.97 ± 3.01 | 8.09 ± 2.89 | 10.55 ± 2.42 | 89.91 ± 13.99 |
|          |              |          | c = 0.5 | 0.17 ± 0.25 | 0.17 ± 0.25 | 0.17 ± 0.25 | 0.17 ± 0.25 | 51.88 ± 0.25 |
|          |              |          | c = 0.8 | 0 ± 0 | 0 ± 0 | 0 ± 0 | 0 ± 0 | 39.69 ± 0.55 |
| XGBoost  | German Credit| 75.29% ± 3.13% | c = 0.2 | 42.29 ± 8.56 | 42.29 ± 8.53 | 25.39 ± 7.32 | 41.49 ± 8.80 | 72.91 ± 2.24 |
|          |              |          | c = 0.5 | 18.19 ± 11.81 | 17.79 ± 11.52 | 14.29 ± 9.25 | 22.39 ± 12.01 | 67.19 ± 5.15 |
|          |              |          | c = 0.8 | 14.39 ± 9.33 | 14.59 ± 9.27 | 8.49 ± 5.81 | 18.89 ± 11.53 | 61.64 ± 8.43 |
|          | Adult Salary | 85.28% ± 1.68% | c = 0.2 | 0.76 ± 0.02 | 0.87 ± 0.03 | 0.82 ± 0.02 | 0.98 ± 0.02 | 44.66 ± 0.45 |
|          |              |          | c = 0.5 | 0.42 ± 0.02 | 0.42 ± 0.05 | 0.34 ± 0.04 | 0.66 ± 0.01 | 32.68 ± 0.02 |
|          |              |          | c = 0.8 | 0.42 ± 0.0 | 0.41 ± 0.0 | 0.05 ± 0.03 | 0.63 ± 0.09 | 26.78 ± 0.19 |
|          | Breast Cancer| 95.95% ± 0.89% | c = 0.2 | 7.56 ± 2.23 | 7.74 ± 2.18 | 7.48 ± 2.41 | 9.14 ± 2.39 | 86.53 ± 2.54 |
|          |              |          | c = 0.5 | 0.17 ± 0.25 | 0.17 ± 0.25 | 0 ± 0 | 0 ± 0 | 49.81 ± 2.53 |
|          |              |          | c = 0.8 | 0 ± 0 | 0 ± 0 | 0 ± 0 | 0 ± 0 | 39.78 ± 1.01 |

- **RQ3**: What is the effect of tuning the temperature hyper-parameter during model smoothing?
- **RQ4**: How does noise injection impact the search results?
- **RQ5**: Does the trajectory sampling approach work well compared to the exhaustive search?

### 4.1 Experimental Settings

We evaluate the proposed adversarial robustness testing approach on multiple pre-trained Random Forest and XGBoost models learned from multiple UCI datasets. All of the random forest models have 100 estimators with maximum tree depth 4. Other hyper-parameters of the tree ensembles remain default values. To evaluate performance, we show the accuracy degradation as evidence of the effectiveness of the adversarial attack. To evaluate the inference efficiency, we show the running time as the metric of comparison.

In the experiments, we call our proposed approaches STA-Exhaustive and STA-Sampling. Here, STA stands for Smoothed Tree Attack. STA-Exhaustive denotes a whitebox attack that exhaustively searches adversarial examples by collecting gradients from all decision trajectories of smoothed trees. In contrast, STA-Sampling denotes the sampling-based whitebox attack we described in Section 3.2.2 that reduces the inference time by sampling a single trajectory for each tree. The other candidate approaches in the experiments are GenAttack [2], NES [16], and Random, where Random denotes uniformly random perturbation on inputs to serves as a baseline attacking approach.

### 4.2 Performance Evaluation on Benchmark Datasets

We evaluate the effectiveness of the proposed methods (STA-Exhaustive and STA-Sampling) in terms of generating adversarial examples given a perturbation tolerance. Table 1 shows the experiment results. Here, we highlight our observations:

- The proposed approaches are effective in terms of looking for adversarial examples. When comparing to the random search baseline, there is a significant performance gap between STAs and Random.
- The proposed approaches show performance competitive with the state-of-the-art approaches, GenAttack and NES. In multiple cases (e.g. XGBoost trained on Adult Salary), the proposed approaches show significantly better performance than NES. Here, we want to highlight that the computational cost of GenAttack is exponentially more expensive than our proposed approaches, as we will show next.
- The sampling-based approximation shows a slightly worse performance than the exhaustive approach. However, such performance degradation is not statistically significant as their confidence intervals heavily overlap with each other.
- The proposed approaches show stable performance on both Random Forest and XGBoost models.
ExhaustiveSamplingGenAttack
NES
100
101
102
103
104
Runtime(sec) (log scale)
0.330.33
89.68
1.49
0.320.32
45.29
1.64
0.360.36
33.85
1.7
German Credit
ε=0.2
ε=0.5
ε=0.8

ExhaustiveSamplingGenAttack
NES
100
101
Runtime(sec) (log scale)
0.290.29
22.81
1.3
0.280.28
2.01
0.64
0.280.28
1.12
0.3
Breast Cancer

ExhaustiveSamplingGenAttack
NES
100
101
Runtime(sec) (log scale)
0.340.34
18.94
1.66
0.340.34
2.01
0.95
0.340.34
1.45
0.56
Breast Cancer

ExhaustiveSamplingGenAttack
NES
100
101
Runtime(sec) (log scale)
2.86
0.39
180.72
4.41
2.86
0.38
123.88
4.41
2.86
0.41
126.26
4.52
Adult Salary

Figure 4: Search time comparison between proposed and existing approaches. We use a log scale for the comparison as the GenAttack shows exponentially more time consumption than other approaches. For bars, lower is better. Legends (colours) show different perturbation tolerance. Values on top of bars are the actual run time in seconds. Lower is better. We omit error bars as the variance is negligible comparing to the significant run time gap among candidates.

4.3 Computational Efficiency against Combinational Optimization
In this experiment, we show the computational efficiency of the proposed approaches. Figure 4 shows the run time estimation that was conducted on Random Forest models. Experiments are done on a cluster with NVDIA Titan V GPUs. Here, we list two important observations:

- the exhaustive variant is more than ten times faster than the NES approach and over 100 times faster than the GenAttack with similar performance. The sampling-based approach is even faster than the exhaustive variant (2-8 times faster depending on the application domain.).

- For GenAttack, a smaller perturbation tolerance $\epsilon$ usually results in longer run time as it is hard to trigger early stopping due to the difficulty of searching for adversarial example with a small tolerance. In contrast, the efficiency of the proposed approaches is not sensitive to the size of epsilon.

- Combining the observations of Figure 4 and Table 1, we note that the proposed approaches show a significant advantage in terms of efficiency while maintaining competitive adversarial attack performance, which make them more practical for large-scale testing purposes.

4.4 Effectiveness of Tuning Hyper-Parameters
As we demonstrated in Figure 4, the temperature hyper-parameter controls the smoothness of the smoothed model. In this experiment, we show how the temperature would impact the adversarial example search. As shown in Figure 5, with a relatively larger smoothing temperature ($10^{-1}$), the whitebox attack usually shows better performance than very low temperature ($10^{-3}$). This is because the low temperature preserves the original model’s piece-wise property, which prevents gradient descent since the sigmoid functions are nearly saturated. However, this does not mean that a very high temperature is the best setting for all application domains. For the German Credit dataset (Figure 5(a)), we note that a large temperature ($10^{2}$) could result in poor performance. We note that the problem comes from the large approximation gap between the smoothed model and the original model. The adversarial examples of the smoothed model are no longer valid examples of the original model. Hence, tuning the temperature is a critical step to guarantee the performance of the
proposed approaches. In this work, we tune the hyper-parameters through grid search in range of \([10^{-3}, 10^{-2}, 10^{-1}, 10^0]\).

4.5 Effectiveness of Noise Injection on Gradient Descent

Figure 2 shows the effect of adding noise during the adversarial example search. We note that the proposed approach (STA-Exhaustive) demonstrated remarkable performance improvement for two of three datasets in our experiment with noise injection. This observation reflects our intuition (as shown in Figure 2) – it is critical to add noise during the search on smoothed trees. Since the smoothed tree ensembles still preserve some piece-wise property, pure gradient descent-based adversarial example search would either misguide the search direction or cause the search to get stuck from the beginning as demonstrated in Figure 2.

5 Conclusion and Discussion

This paper presents a novel adversarial robustness testing approach, STA, (with two variants) for tree ensemble models. The proposed method involves two steps. First, it smooths the tree ensemble to support auto-differentiation. Second, it conducts whitebox gradient-based attacks on the smoothed model for adversarial example search. To facilitate the adversarial example search, we introduce a number of techniques that yield remarkable performance improvement (in terms of effectiveness and efficiency), including temperature control, noise injection, feature-dependent perturbation bound, and log-derivative-based sampling. Our experiments in four application domains show that the proposed approach has a remarkable advantage over other state-of-the-art approaches in efficiency (more than ten times faster) while maintaining competitive effectiveness.

For as successful as our technique is, we emphasize we cannot guarantee it will find all model weaknesses. Adversarial examples present a distinct risk in using machine learning models outside of the lab, as their vulnerabilities may be exploited for malicious intents. Accordingly, if our test incorrectly declares a model robust, there may be negative societal impact. In addition, because our attack itself is powerful, it may be directly employed with malicious intent. However, as our attack requires access to the model’s internals, the likelihood of our test being misused in this way is reduced.
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