Multiple Instance Learning for Malware Classification

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Abstract—This work addresses classification of unknown binaries executed in sandbox by modeling their interaction with system resources (files, mutexes, registry keys and communication with servers over the network) and error messages provided by the operating system, using vocabulary-based method from the multiple instance learning paradigm. It introduces similarities suitable for individual resource types that combined with an approximative clustering method efficiently group the system resources and define features directly from data. This approach effectively removes randomization often employed by malware authors and projects samples into low-dimensional feature space suitable for common classifiers. An extensive comparison to the state of the art on a large corpus of binaries demonstrates that the proposed solution achieves superior results using only a fraction of training samples. Moreover, it makes use of a source of information different than most of the prior art, which increases the diversity of tools detecting the malware, hence making detection evasion more difficult.

Index Terms—Malware, dynamic analysis, sandboxing, multiple instance learning, classification, random forest.

I. MOTIVATION

Since malware is presently one of the most serious threats to computer security with the number of new samples reaching 140 million in 2015 [3], battles against it are fought on many fronts. Signature matching remains the core defense technology, but due to evasion techniques such as polymorphism, obfuscation, and encryption, keeping good recall is difficult for static analysis and methods based purely on string matching. A popular approach to tackle these problems is to execute a binary in a controlled environment (sandbox) [45], monitor its behavior, and based on this behavior classify the sample into benign or malware class (or as a particular malware family). The assumption of these dynamic analysis methods is that behavior should be more difficult to randomize and therefore it should constitute a more robust signal.

Most approaches to dynamic analysis rely on system calls [32], [1], [45], as they are the only means how the binary can interact with the operating system and other resources. This popularity has however already triggered many evasion techniques, such as shadow attacks [29], system-call injection attacks [22], or sandbox detection [16].

A perpendicular approach to modeling system calls is to model resources the binary has interacted with together with the type of the resources. The rationale is that if malware wants to provide revenue to its owner, it has to perform actions, such as downloading advertisements in the case of adware, encrypting hard drive in the case of ransomware, exfiltrating sensitive data in the case of credential stealers, etc. This work assumes that execution of these actions involves interactions with resources visible at the operating system level, and this interaction can be viewed as a signal which is hard to hide and which can be indicative of malware families.

Modeling interactions with system resources has been already exploited by the prior art. Mohaisen et al. [30] extracts a manually predefined set of features such as number of files created in specific folders, number of HTTP requests, etc., and use it in supervised classification. However, we believe that the rapidly changing threat landscape makes it difficult to manually design features that are indicative while also being stable over time. An alternative paradigm is to avoid manual design and to use a bag-of-words model (BoW model), where each interaction with a particular resource identified by its name is considered as a unique feature [38]. The price paid for circumventing manual feature design using BoW is an explosion of the problem dimension, which can easily reach millions.

This work circumvents the problem of manually designing features while at the same time avoiding the problem dimension explosion. The approach is to first cluster resource names with similarity functions tailored for each resource type (file names, mutexes, registry names, and domain names), and then use this clustering to represent a sample (a binary executed in the sandbox) in a lower-dimensional space. This enables us to use a random forest classifier (or any other classifier of choice) to separate malware from legitimate samples. The clustering also effectively removes randomization used to evade detection.

The proposed approach is extensively evaluated on a large number of samples (more than 200 000) and compared to relevant prior art. Experimental results show that the proposed approach indeed improves the accuracy of detecting malware binaries.

The contributions of this paper are manifold including a novel approach to representing malware using raw data, definition of a similarity measure reflecting directory structure, optimization of similarity function over binaries, improvements to Louvain clustering in order to scale to large scale datasets, and finally evaluation and comparison to state-of-the-art approaches on real-world malware using large-scale dataset.

II. CLASSIFICATION OF SANDBOXED SAMPLES

To capture the malware behavior, this work assumes that execution of malware’s actions involves interactions with resources visible at the operating system level. Examples of such interactions include operations with files during encryption of a victim’s hard drive, network communication during...
data exfiltration or displaying advertisements, operation with mutexes used to ensure a single instance of malware is running, or manipulation with registry keys to ensure persistency after reboot. An additional source of information are error messages of the operating system itself. Such information is provided by the sandboxing environment as the following warnings: all not found indicating missing dynamic library, incorrect executable checksum indicating corrupted binary, and sample did not execute indicating the fact that the binary was not executed at all due to various reasons (corrupted binary, sandbox was not able to copy the binary into VM, etc).

To model the interactions of a malware binary with resources, this work views each binary executed in a sandbox as a set of pairs of names and types of resources the binary interacted with. This view frames the problem as a multiple instance learning (MIL) problem where each sample (binary) consists of a set of instances of different size. In our scenario an instance represents the pair of name and type of a resource the binary interacted with during sandboxing.

### Algorithm 1: High-level overview of training (function TRAIN) and classification (function PREDICT) of malware samples.

1. **function** $\text{TRAIN}(S, y)$ ▷ Training samples and labels
   2. $I \leftarrow \text{extractInstances}(S)$
   3. $C \leftarrow \text{cluster}(I)$ ▷ Clustering of instances (separately for individual types)
   4. $X \leftarrow \text{project}(S, C)$ ▷ Projection of samples into binary vector (Alg. 2)
   5. $M \leftarrow \text{trainClassifier}(X, y)$
   6. **return** $M, C$ ▷ Returns cluster centers $C$ and trained classifier $M$
   7. **end function**

8. **function** $\text{PREDICT}(S', C, M)$ ▷ Testing samples $S'$, clusters $C$ and classifier $M$
   9. $X' \leftarrow \text{project}(S', C)$ ▷ Projection of samples into binary vector (Alg. 2)
   10. $\hat{y} \leftarrow \text{predict}(M, X')$ ▷ Classification of testing samples
   11. **return** $\hat{y}$
   12. **end function**

Variable sizes of samples and lack of order over their instances pose a challenge to traditional machine learning methods that expect samples to have fixed size. A recent review of MIL algorithms [2] lists various approaches to overcome this variability in sample sizes. One of the most popular (also adopted in this work) is vocabulary-based method outlined in Algorithm 1. It employs clustering of instances to describe the sample by a fixed-dimensional vector with length equal to the size of vocabulary, i.e. a set of clusters, so that an ordinary machine learning method can be applied.

To convert a sample into a fixed-dimensional vector, all instances $I$ from all training samples $S$ are extracted and clustered by a suitable method per given resource type—files, mutexes, registry keys, network communication. Note that warnings generated by the sandboxing environment are used directly, i.e. every warning is considered as a separated cluster. The resulting clusters represent the vocabulary. Next, for every instance $i$ the closest cluster prototype $c^*$ (a small random subset of the cluster of instances) of corresponding type is located. Finally, the binary representation is then used such that element of the vector equals to 1 iff there was an instance close to the particular cluster prototype. Once all samples are encoded as fixed-dimensional vectors, one can use a machine learning algorithm of choice to implement the classifier. This work uses the random forest classifier [8] due to its versatility, accuracy, and scalability, which make it a popular choice for many different machine learning tasks including malware classification [17].

Since the clustering is an essential component of the above algorithm, the definition of similarity over instances (resource names) greatly influences the accuracy of the system, and therefore it should reflect properties of the application domain. The rest of this section defines a specific similarity metric for each type of resources the malware interact with, namely on files, mutexes, network hostnames, and registry keys, and also justifies our choice of the clustering method.

### A. Similarity between file paths

Although viewing file paths as strings would allow to use vast prior art such as Levenshtein distance [25],
Hamming distance, Jaro-Winkler distance [33], or string kernels introduced in [28], the file systems were designed as tree structures with names of some folders (fragments of the path) being imposed by the operating system and the distance should reflect that. For example two files with paths /Documents and Settings/Admin/Start Menu/Programs/Startup/tii9fwlliv.lnk and /Documents and Settings/Admin/Start Menu/Programs/Accessories/Notepad.lnk share large parts of their paths and common string similarities will return high similarity score, but they serve very different purposes, since the first file is a link to an application executed after the start of the operating system (OS), while the second is a regular link in the Start menu in Windows OS. Another aspect that prohibits the use of common string similarities is their computational complexity (typically $O(n^2)$ where $n$ is the length of the string). The complexity combined with the number of resources to be clustered (in order of millions) leads to unfeasible time requirements. This motivates the design of a similarity that is fast and takes into the account the tree structure of the file system, special folders, and differences between folders and filenames.

The proposed similarity $s(x, x')$ of two file paths $x$ and $x'$ is defined as

$$s(x, x') = \exp (-w^T f(x, x')),$$  \hspace{1cm} (1)

where $w$ is a vector of weights and $f(x, x')$ is a function extracting a feature vector from file paths $x$ and $x'$. Both the weight vector $w$ and function $f$ play an essential role and are both discussed in detail below.

The function $f$ in (1) captures differences between the two paths $x$ and $x'$ by a fixed-dimensional vector. It first splits both paths $x$ and $x'$ into fragments $x_i$ and $x'_i$ using OS specific path separator in the cases of MacOS and Windows changes all characters to lowercase, and assigns all fragments into one of the following four categories:

1) **known folder** – fragment $x_i$ is a well known folder in the list of folders imposed by the operating system (e.g. Windows, Program Files, System32, etc.),

2) **general folder** – fragment $x_i$ is a not-well-known folder (e.g. unknown folders in Program Files, randomly generated folders in Internet Explorer cache folder, etc.),

3) **file** – fragment $x_i$ is file,

4) **empty** – artificial fragment used for padding the paths in cases when paths $x$ and $x'$ have different depths.

When all fragments are assigned to one of the above classes, their dissimilarity is captured by the function $f$ as

$$f(x, x') = (f_{KK}, f_{KG}, f_{KF}, f_{KE}, f_{GF}, f_{GE}, f_{FF}, f_{FE})$$

where

- $f_{KK}$ is the number of fragments on the same level that were both classified as known folder and were not equal,
- $f_{GF}$ is the sum of Levenshtein distances between all fragments on the same level that were classified as general folder,
- $f_{FF}$ is the sum of Levenshtein distances of all fragments on the same level that were classified as file,
- $f_{KG}, f_{KF}, f_{KE}, f_{GF}, f_{GE}, f_{FF}, f_{FE}$ are the sums of all fragments of the same level and were classified as known and general folder, known folder and file, known folder and empty, general folder and file, general folder and empty, and file and empty respectively.

To illustrate the calculation of $f(x, x')$, let’s consider the same two paths used above. At first, function $f$ splits both paths into fragments and assign them into one of four categories (see Table I). Assigning fragment to classes requires a list of known folders, which for the purpose of this example we assume to contain Documents and Settings, Start Menu, Programs and Startup, which are present in all windows installations. All corresponding folders from those two paths are therefore assigned to known folder class, while Admin and Accessories are labeled as general folders.

Individual elements of the vector $f(x, x')$ are calculated using the above rules as follows: the first rule applies to three fragments 1, 3, and 4 belonging to known folder class, but as they are all equal $f_{KK} = 0$; the second rule returns 0 based on analogous reasoning but for general folders; the third rule returns $f_{FF} = 0.7143$, which is the Levenshtein distance between tii9fwlliv.lnk and Notepad.lnk; the only mismatch is on fragment 5–known folder and general folder yielding $f_{KG} = 1$; and finally all remaining elements of feature vector are 0. The output of $f(x, x')$ is captured by the feature vector

$$f(x, x') = (0, 0, 0, 71431, 1, 0, 0, 0, 0).$$

The weight vector $w$ in (1) captures the contribution of individual elements of the feature vector $f(x, x')$. Imposing condition $w \geq 0$, in combination with construction of function $f$, $s(x, x') \in [0, 1]$ such that the similarity functions returns 1 (or values close to 1) if $x$ and $x'$ belong to the same class (files in /temp/ directory, cache of the Internet Explorer, files in system directory, etc.) and values approaching 0 if they belong to different classes. Since the similarity function was inspired by the popular Gaussian kernel, the parameter vector $w$ was optimized using the Centered Kernel Target Alignment (CKTA), which is a method to optimize kernel parameters. CKTA assumes training data $\{(x_i, y_i)\}_{i=1}^m$ where $x_i$ is a file path and $y_i$ is the class of the path $x_i$, and defines centered kernel matrix as

$$[S_w^w]_{ij} = S_{ij}^w - \frac{1}{m} \sum_{i=1}^m S_{ij}^w - \frac{1}{m} \sum_{j=1}^m S_{ij}^w + \frac{1}{m^2} \sum_{i,j=1}^m S_{ij}^w,$$ \hspace{1cm} (2)

2Full list of known folders is available online: https://github.com/SfinxCZ/Malware-analysis-using-multiple-instance-learning

3The first three known folders are embedded in the functionality of the Windows OS. The Startup folder has a specific meaning altering the behavior of the operation system since all programs listed in this folder are executed after the boot of the OS. On the other hand Accessories can be easily changed without major consequences.
Table II: Example of two paths $x$ and $x'$ separated into individual fragments with labels ($K$ – known folder, $G$ – general folder and $F$ – file).

$S_{ij} = s_{w}(x_i, x_j)$ is the kernel matrix corresponding to the similarity function \( \mathbf{1} \) parametrized by the weight vector $w$. CKTA maximizes correlation between labels and a similarity matrix by solving the following optimization problem

$$w^* = \arg \max_{w \geq 0} \frac{(S^w_{ij}, Y_c)_F}{\|S^w_x\|_F \cdot \|Y_c\|_F}, \quad (3)$$

where $Y$ is target label kernel with $\|Y\|_{ij}$ equals to 1 when $i^{th}$ and $j^{th}$ paths from training data belongs to the same class and $-1$ otherwise, $(\cdot, \cdot)_F$ is Frobenius product and $\| \cdot \|_F$ is Frobenius norm (see Appendix A for more details). In below experiments (3) is solved by stochastic gradient descent (SGD) algorithm \( \mathbf{6} \). Note that although the path similarity $s(x_i, x_j)$ is not a valid kernel because it is not positive definite, the use of centered kernel alignment is still possible as the only limitation is that the global optimum might not be found.

To finish the example, the similarity function \( \mathbf{1} \) with weight vector $w = (2, 10^{-5}, 1, 2.3, 1.6, 1, 0.36, 0.7, 0.9)$ returns the value $s(x, x') = 0.049$, which correctly indicates that the two paths are different.

B. Similarity of network traffic

To define the similarity between network resources one has to overcome the randomization often employed by malware authors that render trivial similarity based on names of network resources (domains, IPs) ineffective. To escape blacklisting command and control (C&C) channels of malware, its authors use various techniques to hide and obscure C&C operation. Popular approaches include randomization of domain names by fast flux, or using large hosting providers like Amazon Web Services to hide among legitimate servers, etc. These techniques are relatively cheap (e.g. registering a new .com domain costs ~3USD per 1 year) and they allow for variation in domain names without updating disseminated malware binaries. In contrast, switching from one C&C paradigm to another requires such an update and therefore occurs relatively infrequently. These two properties contribute to each malware family using specific patterns of domain names, paths, and parts of URLs. Exploiting these patterns allows to group domain names into clusters. In this work the similarity in network traffic is defined only for HTTP/HTTPS protocol, because it is presently the default choice for malware authors as it is rarely filtered. The extension to other network traffic is possible \( \mathbf{23} \).

The similarity in URL patterns used in this work has been adopted from \( \mathbf{21} \), which has proposed to cluster domain names so that each cluster contains domains of one type / for one family of malware. The calculation of similarity starts by grouping all HTTP/HTTPS requests using the domain names. Then the model of each domain name is built from path and query strings, transferred bytes, duration of requests and inter-arrival times (time spans between requests to the same domain) of individual requests to it. Finally, these models are used to calculate the similarity function between two domain names in the clustering. Since the calculation of the similarity is out of scope, we refer to an original publication \( \mathbf{21} \) for details.

C. Similarity between mutex names

Mutex (Mutual exclusive object) is a service provided by most modern operating systems to synchronize multi-threaded and multi-processes applications. This mechanism is popular among malware authors to prevent multiple infections of the same machine, because running two instances of the same malware can cause conflicts limiting the potential revenue. Mutexes are identified by their name, which can be an arbitrary string. The naming scheme is challenging for malware authors, because the names cannot be static, which would make them good indicators of compromise of a particular malware, but they cannot be completely random either, because two independent binaries of the same family would not be able to check the presence of each other. Therefore malware authors resorted to pseudo-deterministic algorithms or patterns for generating mutex names. For some malware families these patterns are already well known, for example Salty \( \mathbf{43} \) uses mutex names of the form "$<process name>.exeM_<process ID>_M-<explorer.exeM_<process ID>"$.

Since operating systems do not impose any restrictions on the names of mutexes, they can be arbitrary strings. Therefore standard string similarities such as Levenshtein distance, Hamming distance, Jaro-Winkler distance, etc. can be used. In experiments presented in Sections III Levenshtein was used, as it gives overall good results.

D. Similarity between registry names

In Microsoft Windows operating system, the primary target of the majority of malware, registry serves as a place where programs can store various configuration data. It is a replacement of configuration files with several improvements such as strongly typed values, faster parsing, ability to store binary data, etc. The registry is a key-value store, where key names have the structure of a file system. The root keys are HKEY_LOCAL_MACHINE, HKEY_CURRENT_USER, HKEY_CURRENT_CONFIG, HKEY_USERS and HKEY_PERFORMANCE_DATA; some root keys also always have sub-keys with specific names (Software, Microsoft, Windows, etc.). Due to similarity with a file system, the similarity distance is the same as the one defined in Subsection II-A, but with a different set of
names of known folders and a weight vector optimized on registry data rather than on files.

E. Clustering of resource names

The above similarities are not true distances, which limits the choice of applicable clustering methods to those that do not require proper distance metric between points. The Louvain method [27] is a popular choice and it is used in experiments below, because it also automatically determines the number of clusters and thus removes the need to set it manually. The use of the Louvain method is the authors’ preference, but other clustering methods can be used as well; the reader is referred to [15] for an overview of methods requiring only similarity.

Algorithm 3 Approximative clustering algorithm for instances I (resource names).

1: function APPROXCLUSTER(I; k, m, \epsilon)  
2: C = \emptyset  
3: while I \neq \emptyset do  
4: I’ \leftarrow \text{Random subset of size } k \text{ from } I  
5: C’ \leftarrow \text{cluster}(I’, m) \quad \triangleright \text{Cluster instances } I’ \text{ and create cluster prot. of size } m.  
6: for all i \in I \setminus I’ do  
7: c^* \leftarrow \text{nnSearch}(i, C’ \prime) \quad \triangleright \text{Find cluster prot. } c^* \text{ closest to instance } i.  
8: if s(i, c^*) > \epsilon \text{ then}  
9: c^* \leftarrow c^* \cup \{i\}  
10: end if  
11: end for  
12: C \leftarrow C \cup C’  
13: end while  
14: return C  
15: end function

The use of the Louvain method is not straightforward in the scenario of this paper because it requires a full adjacency matrix in advance. This results in a lower bound to computational complexity being \(O(n^2)\) in the number of resources, which is clearly prohibitive as the number of unique resource names to cluster can easily reach the order of millions. To decrease the number of calculated similarities, an approach inspired by [46], [47], [20] is adopted where the Louvain clustering is used iteratively as summarized in Algorithm 3. Given a set of instances \(I\) of a particular type, in every iteration the algorithm selects a random subset \(I’ \subset I\) of the data of size \(k\) small enough for the Louvain method to be computationally feasible. The results of the Louvaine clustering are then transformed to cluster prototypes—random subsets of clusters with size limited to \(m\). Remaining data \(I \setminus I’\) are then traversed and all samples with similarity larger than \(\epsilon\) to some cluster prototype \(c^* \in C’\) are added to \(c^*\) and removed from \(I\). Finally, \(C’\) is merged with the clustering \(C\) obtained in the previous iteration, and if \(I\) is not empty, the process is repeated.

Clearly the algorithm is an approximation of a clustering with complete data and its performance depends on the choice of parameters \(k\) and \(\epsilon\). Experiments indicate that if parameter \(k\) is large enough (\(k = 10^5\)) and parameter \(\epsilon\) is set reasonably (in the experimental evaluation we use \(\epsilon = 0.4\), see Section III-B for details), the results are comparable with clustering methods applied to the complete data. The computational complexity of this sequential approximation is \(O(l \cdot (k \cdot (k - 1)^2 + c_1 \cdot m \cdot (n_l - k)))\) where \(l\) is the number of iterations of algorithm (typically \(l \leq 10\)), \(n_l\) is the number of non-clustered samples in \(l\)-th iteration, \(k\) is the number of randomly selected samples, \(c_1\) is the number of cluster prototypes produced by the clustering algorithm in \(l\)-th iteration and \(m\) is the maximal size of a cluster prototype (typically \(m = 10\)). Since the parameter \(k\) is fixed and \(k \ll n\), we can see that the number of evaluations of the similarity function is linear in the number of samples, which clearly outperforms the quadratic complexity required by the vanilla Louvain method.

III. Evaluation

In this section the proposed approach is compared to the approach proposed by Rieck, et al. [38] (further referred to as Rieck) and the approach proposed by Mohaisen, et al. [80] (further referred to as AMAL). Rieck has been selected as a representative of the prior art that encodes malware behavior into a high-dimensional feature space using bag-of-words model built directly from data; it uses kernelized SVM to classify binaries. The second approach, AMAL, encodes malware behavior using a relatively low number of hand-made features; to classify unknown binaries AMAL trains multiple classifiers (SVM, decision trees, k-nearest neighbor, etc.) and selects the optimal classifier for given data using cross-validation.

A. Data set description

The dataset used for experiments contained 250527 files collected from October 24, 2016 to December 12, 2016 using AMP ThreatGrid [18]. All files were also analyzed by VirusTotal.com service [19] and labeled using its verdicts as follows: a file was labeled as malicious if at least 4 out of 10 selected AV engines (see Table IV for details) detected the file as malicious, and it was labeled as legitimate if none of the AV engines detected the file. Remaining files were discarded as unknown and removed from both training and testing sets in order to limit the effect of misclassifications by individual AV engines. The final numbers of files were: 144229 malicious, 87026 legitimate, and 19272 discarded as unknown. The numbers of samples of individual malware families are summarized in Table III.

All files were executed in sandbox by AMP ThreatGrid [18] service, using Windows 7 64bit (71\% samples) environment, as it is the most popular OS at the time of writing 4 and Windows XP (29\% samples) environment, since it is still widely deployed on embedded machines such as ATMs. Virtual machines were connected to the Internet without any filtering or restrictions that could by any mean prevent connections to

4According to http://www.w3schools.com/browsers/browsers_os.asp Windows 7 has 34.6\% market share against 1.0\% covered by Windows XP, 11.1\% covered by Windows 8 and 30.9\% covered by Windows 10.
for training, and remaining samples (71 266) perform such optimization during training in order to select using grid search (detailed below), AMAL is designed to and the proposed method the parameters have to be optimized since it does not overestimate the detection performance as [12], or CWSandbox [44]. 

Table IV: Selected AV engines that received full 6 points for performance in AV-Test report from December 2016 [3].

| Malware family | #samples | Malware family | #samples |
|----------------|----------|----------------|----------|
| nemucod        | 13 781   | amonetize      | 1172     |
| cerber         | 12 829   | nanocore       | 1032     |
| bladabindi     | 10 945   | loadmoney      | 964      |
| locky          | 9 894    | yakes          | 892      |
| gamarue        | 7 694    | bifrose        | 804      |
| darkkomet       | 4 664    | autotit        | 781      |
| hupigon        | 35 555   | kolabe         | 707      |
| upatre         | 32 695   | waldek         | 686      |
| tinba          | 31 014   | pdfka          | 649      |
| scar           | 29 661   | shipup         | 625      |
| swort          | 28 686   | rebhip         | 613      |
| zbot           | 24 262   | razy           | 599      |
| virlock        | 17 067   | agentb         | 579      |
| fareit         | 17 063   | poisson        | 551      |
| farfi          | 17 049   | xtrat          | 511      |
| zegost         | 17 199   | onlinegames    | 502      |
| virut          | 15 566   | ramin          | 493      |
| adwind         | 15 373   | magania        | 463      |
| zaky           | 15 055   | atraps         | 461      |
| ircbot         | 14 477   | softpulse      | 460      |
| zerber         | 13 299   | banload        | 387      |
| paleo          | 12 707   | ruskil         | 374      |
| vobfus         | 12 444   | downloadassistant | 373 |
| self            | 12 228   | binder         | 350      |
| donoff         | 12 111   | remaining MW families | 31 856 |

| Total malicious | 144 229 |
| Total legitimate | 87 026 |

Table III: Number of samples of malware families in the data set. The malware families for individual samples were determined using AVClass tool [40].

command & control servers or other servers. The work here is not tailored to AMP ThreatGrid, as the same or similar information about binaries can be obtained by a number of different sandboxing solutions such as Cuckoo [35], Ether [12], or CWSandbox [44].

In contrast to the majority of prior art, binaries were divided into training and testing sets according to the dates they were collected rather than randomly. This approach is more realistic since it does not overestimate the detection performance as some malware families may not be known at the time of training, as they might have appeared later. Thus, all training samples collected prior to November 12, 2016 (72 963 malicious binaries and 48 152 legitimate binaries) were used for training, and remaining samples (71 266 malicious binaries and 38 874 legitimate binaries) were used for testing.

B. Hyper-parameter optimization

All compared methods have several parameters that have to be tuned to achieve good detection accuracy. While in Rieck and the proposed method the parameters have to be optimized using grid search (detailed below), AMAL is designed to perform such optimization during training in order to select both the optimal classifier (SVM, linear SVM, decision trees, logistic regression, k-nearest neighbor and perceptron) and its parameters and thus it does not need to optimize its parameters in advance.

Since Rieck uses SVM with L2 regularization and polynomial kernel there are two parameters that need to be tuned: misclassification cost $C \in \{10^{-2}, \ldots, 10^{9}\}$ and degree of the kernel $d \in \{1, \ldots, 5\}$. The optimal configuration achieving highest accuracy estimated by five-fold cross-validation on the training data was $C = 10^4, d = 4$.

The random forest classifier described in Section [11] contains several parameters such as the number of trees $K \in \{10, 20, 50, 100, 200\}$, maximal depth $d_m \in \{5, 10, 30, 50, \infty\}$, minimal number of samples in node to perform split $s_n \in \{2, 4, 6, 10, 20\}$, and criterion $c \in \{\text{gini, entropy}\}$. All remaining parameters (maximal number of features, minimal number of samples in leaf, maximal number of leafs, class weights, minimum weighted fraction of the total sum of weights in leaf, minimal impurity for split) were set to their default values as defined in the Scikit-learn library [36] since according to our experiments they have little influence on detection performance. The optimal configuration of parameters with respect to accuracy estimated by five-fold cross-validation on training data was $K = 100, d_m = \infty, s_n = 2$ and $c = \text{gini}$.

Additional two parameters (size of randomly selected subsets $k \in \{10^4, 2 \cdot 10^4, 5 \cdot 10^4, 10^5, 2 \cdot 10^5, 5 \cdot 10^5, \infty\}$ and minimal similarity $\epsilon \in \{0.1, \ldots, 0.9\}$) affect the clustering of the resource names described in Section [11-2]. The minimal similarity was optimized on a manually labeled set of file paths and registry keys that were clustered with different values of $\epsilon$. The resulting clusters were evaluated with respect to the adjusted rand index [37], a well known score for evaluation of clustering algorithms, and the optimal value of $\epsilon = 0.4$ was selected. To find the optimal size of randomly selected subsets $k$ the accuracy of the whole proposed method with different settings of parameter $k$ was estimated using five fold cross validation on randomly selected subset of training data. Since the differences between various settings were negligible, the value of the parameter $k = 10^5$ was selected as a reasonable balance. Low value of parameter $k$ increases the number of iterations $l$ performed by the clustering algorithm, since too many samples are rejected to be too dissimilar to available cluster prototypes, and high value increases the quadratic cost for computation of adjacency matrix required by Louvain method.

Classification performance was measured with standard evaluation metrics [14]: true positive rate (TPR), false negative rate (FNR), true negative rate (TNR), false positive rate (FPR) and accuracy. Since the experimental scenario is binary (positive malware vs. negative benign), the TPR (FNR) is the proportion of correctly (incorrectly) classified malware samples, TNR (FPR) is the proportion of correctly (incorrectly) classified legitimate samples and accuracy is the rate of correctly classified samples regardless their class.
C. Experimental results

The comparison and evaluation is divided into two parts. The first experiment evaluates the detection performance of the proposed method, Rieck and AMAL trained on the full training set (121 115 samples), while the second experiment measures degradation of detection performance when only a limited number of data are available for training (5%, 10%, 20% and 100% of training samples). Note that to evaluate AMAL on the complete training set, the meta learner was not allowed to use SVM classifier with RBF kernel due to excessive computational requirements. Note that AMAL’s meta-learner has never selected this variant of the SVM classifier in smaller experiments performed in this work, hence removing it most probably does not have any impact on the results.

The detection rates and accuracy of classifiers trained on all 121 115 training samples as estimated on testing samples are shown in Table 5.

![Table 5: True (TPR) and false (FPR) positive rates of evaluated methods estimated on the training and testing set.](image)

|                     | TPR | FPR | ACC |
|---------------------|-----|-----|-----|
| This paper          | 0.954 | 0.067 | 0.943 |
| Rieck               | 0.934 | 0.081 | 0.926 |
| AMAL                | 0.795 | 0.108 | 0.845 |

The differences between evaluation metrics indicate that the proposed approach outperforms both Rieck and AMAL having the lowest false positive rate and false negative rate. A deeper analysis of the misclassifications produced by the proposed approach revealed that most of the false positives (legitimate binaries classified as malware) were software utilities such as TeamViewer that install themselves into system directories without any user interaction. Since their incidence in the training set was relatively low, the random forest was not able to precisely learn this type of behavior. A second source of errors are false negatives (malware samples classified as benign) where almost 70% are caused by insufficient numbers of training samples (less than 100 samples) from corresponding malware families. Another 11% of false negatives was caused by concept drift as a portion of testing samples exhibited different behaviors than training samples, i.e. created files or registry keys followed different pattern, network communication significantly different URLs, etc.

Large gaps between training and testing accuracies for AMAL and Rieck suggest that manually created features and BoW features do not generalize over longer periods of time as well as features created through clustering do. This suggests that clustering removes some randomization of resource names while retaining a large part of information content.

Figures [3] and [4] show graphs of FNR and FPR rates for larger sizes of the training set expressed as fraction of the data available for training. For fair comparison the testing set was kept static containing all 110 140 samples collected after November 12, 2016. Both graphs show that the proposed approach is able to achieve lower FNR and FPR using fewer samples. In fact, the proposed approach achieved FNR of 0.052 using just 5% of samples, while Rieck achieved 0.066 using the full training set. Similarly, the proposed approach needed just 20% of samples to achieve the same FPR 0.081 as Rieck on all samples.

Figures [3] and [4] also shows that while false negative rates almost do not change with respect to the size of the training set (especially for the proposed approach), the false positive rates decrease dramatically. This suggests that learning behavior of legitimate applications is more difficult than that of malware, which can be caused by the fact that the behavior of malware is more uniform than that of legitimate applications. This corroborates the motivation of this work, that even though malware authors try to randomize, they tend to randomize with same sort of regularity, which leads to uniformity.

D. Detection limits

The experimental results hint at where are the limits of classifying binaries executed in sandbox. When a binary (or all binaries of some malware family) does not perform any actions changing the data used by the proposed or other methods (files, mutexes, network communication, registry keys) it clearly evades detection. An example of such malware is bitcoin miner that resides only in memory without any additional footprint (no operations with files, no operations with registry keys, no mutexes, very limited network communication). Such malware has to be carefully crafted to avoid any interaction with system resources (statically compiled to carry all libraries in the executable, limited network communication, no mutexes ensuring that only single instance is running on the same machine, no persistency after reboot, etc.). Fortunately, at the time of writing this work, this is not an easy task and the majority of malware authors choose to interact with system resources rather than sacrifice functionality.

Another limitation is the fact that a growing number of malware families are equipped with advanced anti-VM and anti-sandbox features and/or are targeted to specific environments (Stuxnet [3]). Such malware families do not reveal their true purpose during sandboxing or mimic less severe types of malware (adware, PUA etc.). This fact is recognized by the community as the main factor hindering the performance of dynamic analysis as the whole. Addressing this issue is out of the scope of this paper.

The last aspect we need to discuss is the false positive rate. The analysis of the results from Section III revealed that a large number of false alarms is caused by applications that install themselves into system directories without user’s interaction and since their number is limited, the classifier was unable to fit this behavior. A solution is of course to improve the training data by including a larger number of such samples and thus achieve lower false positive rate.

E. Scalability and computational complexity

The last aspect we will discuss is the scalability of the proposed solution and prior art. Since the proposed solution employs clustering to project the input data into a feature space with a lower dimension, a large portion of the training time

6 Potentially unwanted application.
is spent in the clustering phase. However, the preprocessing of the dataset used in above experiments was much faster (~2h50min) than the highly optimized pre-computation of the full kernel matrix required by Rieck (~7h). This is caused by the fact that the time required by Rieck for preprocessing grows quadratically with the number of training samples in contrast to the proposed solution with linear complexity (up to an additive constant, see Section II-E). Moreover, the proposed solution can be easily distributed since in every iteration the nearest neighbor search depends only on a limited set of current cluster prototypes $C'$. Another benefit of the proposed solution is tied to the representation itself. Since the clustering is performed only on training samples, in order to classify unknown samples we need to store only the cluster prototypes determined during training. For the whole training dataset used in this paper, which contains over 7 million unique resource names projected into ~40000 features, only 400000 instances need to be stored. In contrast, the kernelized SVM classifier used by Rieck et al. requires to store all training samples (over 120000 samples in the data discussed in Section III) with all actions (on average 2000 actions per sample) in order to make prediction on unknown samples.

In contrast to both the proposed solution and Rieck, AMAL does not need any preprocessing since the features can be extracted per sample. However, the complexity arises from the design of the training process. Authors in [30] argue that the dynamic selection of both optimal algorithm and its parameters provides optimal results, but this design makes the training process computationally expensive since every training of the meta-learner requires to evaluate all possible combinations of parameters for all its classifiers. Another aspect is the selection of classifiers itself. Authors propose to use an array of classifiers such as kernelized SVM, linear regression, decision trees, perceptron, etc. However, the complexity of some classifiers (e.g. kernelized SVM) prevents any large-scale training. Moreover, according to the evaluation the AMAL’s detection capabilities are not sufficient for real-world deployment since both FPR and FNR are nearly 20%, which is clearly insufficient.

IV. RELATED WORK

Since the analysis of malicious binaries and recommending them for further analysis has important practical applications, there exists rich prior art. Although it is frequently divided into two categories, static and dynamic, the boundaries between them are blurred since techniques such as analysis of the execution graph is used in both categories.

A. Static malware analysis

Static malware analysis treats a malware binary file as a data file from which it extracts features without executing it. The earliest approaches [27] looked for a manually specified set of specific instructions (tell-tale) used by malware to perform malicious actions but not used by legitimate binaries. Latter works, inspired by text analysis, used $n$-gram models of binaries and instructions within [26]. Malware authors reacted quickly and began to obfuscate, encrypt, and randomize their binaries, which rendered such basic models [41] useless. Since reversing obfuscation and polymorphic techniques is in theory an NP-hard problem [31], most state of the art [9], [1], [42] moved to a higher-level modeling of sequences of instructions / system calls and estimating their action or effect on the operating system. The rationale behind is that higher-level actions are more difficult to hide.
B. Dynamic malware analysis

An alternative solution to analyzing obfuscation and encryption is the execution of a binary in a controlled environment and analyzing its interactions with the operating system and system resources.

A large portion of the work related to dynamic malware analysis utilize system calls, since in modern operating systems system calls are the only way for applications to interact with the hardware and as such they can reveal malware actions. The simplest methods view a sequence of system calls as a sequence of strings and use histograms of occurrences to create feature vectors for the classifier of choice \[17\]. The biggest drawback of these naive techniques is low robustness to system call randomization. Similarly to static analysis, this problem can be tackled by assigning actions to groups (clusters) of system calls (syscalls) and using them to characterize the binary \[32, 45, 5\].

A wide class of methods identifying malware binaries from sequences of syscalls rely on \(n\)-grams \[24, 54\]. Malheur \[39\] uses normalized histograms of \(n\)-grams as feature vectors, which effectively embeds syscall sequences into Euclidean space endowed with \(L_2\) norm. In this space the algorithm extracts prototypes \(Z = \{z_1, \ldots, z_n\}\) using hierarchical clustering. Each prototype captures the behavior of the cluster, which should match corresponding malware family. An interesting feature of Malheur is that if a cluster has less then a certain number of samples, the prototype is not created. The classification of an unknown binary is determined by searching for the nearest prototype within certain range. If the nearest prototype is outside of this range, the sample is not classified.

To counter dynamic analysis advanced malware detects the presence of a sandbox and does not execute within it. Since most sandboxes rely on a detectable system call interposition, Das et al. \[11\] propose to extend hardware with FPGA that would extract system calls from their execution on processor. Syscalls are then grouped by comprehensive yet hand designed rules, and these groups are then fed into multi-layer neural network classifier. The classifier itself is also part of the FPGA, such that the system can simultaneously extract training samples and classify them.

AMAL uses its custom sandbox to extract features describing files, network communication and registry features \[30\] and tunes various classification algorithms. The main difference between AMAL and this work is the construction of features. Whereas AMAL uses numeric features such as counts or sizes of created, modified or deleted files, counts of created, modified or deleted registry keys, counts of unique IP addresses, etc., we assume that individual resources (files, registry keys, mutexes and network communication) have specific role in the operation system, which can be different even though the characteristics exhibited by the file are the same.

The approach proposed by Rieck et al. \[38\] creates a representation of the analyzed binaries directly from the data which is at the first sight similar to the proposed approach, however there are two key differences. The first one is the source of data, because Rieck et al. model actions triggered by the malware (writing into a file, communication with remote server, reading data from registry keys, starting new thread, etc.), whereas the proposed approach models only affected resources. This enables to deploy the proposed approach in environments without access to low-level actions (VMs without such access, user machines without API hooking). Another difference is in handling the randomization of resource names. Instead of clustering resource names used in this work, Rieck et al. remove parameters of actions, which increases the dimensionality of the model since for every action with \(n\) parameters it creates \(n + 1\) features representing the action at different levels of granularity by removing parameters from the end: from full description with all parameters to the most coarse description where only name of the action is used. This leads to a massive increase in the already large number of features.\[7\] Even though the resulting feature space, is sparse the scalability of such an approach is limited.

V. Conclusion

Dynamic malware analysis is a popular approach to automatically identify malware binaries and analyze them. This paper has proposed a model of malware behavior observed through its interactions with the operating system and network resources (operations with files, mutexes, registry keys, operations with network servers or error messages provided by the operating system). It employs an efficient clustering of resource names to reduce the impact of randomization commonly employed by malware authors to avoid detection and projects malware samples into a low-dimensional space suitable for classifiers such as random forest.

The proposed solution was extensively compared to related state of the art on a large corpus of binaries where it demonstrated significant increase in precision of malware detection. Moreover, we believe that the availability of solutions relying on widely different types of features increases the overall reliability of malware detection techniques, because malware authors have to evade more detectors to stay undetected.

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APPENDIX

A. Frobenius product and Frobenius norm

For two matrices $A \in \mathbb{R}^{n \times m}$ and $B \in \mathbb{R}^{n \times m}$ we define Frobenius product $\langle \cdot , \cdot \rangle_F$ and Frobenius norm $\| \cdot \|_F$ as follows

$$\langle A, B \rangle_F = \sum_{i=1}^{n} \sum_{j=1}^{m} A_{ij} \cdot B_{ij}$$

$$\| A \|_F = \sqrt{\langle A, A \rangle_F} = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{m} A_{ij}^2}$$

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