Evading Malware Classifiers via Monte Carlo Mutant Feature Discovery

John Boutsikas 1 Maksim E. Eren 1 Charles Varga 1 Edward Raff 1,2 Cynthia Matuszek 1 Charles Nicholas 1

Abstract

The use of Machine Learning has become a significant part of malware detection efforts due to the influx of new malware, an ever changing threat landscape, and the ability of Machine Learning methods to discover meaningful distinctions between malicious and benign software. Antivirus vendors have also begun to widely utilize malware classifiers based on dynamic and static malware analysis features. Therefore, a malware author might make evasive binary modifications against Machine Learning models as part of the malware development life cycle to execute an attack successfully. This makes the studying of possible classifier evasion strategies an essential part of cyber defense against malice. To this extent, we stage a grey box setup to analyze a scenario where the malware author does not know the target classifier algorithm, and does not have access to decisions made by the classifier, but knows the features used in training. In this experiment, a malicious actor trains a surrogate model using the EMBER-2018 dataset to discover binary mutations that cause an instance to be misclassified via a Monte Carlo tree search. Then, mutated malware is sent to the victim model that takes the place of an antivirus API to test whether it can evade detection.

1. Introduction

The number of malware in the wild has increased significantly in recent years. 1.1 billion total malware was recorded in 2020 alone. That is an over 139% increase from 2015 (The Independent IT Security Institute, 2020). The influx in the quantity of malware makes Machine Learning (ML) approaches such as statistical modeling, behavior analysis, and deep learning an ideal choice for malware analysis by cyber defenders. When used as a helper in the cyber domain, ML has shown to be one of the most effective ways to reduce risk, drive precise detection, reduce cost, and reduce response and recovery time (Bissell et al., 2020). Because of its advantages, ML and Artificial Intelligence (AI) are utilized by 38% of organizations (Bissell & Ponemon, 2019), and 83% of these spend more than 20% of their cybersecurity budget on such technologies (Bissell et al., 2020). At the same time, antivirus (AV) vendors have begun to widely utilize ML based malware detection techniques (Microsoft 365 Defender Threat Intelligence Team, 2020; Quintero, 2019b,a; Fleshman et al., 2018).

Recent work has shown that top AV that utilize some form of ML technology can be bypassed with simple modifications on the malware such as by adding a new section, appending a single byte, removing the debug and certificate values, or renaming a section (Song et al., 2020; Anderson et al., 2018). In our work, we borrow the feature changes that are shown to be effective in prior research, and explore a new mutant malware discovery methodology that is based on Monte Carlo Tree Search (MCTS).

We approach classifier evasion as a game playing exercise between the adversary and the ML model where a winning hand is a successful mutation that makes the malware undetectable. Similar to chess, there are numerous state permutations – mutations in our case – that can yield a winning play at any stage of our “game”. MCTS can find the winning hand by simulating a subset of all possible mutations, and discover an optimal path using an empirical scoring method. This allows empirical evaluation of mutations while minimizing error, and examines paths without actually computing all the possible permutations of changes. At the end, MCTS prioritizes minimizing the number of trackable changes that lead to evasion, hence avoiding excessive changes to the binary.

In this experiment, we stage a grey box adversarial scenario where the target classifier algorithm, decisions made by the classifier, and the data used in training are unknown, but the features used in training are known. The attacker
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trains a local Decision Tree (DT) with the test portion of the EMBER-2018 dataset (Anderson & Roth, 2018) and discovers evasive feature modifications via MCTS while using the surrogate model (DT) for confirmation. This allows attackers to circumvent querying AV APIs to verify their modifications. Such a scenario is feasible for an adversary when an API for verification is unavailable because it is part of an internal defense system at an organization, or if the malicious actor wants to avoid attention. The performance of the mutations is then evaluated against the victim Multilayer Perceptron (MLP), which is trained on the training portion of EMBER-2018, that takes the place of the target antivirus engine.

Our results show that MCTS finds successful mutations on the surrogate model for 52.18% of the malware, out of which 8.78% evades detection by the victim model, performing slightly better than our random mutation baseline with a 5.26% evasion rate. Our contributions in this paper include:

- Demonstrating an evasive malware feature discovery technique with Monte Carlo tree search.
- Analyzing the detection avoidance success rate when the adversary does not have access to the ground truth via an AV API.

2. Relevant Work

Adversarial attacks against ML models and defenses for these attacks are widely studied research areas (Jia et al., 2020; Papernot et al., 2017; Tramèr et al., 2017). Consequently, an open source toolbox for adversarial training has become popular in recent years 1. These attacks include modifications on the training data, poisoning the feature vector, or extracting the ML model parameters. When it comes to malware data science, however, there are special considerations to be taken.

Song et al. argues that some attacks are not always realistic or have an effect on the end user in the malware domain (Song et al., 2020). Attacks performed on feature vectors are not realistic as the poisoned feature vector may not possess the corresponding binary representation. Conversely, the attacks on byte-based models like MalConv (Raff et al., 2021; 2018) insert adversarial content into an executable that maintains validity while attempting to hide the evasive payload (Suciu et al., 2019; Kolosnjaji et al., 2018; Kreuk et al., 2018). An additional constraint (to the defender’s advantage) is that attacks are one-way, as benign authors do not attempt to alter their files to become falsely detected as malicious – only malicious authors alter their files to avoid detection (Fleshman et al., 2019; Incer et al., 2018). Therefore, in our analysis we avoid performing attacks towards feature vectors and focus on modifying the malware itself.

Similarly, changing malware requires additional ruminations as the direct modifications of the compiled malware may make the binary non-functional (Fleshman et al., 2018; Song et al., 2020). Malware that is generated in such a manner can evade the detector, but at the same time it may no longer demonstrate the malicious behavior. A keylogger could, for example, obtain permanence and display some of its malware characteristics, but may no longer actively log keystrokes, as that portion of the code has been altered during the modifications to avoid identification. We recognize this problem by developing heuristics that limit the possible changes in the Monte Carlo Tree Search. With that, we introduce a strong assumption that after the modification(s), the malware is still functional. In a real world example, an adversary can alter this rule set if the changes break the malware. Nevertheless, malware functionality can be verified on a virtual sandbox environment, and we leave this significant step to future work.

Additionally, Song et al. points out that some of the attacks demonstrated by other research assume inside knowledge with a white box setup, which is not realistic for an adversary to possess in real world scenarios (Song et al., 2020). For example, an attacker may not have access to the malware classifier’s architecture when it is part of the internal company infrastructure, unless the attacker obtains such knowledge via other means in the reconnaissance stage of the attack. Furthermore, in such a scenario, the attacker does not have access to the decisions the malware classifier makes. With this in mind, we stage a grey box attack where it is assumed that the attacker lacks access to the malware classifier but knows the features used in training; hence, the attack must be conducted without the ground truth in classification. Consequently, in our setup an adversary trains a surrogate model using a different set of data to verify the success of mutations.

With all the important considerations above, Song et al. develop a malware modification and mutant malware functionality verification system, and show that the static classifiers of real AV programs can be evaded 24.3% to 41.9% of the time with changes as simple as a single byte modification (Song et al., 2020). Finally, they discuss the fact that even though a sample can evade the classifier, it is not known what factors contribute to this evasion. In order to alleviate this concern, they provide a framework that can generate malware mutations while preserving the original malicious behavior of the sample, and also providing a way to trace back those modifications in order to explain which features were responsible for the evasion. Similarly, our mutant feature searching method can re-track the changes that caused the original mutation with a minimal number of steps.

1https://github.com/Trusted-AI/adversarial-robustness-toolbox
3. Dataset

We base our analysis on the EMBER-2018 dataset (Anderson & Roth, 2018). EMBER contains features extracted from 1.1M Windows PE files in a human friendly, JSON format, along with their label indicating whether the sample is malicious or benign. The main reason for our choice is the same that drove the creation of EMBER. A large collection of binaries is bound by many difficulties including logistical ones (i.e. storage, safe distribution) and legal ones (i.e. copyrighted binaries). EMBER resolves that by not sharing the binaries themselves – or even their name for that matter – but by sharing a parsed representation of various metadata that can be extracted from the PE header. We use this metadata to train our surrogate and victim models.

The default training and test set split in the EMBER dataset has a significant factor in our grey-box setup. Our victim malware classifier is trained on the EMBER-2018 training portion which consists of 299,867 benign and 299,851 malware instances for a total of 599,718 samples. On the other hand, our surrogate (adversary’s local model) will only utilize the EMBER-2018 test set that contains 199,800 samples, of which exactly half are malicious. This split supports the idea that malware is developed for more specific tasks requiring a smaller number of imports and exports. We then proceed to the pre-processing of our dataset, utilizing the tools available in the Scikit-learn library (Pedregosa et al., 2011).

3.1. Pre-processing

During training, both the surrogate model and the victim classifier utilize numerical and categorical static malware analysis based features. The numerical features used in training are String Entropy, Number of Strings, File Size, Timestamp, Size of Code, Number of Exports, and Number of Imports. These features are scaled to unit variance during pre-processing, and missing values are replaced with the median.

Categorical attributes include the Has Debug flag which indicates if the binary has the debug value set, the Has Signature which is used to indicate the existence of the binary certificate, and the Entry string that names the section name the binary uses to start the code execution. Categorical features are vectorized via one-hot encoding and missing values are replaced with the most frequent element for each feature. Unknown categorical attributes in the validation set are ignored. We also used imported libraries and imported functions during training. Unlike the previous categorical features, imported libraries and imported functions are vectorized by hashing their values while limiting the number of dimensions to $2^{10}$ for libraries and $2^{13}$ for the functions. Finally, all the features that are mentioned above are combined via multimodal feature fusion to create a single features vector $X$ representing each $n$ malware sample.

4. Adversarial Model

Adversarial scenarios differ in terms of the knowledge that an attacker possesses about the target. In a white-box adversarial setting, it is assumed that the attacker has significant knowledge about the target model, including the algorithm and the features-set used in training. On the other hand, black-box attacks are more realistic as the only known information is the output label of an otherwise unknown algorithm. For the malware classifiers; however, the output label may also be unavailable when the model is part of an internal defense system at an organization. Therefore, an attacker needs to verify the validity of modifications locally before the attack is deployed.
Our adversarial setup follows a grey-box scenario, a structure that is in between the white-box and the black-box setting, where the malware features and their corresponding pre-processing steps are the same for the surrogate and the target model. All the other information about the victim model is assumed to be unknown, including the prediction labels. To this extent, we train two different models where one replaces the place of the victim malware classifier an AV would have used, and a separate surrogate classifier that the malicious actor trains to identify the evasive feature mutations. In this section we describe both of these models, and provide their performance with receiver operation characteristics (ROC) and area under the curve (AUC), and with a precision-recall (PR) curve and the F1 scores.

4.1. Grey-box Surrogate Learner

Because the malicious actor does not have access to the decisions made by the target classifier, a local Decision Tree is trained, using Scikit-learn (Pedregosa et al., 2011), on a random subset of 60% of the EMBER test set. Predictions made by the Decision Tree are used to identify the features which makes the mutation valid. A valid mutation is when a malware sample is predicted to be benign by the surrogate after a mutation or combination of mutations.

We set the Decision Tree (surrogate) maximum depth hyper-parameter to 12. Our model obtains an ROC-AUC of 0.956 and an F1 score of 0.916 when classifying the remaining 40% of the EMBER-2018 test set.

4.2. Victim Malware Classifier API

We train a Multi-layer Perceptron (MLP) that takes the place of the AV. We train our model on the EMBER training set with a 20% split for the validation set which is used in hyper-parameter tuning. Our model consists of seven hidden fully connected layers with 512, 256, 128, 256, 128, 256, and 128 hidden nodes, respectively. In the hidden layers of the MLP we use the Rectified Linear Unit (ReLU) activation function (Nwankpa et al., 2018; Nair & Hinton, 2010). The output layer with a single node transfers the input $x_i$ with the Sigmoid activation function $\frac{1}{1 + e^{-x_i}}$. For the model optimizer, we use Adaptive Moment Estimation (Adam) (Kingma & Ba, 2019). Adam’s exponential decay hyper-parameters $\beta_1$ and $\beta_2$ are left at default $\beta_1 = 0.9$ and $\beta_2 = 0.999$ as suggested in (Kingma & Ba, 2019).

With this setup, our model obtains the ROC-AUC score of 0.964 and F1 score of 0.934 when classifying the 200,000 benign and malicious instances in the held out EMBER-2018 test.

5. Mutant Malware Generation

As discussed earlier, our goal is to generate mutations of the malware in the EMBER-2018 dataset, such that the mutated malware will not be detected by the API classifier. However, it is very important that those samples remain malicious after the modification. To that end, we provide a way to limit the mutations that can be applied to any given sample – mutated or otherwise. We will next explain these limitations and their purpose. There is a difference in the complexity of the mutations, as some imply that a number of different, simpler mutations also happen, and can be thought of as aggregate mutations.

5.1. Target Features

Here we list the set of possible mutations available to our Monte Carlo implementation, and their corresponding heuristic that limits the changes:

1. **Add String**: Any sample can have a total of 15 strings added to it, the reason being that there is a limit to the free, unused space in an already compiled binary, and as such there is a limit to how many strings can be added by using that space.

2. **Add String with Size**: This mutation shares the same 15 strings limit as the previous mutation; however, only 5 of those strings can also modify the size of the binary. The purpose of this simulation is to account for strings that can be added by small extensions to existing sections of the binary. Our implementation changes the size of the binary by 30 bytes.

3. **Change String Entropy**: This mutation attempts to modify the string entropy of the binary, towards a "benign" value. For our benign value we use the average entropy of all benign samples. There can be a total of 7 entropy modifications per sample. It represents adding specific strings with the goal of modifying the entropy towards a target value, versus just adding any string like the previous 2 mutations did.

4. **Change String Entropy with Size**: This mutation is similar to the previous one, and shares the same 7 applications cap. However, only 3 of those 7 mutations can also affect the size of the binary. The major difference with this mutation, is that since the attacker can specify the size, it is easier to construct strings that provide a more significant change to the overall entropy. Both entropy mutations imply the addition of a string.

5. **Remove String**: By removing a string, we are trying to simulate the act of the attacker finding a series of random bytes that are interpreted as strings, but they are in fact not strings, and changing those bytes so
they are no longer detected as strings by the feature extraction. We limit these removals to 4 per sample, as those type of strings should be less frequent.

6. **Add Section**: With this mutation we add a section with benign contents to the sample. There is no limit to how many times this can be applied, as after some testing we found that our algorithm would avoid adding a large quantity of sections, and instead use a shorter route to evasion. Each section adds 512 bytes to the sample’s size.

7. **Add Bytes**: In this mutation we simulate appending benign bytes to any of the existing malware sections. This mutation adds 128 bytes to the size of that section and the overall size of the file. The mutation can be applied as many times as desired.

8. **Add Code Bytes**: Appends 64 benign bytes to the code section specifically. This mutation be applied as many times as desired, but again our algorithm seems to avoid extensive application of these.

9. **Import Function**: This mutation will add a function to the import table of the malware, as well as the matching DLL if it is missing. In order to decide what those functions would be, we made a list of the most common functions in the benign samples that do not appear in malware samples. This gave us 14 candidate functions, so each application of this mutation will select one of those 14 at random, provided it is not already present in the sample.

10. **Change Timestamp**: This mutation will modify the timestamp of the sample towards a target timestamp, by the given step size. For our target timestamp we used the average timestamp of all benign samples, with a step of 1000 milliseconds. The mutation can be applied as many times as desired, as it can adjust the direction of the step to move towards the target timestamp.

11. **Remove Debug**: This mutation will set the debug flag to false. The mutation can only be applied if the sample’s debug flag is set to true.

12. **Change Signature**: This mutation sets the certificate flag to true. The mutation can only be applied if the sample does not have a certificate already.

We use this list of feature modifications as they seemed to provide reasonable results and prior work showed that successful evasion is possible with some of them (Song et al., 2020). Our framework allows for easy modification of the mutation values – by the researcher – to match any given dataset, including restricting the heuristics if the modifications break the malware. It also allows for easy extension of these mutations to accommodate for the samples at hand.

5.2. Monte Carlo Mutant Feature Search

We decided to approach the mutation finding activity as a game playing problem where a winning hand is a successful mutation that makes the sample undetectable. This fits well with our problem because at any stage of our “game”, there are many different possible combinations of mutations that can be the winning hand. There are multiple algorithms that can be used in this context, including, but not limited to, the mini-max alpha beta pruning and the expectimax tree search algorithms. The main drawback of these algorithms is that they rely on the existence of two opponents playing the game. Thus, our analysis direction changed towards a game playing algorithm that could be adapted to a “single player” context as our only player would be the program that is trying to beat the surrogate model (i.e. the surrogate model cannot make any “plays”). As such, we decided to proceed with the Monte Carlo Tree Search (MCTS) algorithm. This algorithm still shares all the tree-related pitfalls – like state explosion and extreme redundancy – with the previously mentioned algorithms. We address those issues in our implementation.

MCTS has gained popularity based on its application for the game Go as described by (Coulom, 2009), as well as its latest implementation in Google’s AlphaZero (Silver et al., 2018). The algorithm consists of 4 conceptual stages. All stages happen once per iteration.

1. **Tree Traversal**: In this phase, the algorithm traverses the existing nodes of the tree. A node is a combination of the mutations that have happened to the sample up to that point. The goal is to reach a node that is currently a leaf, and expand it if it is not a terminal node. We consider a node terminal when a benign classification is reached. We name this behavior the **Tree Policy**.

2. **Expansion**: During expansion the algorithm will add a number of children nodes to the node found during tree traversal. Each child will represent a mutation allowed by our rules. The expansion of a given node happens only once; the second time a non-terminal, leaf node is visited. The first time we visit a leaf node, we simulate it on its own; therefore, we cannot also expand it at the same time. We name this the **Expansion Policy**.

3. **Simulation**: The application of Monte Carlo methods happens in this phase. Starting from the node that is currently evaluated, the algorithm generates subsequent states at random until it reaches a terminal node or we reach our simulation depth. At the end of this phase, a score is calculated for the node that is under evaluation by accounting for the simulated number of mutations, then the simulation states are discarded. Finally, the score is then propagated back up the tree. We name this behavior the **Simulation Policy**.
4. **Back propagation**: In this phase, we update the score of the node we just evaluated as well as its visit count, and then propagate this change up the tree until we reach the root node. This way the tree policy can select a more suitable path to explore in the next iteration.

MCTS on its own does not suffice. Even successful implementations – AlphaGo Zero for instance – do not rely on the algorithm alone, and make modifications. Similarly, we implement the following modifications to the various phases of MCTS, to better suit our problem.

We borrow inspiration from the Upper Confidence Bounds algorithm as applied to trees (UCT) for the Tree Traversal phase (Kocsis & Szepesvári, 2006). UCT allows selecting the next best child to explore using an empirical score, through the use of bandit methods, instead of relying on obtaining the actual score. Computing the real score of the child is expensive, and quite often impossible for our case as finding a successful mutation from any given node is not always achievable. However, the use of the empirical score introduces a potential divergence from the true value. Thankfully, the algorithm is shown in the original paper to be consistent within the estimation error caused by sampling. We apply a modification on that algorithm, and use the UCB1 function to evaluate the next child to traverse:

\[
ucb1 = \frac{score_{child}}{visits_{child}} + c \sqrt{\frac{\ln(visits_{parent})}{visits_{child}}}
\]

where the first element in the sum is the empirical score of the child node we want to evaluate, \(c\) is the exploration coefficient, and the squared root factor gives a higher score to the children that we have visited the least. In this context, a 0 visit means always exploring the child node. Finally, a high exploration coefficient makes our traversal more akin to breadth-first search, while a lower value makes the traversal similar to a depth-first search. We put these modifications in place with the hope that our search will not limit itself into exploring a few specific mutations, but instead explore a larger portion of the mutation space.

By using the above evaluation score the Tree Policy selects the child with the highest evaluation to traverse next with:

\[
next_{child} = \arg \max_{ucb1} children
\]

This allows our search to change which part of the tree it explores in each iteration, and give high prioritization to the nodes that have not been explored before using the UCB1 based evaluation.

Similarly, we apply some modifications in the expansion phase. We begin with our mutations rules – or invariants mentioned in Section 5.1. In the original MCTS, a child is added for each potential action from the current node when a node is expanded. Specifically, we limit the available children nodes to the ones with applicable mutations according to our invariants. This reduces the potential state explosion, and limits generating mutations that are likely to break the malware. Finally, we need to address the redundancy present in a tree structure. If 0, 1, 4 are 3 different mutations, the classification result for [0, 4, 1] and [4, 1, 0] should be the same since we examine the mutation set as a whole instead of each mutation individually. By sorting the proposed path and hashing it, we can cross-reference the hash of the sorted new mutation with all the other, sorted paths which we have already examined. If we have a match for this proposed path for the malware sample \(n\), the mutation is not added during the expansion phase as a child node. This further reduces the potential state expansion as well as our runtime, as we no longer spend time on the previously seen combinations.

**Algorithm 1** Tree Policy

```
Input: node root
Initialize node = root
while node.is_expanded do
    node = arg max<sub>ucb1</sub> node.children
end while
```

Our simulation phase is not that different from the original algorithm. However, we do still enforce our invariants when expanding the randomly selected nodes. If we skip this step, the algorithm could generate a successful mutation that is not allowed by our invariants. Therefore, this part of the tree would get a high score, but the search would never be able to construct the path as it is not considered valid during the expansion phase. During the simulation phase, child selection happens through random sampling instead.
Finally, before we move onto back propagation, we need a value to assign as the score of the newly evaluated node. We elected to use the length of the simulated path to a benign mutation. So for example, if our simulation policy produced the path \([7, 8, 4, 4, 9, 10]\) from some node \(n\), then the score of \(n\) will be \(\text{length}(\text{path}) = 6\). However, since we care about the shortest mutation paths we use the negative of that score. This allows the shortest paths to produce the higher scores. If no benign classification was found, we set the score to \(-\infty\):

\[
    s = \begin{cases} 
        -\text{length}(\text{min}(\text{path})), & \text{if benign} \\
        -\infty, & \text{otherwise}
    \end{cases}
\] (1)

We should note that this score is produced only once, as each node is simulated only once. It can be, however, updated since in the subsequent iterations the search can explore the children of \(n\). The back propagation phase of these children will modify the score of \(n\).

Algorithm 3 Monte-Carlo Tree Search

**Input:** sample \(s\), iterations \(it\)

1. Initialize \(it\) = 0.
2. Initialize root from sample
3. \(node = root\)
4. **repeat**
   1. **while** node.isExpanded **do**
      1. \(node = \text{TreePolicy}(node)\)
   2. **if** node.visitCount \(\neq 0\) **then**
      1. ExpansionPolicy(node)
      2. \(node = \text{TreePolicy}(node)\)
   3. **end if**
5. \(path = \text{SimulationPolicy}(node)\)
6. \(score = \text{EvaluatePath}(path)\)
7. \(\text{BackPropagate}(score)\)
8. **until** iterations is \(it\)

Algorithm 4 Back propagation

**Input:** Node’s ancestors \(ancestors\)

1. **for** node \(\in\) ancestors **do**
   1. **if** node.score \(\neq -\infty\) **AND** \(s \neq -\infty\) **then**
      1. node.score += \(s\)
   2. **else**
      1. node.score = \(s\)
   3. **end if**
2. node.visits += 1

Algorithm 5 Path recovery

**Input:** node \(root\)

1. **Output:** Mutation Path \(path\)
2. Initialize \(node = root\).
3. Initialize \(path = \) empty list
4. **while** node.isExpanded **AND NOT** node.isTerminal **do**
   1. \(node = \arg\max_{\text{score}} node.children\)
   2. \(path = path \cup node\)
5. **end while**

The last missing piece of our algorithm is the recovery of the path once MCTS has finished all of its iterations. MCTS is often used to select the next action or state transition. Our goal, however, is to create a serializable version of the shortest mutation path so that we can apply it later against a different classifier. Therefore, we need to recover the whole mutation path. The algorithm is very intuitive, as our scoring ensures that the best evaluated nodes will have the highest – although still negative – scores and visit counts. With that, recovering the path is as simple as starting from the root of the tree then always selecting the child with the highest score until we reach a terminal node. If after this process we cannot reach a terminal node, it means that the search was unable to find a mutation for this sample.

6. Results

Here we present the mutant feature discovery results and their performance when evading the target classifier introduced in Section 4.2. Additionally, we compare the Monte Carlo search and its corresponding classifier evasion performance to a Random Search baseline. The longest mutation chain that was produced by MCTS was 5; as such, we limit the Random Search to mutate the malware a maximum of 5 times for our comparison. The reasons will become apparent soon through the rest of this section.

6.1. Search Results

We begin by introducing the feature changes discovered by the MCTS. Using the surrogate Decision Tree, MCTS was able to find successful mutations for over 56% of the total malware samples in the EMBER-2018 test set. This is shown in Figure 1 with the distribution of a total number of mutations needed for samples to be misclassified. If the algorithm was unable to find a successful mutation in the given setup/time, the sample is classified as a “Failed mutation”. Around 52% of the malware needed only a certificate signature change (Change Signature) to be misclassified as shown in Table 2. Specifically, changing the signature alone was enough to alter the prediction for 71% of the successful mutations. This behavior could be an artifact of the binary
Table 2. Statistics from mutation discovery via Monte Carlo and Random Search on the surrogate Decision Tree (DT). The Alone column presents the number of malware where one type of feature change was enough for misclassification. In Group shows the number of samples where the mutation appeared in combination with other mutations. The Repeats column provides the instance count where the mutation type appears more than once. Affected Instances is the number of mutated malware, and Total Occurrence is the total number of times our tree search yielded the mutation across all of the successfully modified malware samples.

| Mutations over DT with MCTS | Mutations over DT with Random Search |
|-----------------------------|-----------------------------------|
| Alone | In Group | Repeats | Affected Instances | Total Occurrence | Alone | In Group | Repeats | Affected Instances | Total Occurrence |
| Add String | 0 | 79 | 23 | 79 | 115 | 0 | 496 | 27 | 496 | 523 |
| Add String with Size | 6 | 137 | 0 | 143 | 143 | 1 | 4355 | 0 | 4356 | 4356 |
| Change String Entropy | 0 | 2223 | 90 | 2223 | 2313 | 0 | 615 | 30 | 615 | 645 |
| Change String Entropy with Size | 9724 | 3223 | 5 | 12947 | 12952 | 1144 | 6754 | 1 | 7898 | 7899 |
| Remove String | 0 | 35 | 0 | 35 | 35 | 0 | 4389 | 510 | 4389 | 4937 |
| Add Section with size | 698 | 249 | 151 | 947 | 1153 | 186 | 4609 | 306 | 4795 | 5339 |
| Add Bytes | 0 | 33 | 0 | 33 | 33 | 21 | 4424 | 508 | 4445 | 4993 |
| Add Code Bytes | 0 | 31 | 2 | 31 | 37 | 20 | 4416 | 481 | 4456 | 4951 |
| Import Function | 502 | 634 | 559 | 1136 | 1949 | 66 | 4451 | 575 | 4537 | 5128 |
| Change Timestamp | 0 | 32 | 1 | 32 | 33 | 0 | 4465 | 536 | 4465 | 5036 |
| Remove Debug | 10 | 39 | 0 | 49 | 49 | 33 | 686 | 0 | 686 | 686 |
| Change Signature | 37214 | 1238 | 0 | 38452 | 38452 | 4150 | 17470 | 0 | 17470 | 17470 |

Figure 1. Distribution of number of mutations needed for misclassification over the EMBER test set while using MCTS on the surrogate model. A sample failed mutation, when the algorithm was not able to find a mutation in the given setup/time (for example number of iterations limit is reached).

The second most potent mutation with MCTS is adding a string that would simultaneously modify the string entropy of the sample, increase the file size, and the number of strings (Change String Entropy with Size). This result is not unexpected as it is an aggregate mutation affecting 3 of the binary features simultaneously. Change String Entropy with Size was a desired path for 19% of the mutations, and 9,724 malware instances were mutated (i.e. successfully misclassified) with this modification alone.

When using Random Search, the feature that was used the most was Change Signature, and the distribution of the number of mutations needed until evasion can be seen in Figure 2. Random Search mutated significantly fewer malware samples. In the times where the mutation was successful, it required a higher number of changes.

Figure 2. Distribution of the number of mutations needed for misclassification over the EMBER test set while using Random Search on the surrogate model. A sample failed mutation, when the algorithm was not able to find a mutation in the given setup/time (for example number of iterations limit is reached).

6.2. Classifier Evasion Results

The performance of the mutations is evaluated against the target API, or victim model, after the modifications found by MCTS and Random Search with the Decision Tree are serialized to mutate the malware samples in the EMBER-2018 test set. The mutated malware is then transformed using the pre-processing pipeline introduced in Section 3.1. Finally, the victim classifier predicts the new labels, and the results from the MCTS and Random Search are compared.

As seen in Figure 3, approximately 8.79% of the mutations found by MCTS managed to evade the model. While the majority of the malware is still detected, the increased number of malware passing through the security parameters carry high risk. In comparison, 5.26% of the mutations found by Random Search evaded detection, and it was able to mutate less than 23% of the samples. The reduced mutation rate of Random Search is an artifact of limiting the search space to the maximum number of changes performed by
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MCTS in order to create a more equal comparison. If we were to allow Random Search an unlimited search space, we would be measuring the number of mutations required before mis-classification, instead of finding targeted mutations. In theory, if we were to apply an infinite number of mutations, malware would eventually evade the classifier. However, this would also be detrimental to the functionality of the sample.

These results show MCTS being able to find more mutations and yield a higher evasion rate in comparison to Random Search in our setup. It should also be noted that our Monte Carlo implementation is flexible for more targeted settings. If we were to narrow down our samples and adjust the various Monte Carlo search hyper-parameters, we could potentially get better results even with the Decision Tree as the surrogate model. In addition, our system is flexible in what model is used as the surrogate. Therefore, an attacker may consider using a more complex surrogate model like a deep learning architecture, or an ensemble of models.

Our intuition, along with the results we have seen in this paper, points to the surrogate model playing a considerable role in the performance of the search. Specifically, we are using a binary decision tree as our surrogate which will need to grow in depth in order to properly train over the dataset. That makes depth-first searches more likely to find and exploit the decision tree, whereas a breadth-favoring approach might work better against an MLP model. Furthermore, the fact that a completely binary mutation was the most used one in both searches might also be an artifact of the binary decision tree. Therefore, the future work can include examining how different surrogate models affect the search as well as experimenting with favoring mutations of slightly longer length in MCTS.

Conclusion

Growing popularity of ML based malware detection makes the analysis of these systems against evasive attacks an essential part of cyber defense. We show that a malicious actor can reduce the detection rate of malware samples without the knowledge of the output labels of the Machine Learning model that the adversary camouflages against. Utilizing the adjustable Monte Carlo tree search, with the custom rule set, an adversary can discover the modifications that makes the malware undetectable by checking the changes against a surrogate verifier.

Future work can consider model extraction attacks to create a copy surrogate model to be used as the validator. This can include the re-training attack and the equation-solving attack. Another direction for future work is to perform direct modifications on the real malicious binaries and verify their functionality after feature alteration(s) via a sandbox setup. Finally, it would also be interesting to try a black box setup where the adversary does not know the features used during the training of the target.

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