MutantX-S: Scalable Malware Clustering Based on Static Features

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Abstract
The current lack of automatic and speedy labeling of a large number (thousands) of malware samples seen everyday delays the generation of malware signatures and has become a major challenge for anti-virus industries. In this paper, we design, implement and evaluate a novel, scalable framework, called MutantX-S, that can efficiently cluster a large number of samples into families based on programs’ static features, i.e., code instruction sequences. MutantX-S is a unique combination of several novel techniques to address the practical challenges of malware clustering. Specifically, it exploits the instruction format of x86 architecture and represents a program as a sequence of opcodes, facilitating the extraction of N-gram features. It also exploits the hashing trick recently developed in the machine learning community to reduce the dimensionality of extracted feature vectors, thus significantly lowering the memory requirement and computation costs. Our comprehensive evaluation on a MutantX-S prototype using a database of more than 130,000 malware samples has shown its ability to correctly cluster over 80% of samples within 2 hours, achieving a good balance between accuracy and scalability. Applying MutantX-S on malware samples created at different times, we also demonstrate that MutantX-S achieves high accuracy in predicting labels for previously unknown malware.

1 Introduction
According to the Symantec’s latest Internet Threat Report, 403 million new variants of malware were created in 2011, a 41% increase from 2010. This exponential growth of malware samples has created a major challenge for anti-virus (AV) companies: how to efficiently process this huge influx of new samples and accurately labels them? It is practically impossible to manually analyze several thousands of suspicious samples received every day. As a result, a large fraction of samples are left unlabeled, which delays the signature generation. One possible solution is to automatically cluster malware samples and assign them labels according to their similarities. The intuition is that malware programs bearing significant similarities are likely to have been derived from the same code base, and hence from the same malware family. One can thus group similar malware and label them with high accuracy by analyzing only a few representative samples. Moreover, the label of a new sample can be automatically derived and previous mitigation techniques can be re-used if it is determined to belong to an existing family. Therefore, accurate clustering plays a crucial role in helping AV companies categorize large amount of incoming samples by avoiding duplicate work and enabling malware analysts to prioritize limited resources on novel and representative samples [17, 12, 7]. In this paper, we design, implement and evaluate MutantX-S, a novel and scalable system, that can efficiently cluster a large number of malware samples into families based on their static features, i.e., code instruction sequences.

Many existing malware clustering/classification systems are based on dynamic behavioral features such as runtime API or system call traces [6, 7, 24]. The major benefit of using dynamic behavioral features is that they are less susceptible to mutation schemes frequently employed by malware writers to evade binary analysis, e.g., packing or obfuscation. However dynamic-feature-based approaches also suffer from several limitations. First, they may have only limited coverage of an application’s behavior, failing to reveal the entire capabilities of a given malware program. This is because a dynamic analysis can only capture API or system call traces corresponding to the code path that was taken during a particular execution. Different code paths may be taken in different runs, depending on the program’s internal logics and/or external environments. Also, malware often include triggers in their programs and exhibit an interesting behavior only when certain conditions are met. For example bot programs wait for commands from botmasters and some malware are designed to launch attacks on a certain time. Although there exists work that forces a program to run all code paths [21], they are too expensive to analyze large amount of malware. Second, dynamic analysis is inherently resource-intensive and doesn’t scale well. With limited resource and the sheer number of malware, a dynamic-analysis system can execute and monitor each sample only for a short period of time, e.g., a couple of minutes. Unfortunately, this time is often too short for typical malware to reveal all their true behavior.

In this paper, we present MutantX-S, a new and practical system that exploits static features of code instruction sequences for efficient and automatic malware clus-
tering and labeling. MutantX-S is motivated by the common observation that majority of today’s malicious programs are variations of a relative small number of malware families and thus share similar instruction sequences. Analyzing static features of malware offers several unique benefits. First, it has the potential to cover all possible code paths, yielding more accurate representations of the entire functionalities of the program. Moreover, approaches based on static features are much more scalable than their dynamic counterparts, as they do not require resource-intensive and time-consuming monitoring of program behavior. This is particularly important for AV companies to process a rapidly-increasing number of new malware samples. Unfortunately, static analysis is well-known to suffer from run-time packing and obfuscation techniques. Therefore, the goal of MutantX-S is not to replace existing dynamic-behavior-based systems, but to complement them to achieve higher clustering accuracy and better coverage of malware programs.

MutantX-S features a unique combination of techniques to address the deficiencies of static malware analysis. First, it tailors a generic unpacking technique to handle run-time packers without needs to know its specific packing algorithm. Second, it employs an efficient encoding mechanism that exploits the IA32 instruction format to encode a program into opcode sequences that are resilient to low level mutations. In addition, it applies a hashing-trick and a close-to-linear clustering algorithm to allow MutantX-S to efficiently handle large number of malware with very high dimensional features. We have successfully implemented a fully-automated prototype of MutantX-S and evaluated its performance using over 130,000 distinct malicious programs. Our evaluation demonstrates MutantX-S’ efficiency and efficacy of creating clusters corresponding to malware families and accurately predicting labels for new malware.

The rest of the paper is organized as follows. Section 2 surveys related work of malware analysis. Section 3 describes the architecture of MutantX-S followed by elaboration of all subcomponents including unpacking (Section 4), feature extraction (Section 5) and clustering (Section 6). The performance evaluation is presented in Section 7. Section 8 discusses the limitation and potential improvement, and Section 9 concludes the paper.

## 2 Related Work

Malware pose one of the severest threats to computer systems and the Internet. Various schemes have been proposed to automatically cluster/classify malware based on either dynamic behavior or features.

Dynamic-analysis approaches have the major benefit of handling obfuscated malware samples based on their runtime system or API calls. Lee and Mody [18] used a sequence of runtime events (e.g., registry and file system modifications) to cluster similar malware programs. Rieck et al. [23] applied SVM (Support Vector Machine) to learn the frequency of run-time behavior, and classified unknown samples to their closest kin. Later, Bailey et al. [6] applied a hierarchical clustering algorithm to group similarly-behaving malware samples. Unfortunately, the complexity of this clustering algorithm is $O(n^2)$, limiting its applicability only to a small number of samples. To address this problem, Bayer et al. [7] and Rieck et al. [24] developed different methods to scale the clustering. Bayer et al. [7] applies locality-sensitive hashing (LSH) to efficiently compute an approximate hierarchical clustering with a significantly smaller number of distance computations. By contrast, Rieck et al. [24] applied a prototype-based clustering algorithm that reduces the runtime complexity by performing clustering only on representative samples. Comparing to LSH clustering, a prototype-based algorithm facilitates the analysis of behavior groups because each prototype represents a particular malware group [24]. In MutantX-S, we adopt the same prototype-based algorithm as in [24] because of its efficiency and explicit expression of malware features.

Static analysis, on the other hand, uses features extracted directly from malware binaries. Christodorescu et al. [8] discovered malicious patterns from disassembled malware that are resilient to obfuscation. Wicherski [30] utilizes static features from PE headers, e.g., entry point, import table, etc., to group malware programs. Karim et al. [13] demonstrates the effectiveness of N-gram and N-perm on assembly instructions by using them to study the malware evolution. Similar features have also been used in [15] to validate various learning methods. MutantX-S falls into the static-analysis category since it relies on features extracted from the malware instructions. MutantX-S differs from previous approaches in its unique combination of novel techniques to improve its scalability in handling very large malware datasets. Another independently developed system similar to MutantX-S is BitShred [12] which also focuses on malware comparison and triage on a large scale. However, BitShred compares malware using their byte sequences which is susceptible to binary level obfuscation.

## 3 Architecture

Figure 1 shows an overview of MutantX-S. At a high level, MutantX-S takes a set of malicious or suspicious samples as input and extracts their features using static analysis to avoid the computational overhead and maximize code coverage. Specifically, MutantX-S first uses existing tools (e.g., PeID\(^1\) [3]) to identify malware files that are likely processed by packing tools such as UPX.
These files will be unpacked with a generic unpacking technique tailored for MutantX-S. Together with samples that are in their original binary (not packed), they are disassembled to code instructions. These pre-processing steps ensure that features inherent to malware families can be successfully extracted without influence of encryption or compression. Then, all malware samples are processed with three steps to extract representative features: (1) Instruction Encoding for converting each instruction to a sequence of operation codes that capture the underlying semantics of the programs, (2) N-gram analysis for constructing feature vectors used to compute program similarities, and (3) Hashing Trick for compressing the feature vectors, which significantly improves the speed of similarity computation with only a small penalty in accuracy. Finally, a prototype-based clustering algorithm is applied on compressed feature vectors and partitions samples into clusters, each representing a group of similar malware programs.

Figure 1: A system overview of MutantX-S

4 Generic Unpacking Algorithm

Run-time packing is arguably the most popular techniques used by malware writers to circumvent anti-virus detection. More than 80% of malware programs are estimated to be packed [10]. A typical packer like UPX works as follows. UPX first compresses all the code and data sections of a portable executable (PE) binary\(^2\) into a single section. Then, it creates a new PE binary containing the compressed data followed by the unpacker code. The entry point in the new PE header is altered to point to the unpacker code such that when the packed program runs, the unpacker will first be executed. The unpacker decompresses the original program codes into memory and then jump to the first instruction of the restored codes (i.e., the original entry point) to resume execution. This packing process enables malware programs to disguise their malicious instructions as random-looking data while keeping the original functionality intact. Since all static analysis tools including MutantX-S rely on features extracted from original instructions, it is imperative for them to handle packing correctly and efficiently.

While there exist unpacking tools such as UPX itself, ArmaGedoon, etc., they are often targeted specifically at one or a few packers. As more packers appear in the wild, the cost of manually reverse-engineering packers and continually updating unpacking tools is expected to grow over time. In addition, unpacking tools often have to perform expensive processing to ensure that the unpacked program can be successfully executed (e.g., the PE headers and imported tables must be correctly reconstructed), making them too slow for large scale processing. MutantX-S, on the other hand, need not guarantee the executability of unpacked programs as long as the original instructions can be inspected and features extracted. MutantX-S thus exploits this advantage and tailors a generic unpacking mechanism to meet the particular need for efficient malware clustering. The basic idea is to use the inherent property of the unpacking procedure, i.e., a packed binary has to write the unpacked code into some memory space and transfer control to the modified memory locations to continue execution. By continuously monitoring memory accesses, we can learn the occurrence of some form of unpacking, self-modification or on-the-fly code generation if the program executes code at a memory address after writing into it. These written-then-executed memory pages likely contain the original instructions and thus are the targets of MutantX-S.

The unpacking component of MutantX-S exploits the physical non-execution (NX) support in modern x86 CPUs to track memory page status. It consists of a kernel driver responsible for tracking system calls and a user-level component that is injected as a remote thread into a program’s address space. The unpacking component does two things: (1) runs the packed binary and dumps the memory image of the running process at an appropriate time when the binary is likely to finish unpacking, and (2) determines the correct original entry point (OEP) for the dumped image. Finding the correct OEP is critical for correct program disassembling and feature extraction. A wrong entry point may cause a disassembler to miss all the instructions between the original and the misidentified entry points (if there is no other reference to this portion of codes). In addition, if the entry point is incorrectly set in the middle of an instruction, the disassembler will fail or generate completely wrong assembly codes. The unpacking process is summarized in Algorithm 1 and elaborated below:

1. MutantX-S loads the packed program, suspends its execution and injects the user-level hooking DLL into the process’ memory space. It marks all the memory pages as executable but non-writable, and resumes its execution.
2. During the execution, when the unpacker attempts to write unpacked codes into memory (which has been marked as non-writable), a write exception will occur. MutantX-S marks the page as dirty and changes its permission to writable but non-executable.
3. When the unpacker jumps to the the newly-generated

\(^2\)PE is the executable file format used by Windows OS.
code for execution (e.g., after finishing unpacking), the non-executable permission on these pages triggers an exception. MutantX-S intercepts the exception and records the memory address where it occurred. For simple packers (e.g., UPX) that first unpack the entire program and then jump to the restored codes for execution, the memory address where the exception occurs is the OEP (original entry point). However, this is not necessarily true for more sophisticated packers (e.g., self-modifying code that rewrite to the same memory location). Hence, MutantX-S removes the write permission from these memory pages again, grants execution privilege and continues execution. MutantX-S also monitors dynamic allocation of memory pages and removes their write permission to track unpacking on these pages.

4. MutantX-S dumps the process memory image either at the end of program execution or after certain time. The rationale is that after the program has been running for a sufficient amount of time (e.g., 1 minute), it is fairly safe to assume that the program has finished unpacking and the original codes are placed in the memory.

**Algorithm 1** MutantX-S unpacking algorithm

1: **Input:** A packed binary program $B$
2: **Output:** A unpacked PE file with original program codes
3: 
4: Load the packed program into memory
5: for all $p$ in the program's memory pages do
6: Permission($p$) = W/remove write permission
7: end for
8: 
9: while $B$ is running and $T_{runtime} < T_{thresh}$ do
10: $a$: The address of the page fault
11: $t$: The page fault type $t \in \{WRITE, EXECUTE\}$
12: $p \leftarrow Page(a)$
13: if $t = WRITE$ then
14: Permission($p$) = (W|X) // Writable but non-executable
15: last_written($p$) $\leftarrow$ current time
16: end if
17: if $t = EXECUTE$ then
18: Permission($p$) = (W|X) //non-writable but executable
19: last_exec($p$) $\leftarrow$ current time
20: addr_exec($k$) $\leftarrow a$
21: end if
22: end while
23: 
24: Dump process memory
25: reconstruct $B'$ by setting OEP to be addr_exec($k$) where:
26: $k = \arg \min_k (last_exec(k) > \max(last_written(i)))$
27: return $B'$

With the dumped memory image, MutantX-S creates a valid PE file from which a standard disassembler can disassemble instructions. As mentioned earlier, the major challenge in creating a valid PE file is to identify the correct entry point in the PE header. For simple packers like UPX, the entry point is simply the start address of the dirty memory page where the first execution exception occurs. Unfortunately, as adversaries become increasingly sophisticated, various evasion schemes have been developed to obfuscate OEP. A typical method is to fake end-of-unpacking by writing rouge instructions into a reserved memory page, transfer control to it, and jump back to the unpacker code. More advanced packers use incremental unpacking that decrypts only part of the payload and executes them before decrypting more instructions. In such cases, detecting the first execution exception is not enough because only rouge instructions or part of the original program is visible. To address these problems, we developed a new heuristic called LMFE (Last Modification First Execution).

The idea is to keep track of time when the last write exception and a subsequent execution exception occur on each memory page, so MutantX-S can identify the unpacker’s attempts to write to the same memory page multiple times, in which case, the previous modification and execution on the page are likely to be spurious. More specifically, for each memory page, MutantX-S keeps a record of: 1) last modification time (i.e., a write exception occurred), denoted as last_written; 2) last execution exception time, denoted as last_exec; and 3) the address addr_exec where the exception had occurred. At any point of execution, there are 3 types of memory pages:

**Type I:** memory pages that have valid last_written and last_exec, i.e., pages that have been both modified and executed.

**Type II:** memory pages that have valid last_written but not last_exec, i.e., pages that have been modified but not executed. They could either be page containing temporary data or code pages that have not yet been executed.

**Type III:** memory pages that have neither valid last_written nor valid last_exec. These could be initialized data-section pages or unpacker-code pages.

Essentially, type-I memory pages are those that hold the unpacked instructions and thus contain the OEP. When dumping the process memory, MutantX-S uses the following algorithm to pinpoint the correct OEP. Let $P(i)$, $i = 1..n$ represent all type-I memory pages and last_written($i$), last_exec($i$) and addr_exec($i$) respectively represent the time of the last write exception, last execution exception and address where the exception occurred for page $P(i)$. Then, the OEP is addr_exec($k$) in the memory page $P(k)$ where

$$k = \arg \min_k (last_exec(k) > \max(last_written(i)))$$

(1)

where $i = 1..n$. In other words, $P(k)$ is the first memory page that is executed after all type-I memory pages have been written. Below we show that the heuristic is able
to find the correct OEP (i.e. \( \text{addr} \_\text{exec}(k) \)) even when the packers try to fool the MutantX-S using spurious write-and-execute sequences or multi-layer packing.

**Proposition.** For \( k \) satisfying Eq. (1), \( \text{addr} \_\text{exec}(k) \) is the correct OEP of the original program no matter whether the program is packed with simple packers or more advanced packers that fake the end of unpacking.

**Proof.** First, for simple packers like UPX that restore the entire program into memory before executing it, let \( P(j), j = 1..m \) denote memory pages where the unpacker writes the original program codes. Without loss of generality, we can assume that the contents are written sequentially from \( P(1) \) to \( P(k) \), meaning that \( \text{last} \_\text{written}(1) < \text{last} \_\text{written}(2) < \ldots < \text{last} \_\text{written}(m) \). When the packer finishes unpacking and starts executing the restored program by jumping to the OEP, an execution exception will first occur in the page \( P(k) \) that contains the OEP, i.e., \( \text{last} \_\text{exec}(k) > \text{last} \_\text{written}(m) \) and \( \text{last} \_\text{exec}(k) < \text{last} \_\text{exec}(j)/j \neq k \). As a result, \( \text{addr} \_\text{exec}(k) \) is the correct OEP.

Second, assume a more advanced packer with the following spurious unpacking sequence: it writes arbitrary instructions into some memory page, executes them and, at the end of execution, returns to the unpacker code. Such a routine may be called multiple times during the entire unpacking process. As a result, an unpacking tool cannot assume that unpacking ends at the first (or first few) execution exception. MutantX-S is resilient to this type of evasion by enforcing the invariant that the execution exception on the OEP must succeed all the write exceptions. For example, when the spurious unpacking routine touches memory page \( P(s) \), MutantX-S records \( \text{last} \_\text{exec}(s) \) and marks \( P(s) \) as executable but un-writable. Then, the unpacker resumes the normal unpacking and writes more decrypted instructions to memory page \( P(t) \) (\( t \) could be any page including \( s \)). This creates a new write exception on \( P(t) \) at timestamp \( \text{last} \_\text{written}(t) \). Note that because \( \text{last} \_\text{exec}(s) < \text{last} \_\text{written}(t) \), the heuristic determines \( s \) to not contain the OEP. In contrast, after the packer finishes unpacking and transfers control to the real OEP, the execution exception satisfies Eq. (1). By keeping \( \text{addr} \_\text{exec} \) up-to-date and pointing to a valid instruction, MutantX-S is able to keep track of the real OEP accurately. Same arguments hold for multi-layer packing because the write exceptions of code pages will always precede the executable exceptions caused by jumping to the OEP.

### 5 Feature Extraction

With the correct OEP identified, MutantX-S reconstructs a new PE file with dumped memory images. The correct OEP ensures a proper starting point to disassemble instructions and MutantX-S uses the IDA Pro\(^3\) to disassemble a malware program into a sequence of machine instructions that are then used for feature extraction. The key step in MutantX-S is the similarity comparison between malware samples based on the disassembled instruction sequences, e.g., mov eax, ebx; cmp eax, 1h. The main challenge in similarity comparison lies in handling the variations of machine instructions. Malware often undergo changes for many reasons, such as mutation, polymorphism, and obfuscation where semantically-equivalent instruction sequences are used to replace each other. Hence, ensuring exactness in comparing instructions will not tolerate any variation in the syntax. At the other extreme, correctness is compromised if all forms of variation are tolerated. MutantX-S strikes a balance between these two extremes by exploiting the x86 instruction format (Fig. 2) and uses the opcode as a succinct representation of the instruction semantics.

Using opcodes—instead of other features used before, such as control flow graphs, binary sequences or mnemonic sequences—offers several benefits. First, opcodes generalize well to represent variants of a malware family. Malware in the same family are often derived from the same code base and thus share similarities in their instructions. However, due to relinking, rebinding and rebasing, the operands (e.g., registers, memory addresses) of instructions tend to change across the variants. Using opcodes and ignoring the operands (i) make MutantX-S more resilient to low-level mutations while providing a meaningful characterization of semantics and (ii) reflect the functionality of the malware programs. Second, previous approaches often use mnemonic sequences (e.g., mov, push) to represent the instruction functionalities and address the variability of operands. From the evaluation of MutantX-S, we discover that the opcode sequence offers a better representation of instruction semantics. Mnemonics sometimes overly generalize the underlying CPU operations, causing instructions with distinct semantics to appear similar. To illustrate this, consider all the instructions in Table 1. Although all of them have the same mnemonic (i.e., mov), the underlying functionalities are drastically different. For instance, moving a value to a control or debug register of-

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\(^3\) the de-facto disassembler for the analysis of hostile code
ten indicates a critical OS operation, such as interrupt control, switch addressing mode or enable/disable debugging, etc., which should not be treated the same as moving a value between registers. Ideally, moving data from memory to a register (memory load operation) should also be considered as a distinct operation from that of moving from a register to memory (memory store operation). Unfortunately, using mnemonics would cause all these distinct instructions to be represented with a single feature (i.e., mov), which may lead to an accidental similarity between code sequences. As illustrated in Fig. 3, however, features based on opcode provide higher distinguishability between semantically different instructions, thus yielding better clustering accuracy.

<table>
<thead>
<tr>
<th>Op</th>
<th>Instruction</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>89</td>
<td>MOV r/m32, r32</td>
<td>Move from reg to mem/reg</td>
</tr>
<tr>
<td>8B</td>
<td>MOV r32, r/m32</td>
<td>Move from mem/reg to reg</td>
</tr>
<tr>
<td>B8</td>
<td>MOV r32, imm32</td>
<td>Move immediate val to reg</td>
</tr>
<tr>
<td>0F 20</td>
<td>MOV r32, CR0-CR4</td>
<td>Move from control reg to reg</td>
</tr>
<tr>
<td>0F 22</td>
<td>MOV CR0-CR4,r32</td>
<td>Move from debug reg to control reg</td>
</tr>
<tr>
<td>0F 21</td>
<td>MOV r32, DR0-DR7</td>
<td>Move from debug reg to registry</td>
</tr>
<tr>
<td>0F 23</td>
<td>MOV DR0-DR7,r32</td>
<td>Move from registry to debug reg</td>
</tr>
</tbody>
</table>

Table 1: Op (OpCodes) provides fine-grain representations of instruction semantics

![Figure 4: Encoding a function into a feature vector](image)

6 Clustering Algorithm

The next step in MutantX-S is clustering malware samples into groups that share common traits. Considering the enormous amount of malware in the wild, the goal of MutantX-S is to process hundreds of thousands malware files sufficiently fast. Unfortunately, classic clustering algorithms such as hierarchical and partitioning-based clustering, e.g., K-Means or K-Medoids—although they have been successfully applied to cluster malware behaviors and programs [6, 13]—incur a time complexity at least quadratic in the number of samples, which in practice, does not scale to the MutantX-S target. MutantX-S exploits two approaches to address the scalability issue: (1) a hash kernel that compresses the high dimensional feature vector into a low dimensional space, and (2) a prototype-based clustering algorithm that has close-to-linear runtime complexity.

6.1 Hashing Kernel

Kernel methods [25] are powerful tools used in machine learning to allow operation in the high-dimensional feature space without having to compute the coordinates of the input data in that space. This is particularly useful when the input data has a non-linear decision boundary but can be linearly separated in a high dimensional feature space. In MutantX-S, however, we have encountered the opposite problem: the original space is very high-dimensional. The number of dimensions $D$ determines the complexity when computing the vector distance and $D$ increases exponentially with $N$ in $N$-gram (i.e. $D = \lvert \mathcal{O} \rvert^N$ where $\lvert \mathcal{O} \rvert$ is the number of different opcodes and in practice $\lvert \mathcal{O} \rvert > 200$). Therefore even a small $N$ like 3 will result in a (very sparse) feature vector with more than 8 million dimensions, which is computationally prohibitive when calculating similarities for large amount of malware

\[^4\] thus, the input data are likely already linearly separable

Figure 3: Two code pieces with different semantics share same mnemonic representation (i.e., move, cmp, jnz). However, they can be differentiated by their opcode representation: “0F 21 3D 75” vs “8B 3D 75”
samples. Unfortunately, \( N \) has to be at least 3 or 4 to be descriptive enough for capturing the program semantics.

**MutantX-S** addresses the problem by exploiting the **hashing-trick** recently developed in the machine learning community [26], which hashes the high dimensional input vector \( x \in \mathbb{R}^n \) into a lower dimensional feature space \( \mathbb{R}^m \) with the mapping function \( \phi : \mathcal{X} \rightarrow \mathbb{R}^m \). Since \( m \ll n \), the hashing trick reduces a feature vector to a more compact representation, allowing the clustering algorithm to handle a large volume of data, and save both computation and memory requirements. Previous research has shown that the hash kernel approximately preserves the vector distance and the penalty incurred from using a hash for reducing dimensionality only grows logarithmically with the number of samples and groups [26, 14].

Specifically, **MutantX-S** applies a **uniform** hash function \( H : \{N\text{-gram}\} \rightarrow [1..m] \) that hashes \( N\)-gram directly into a position in the feature vector of length \( m \). In case of a collision where two or more \( N\)-grams map to the same position, the sum of their counts is used as the value in the new vector. More formally, for malware \( M \) and \( M' \), let \( v \) and \( v' \) represent their original feature vector extracted from the encoded opcode sequences and \( \xi \) denote the mapping from the \( N\)-gram \( o_1, o_2, \ldots, o_N \) to the index in \( v \). We define the hash feature map \( \phi \) as

\[
\phi_i(v) = \sum_{l : H(o) = i, l \in S} v(\xi(o))
\]

and the distance between \( M \) and \( M' \) as

\[
d_\phi(M, M') = \|v - v'\|_\phi = \|\phi(v), \phi(v')\|.
\]

The choice of \( m \), the length of the low dimensional vector, is a trade-off between clustering accuracy and storage overhead plus computation complexity. Choosing a smaller \( m \) means shorter vector length, thus, faster distance computation and smaller memory footprint to store malware features. However, decreasing \( m \) increases the collision possibility, leading to over-compression of features and negative impact of the clustering accuracy.

### 6.2 Prototype-Based Clustering

Classic clustering algorithms typically incur a complexity that is super-linear in the size of the input data. For example, the running time for two most widely-used clustering algorithms \( k\)-means and hierarchical clustering are \( O(nkd) \) [4] and \( O(n^2 \log n) \) [19], resulting in the computation time that is prohibitively large for the number of malware we have to deal with. Instead, **MutantX-S** adopts the prototype-based close-to-linear clustering algorithm [24].

Despite their simplicity, Prototype-based algorithms have been empirically shown to be very effective and often one of the best performers in real data [11]. Prototype-based clustering extracts a set of prototypes each of which serves as the representative for a small group. The remaining data points are associated with their closest prototype in the feature space. The key idea of Prototype-based algorithm is to perform computation (e.g. clustering) only on the prototypes which are a small subset of original data points, thus reducing the computation time significantly. The algorithm comprises 2 steps.

**Prototype extraction:** The quality of final clusters depends on the choice of the prototypes. Well-positioned prototypes can accurately capture the distribution of input data and allows creating accurate class boundaries in the feature space. Unfortunately, determining the optimal number and positions of prototypes is NP-hard and an approximate algorithm by González [9] was commonly used to iteratively select prototypes. During each iteration, the data point with the largest distance to existing prototypes is selected as the next prototype (the first prototype is selected randomly). The process repeats until the distance from all the data points to their nearest prototype is smaller than a predefined distance threshold \( P_{\text{max}} \), i.e., all the data points are located within a certain radius from their closest prototypes. The run-time complexity of this algorithm is \( O(kn) \) where \( k \) is the number of prototypes selected. Since \( k \) only depends on the distribution of the data (in this case, \( k \) is proportional to the amount of malware families), with a reasonable choice of \( P_{\text{max}} \) the algorithm is linear in the number of input data \( n \).

**Clustering with prototypes.** Instead of working on the huge number of original data, the algorithm performs agglomerative hierarchical clustering only on the prototypes. Specifically, the algorithm starts with individual prototypes as singleton clusters, successively merges two closest clusters, and terminates when the distance between the closest clusters is larger than a predefined distance threshold \( M_{\text{dil}} \). Then, prototypes within the same cluster are assigned the same cluster label and subsequently propagate the label to their associated data points. Because each prototype is a good representation of its associated data points (all within a radius of \( P_{\text{max}} \)), the algorithm avoids expensive distance computation between the original data points without too much loss in the overall accuracy. The respective run-time complexities of clustering and propagation steps are \( O(k^2 \log k) \) and \( O(n) \). Compared to the \( O(n^2 \log n) \) complexity of applying an hierarchical clustering algorithm on the original data points, this algorithm achieves a speed-up with a factor of at least \( (n/k)^2 \).

### 7 Experimental Evaluation

We now evaluate **MutantX-S**’ efficiency and accuracy using two data sets: (1) a reference data set containing 4821 malware files whose labels are generated by security experts from a large anti-virus company and thus
more reliable; and (2) a large malware data set collected from an online malware archive [29] which comprises 132,234 malware samples with unreliable labels derived from AV scanners. The reference data set includes malware samples from 20 different families and their distributions are given in Table 2. Considering its reliable labeling, the reference set is used to evaluate and fine-tune the empirical parameters for the MutantX-S’s clustering engine while the larger set is used to assess its scalability.

Table 2: Malware families of the reference data set

<table>
<thead>
<tr>
<th>Family</th>
<th>#</th>
<th>Family</th>
<th>#</th>
<th>Family</th>
<th>#</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pilleuz</td>
<td>500</td>
<td>Bredolab</td>
<td>301</td>
<td>Tisderv</td>
<td>59</td>
</tr>
<tr>
<td>Koobface</td>
<td>496</td>
<td>Vundo</td>
<td>249</td>
<td>Waledac</td>
<td>34</td>
</tr>
<tr>
<td>Silly</td>
<td>489</td>
<td>Almanaxe</td>
<td>241</td>
<td>Ackantta</td>
<td>32</td>
</tr>
<tr>
<td>Fakeav</td>
<td>489</td>
<td>Sasfis</td>
<td>199</td>
<td>Mebroot</td>
<td>26</td>
</tr>
<tr>
<td>Zbot</td>
<td>459</td>
<td>Graybird</td>
<td>166</td>
<td>Hotbar</td>
<td>21</td>
</tr>
<tr>
<td>Banker</td>
<td>449</td>
<td>Gammima</td>
<td>126</td>
<td>Qakbot</td>
<td>17</td>
</tr>
<tr>
<td>Virat</td>
<td>361</td>
<td>Mabezat</td>
<td>107</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.1 Effectiveness of Unpacking Engine

To evaluate the effectiveness of MutantX-S’s unpacking component, we select and then pack a malware program with 8 popular packers. We then unpack them with MutantX-S and compare unpacked files with the original version. Ideally, the unpacked binary should be byte-to-byte identical to the original file. However, this is neither possible (MutantX-S does not reconstruct the import table, and the unpacker code is also dumped from the memory), nor necessary for the purpose of malware clustering. As a result, we compared the unpacked files with the original one using two metrics: (i) the difference in their instruction count (IC), and (ii) the distance between their N-gram feature vectors (NG), because they are directly related to clustering accuracy. Table 3 summarized the results. For most packers, the MutantX-S successfully recovered their original binaries with only a 1–6% increase of ICs which is often due to the inclusion of unpacker routines in the dumped memory. Besides, the feature vectors of unpacked binaries are very similar to those of the original binary with most normalized distance measurements below 0.1, where 0 means identical and 1 means completely different. However, MutantX-S also failed on certain packers. In particular, the memory dump of Armadillo-packed malware sample still contains a packed version of the binary. A further investigation showed that Armadillo works by unpacking an intermediate executable on disk and creating another process to run this executable [20]. Therefore, memory dump of an Armadillo-packed file does not contain original instructions. After running MutantX-S on the larger data set, we have also observed other causes of unsuccessful unpacking, such as malware samples re-fusing to run in a virtual machine or the time required for unpacking is longer than the threshold. Nevertheless, MutantX-S’s generic unpacking technique is still effective against popular packers without requiring any specialized knowledge of packing algorithms.

Table 3: Unpacking effectiveness (IC: Instruction Count; NG Dist: N-gram Difference)

<table>
<thead>
<tr>
<th>Packer</th>
<th>Diff in IC (%)</th>
<th>NG Dist</th>
<th>Packer</th>
<th>Diff in IC (%)</th>
<th>NG Dist</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEcompact</td>
<td>0.88%</td>
<td>0.068</td>
<td>ASprotect</td>
<td>6.70%</td>
<td>0.133</td>
</tr>
<tr>
<td>EXEcryptor</td>
<td>3.20%</td>
<td>0.176</td>
<td>UPX</td>
<td>0.88%</td>
<td>0.068</td>
</tr>
<tr>
<td>EXEStealth</td>
<td>0.88%</td>
<td>0.071</td>
<td>NSPack</td>
<td>0.87%</td>
<td>0.069</td>
</tr>
<tr>
<td>VMprotect</td>
<td>2.50%</td>
<td>0.10</td>
<td>Armadillo</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

7.2 Malware Clustering Accuracy

We first evaluate and calibrate MutantX-S against the reference data set. All of our evaluations were done on a Ubuntu 10.4 machine with Core i7 3.0G CPU and 12GB memory. We use precision and recall as the main metrics to assess the accuracy of MutantX-S. Suppose that with respect to the original labels (i.e., family names in Table 2), n input malware samples can be grouped into a set of clusters \( O = \{O_1, O_2, \ldots, O_n\} \). Assume MutantX-S outputs a set of clusters \( C = \{C_1, C_2, \ldots, C_c\} \). Then, precision \( P \) measures how well individual clusters agree with the original classes (i.e., the exactness of clusters), and recall \( R \) measures how much the malware classes are scattered across the clusters (i.e., the completeness of each cluster). Formally, we define

\[
P = \frac{1}{n} \sum_{i=1}^{c} \max(|C_i \cap O_1|, |C_i \cap O_2|, \ldots, |C_i \cap O_n|)
\]

\[
R = \frac{1}{n} \sum_{j=1}^{o} \max(|O_j \cap C_1|, |O_j \cap C_2|, \ldots, |O_j \cap C_c|)
\]

\( P \) will be 1 if all the samples in every cluster \( C_i \) are from the same family and \( R \) will be 1 if all malware samples from the same family fall into a single cluster (but not necessarily the only family in this cluster). Fig. 5 shows the precision and recall of MutantX-S’s clustering with varying thresholds \( P_{\text{max}} \) and \( Min_d \) (defined in Section 6). The experiment uses 4-gram and 12 hash bits (i.e., the 4-gram is mapped into 2^{12} hash bins).

From the figure, we observe that MutantX-S is able to cluster the samples with the precision ranging from 0.72 to 0.89 (average=0.80). The precision number is smaller than those reported in previous dynamic-behavior approaches, e.g., 0.996 in [24] and 0.984 in [7]. We conjecture that this difference may be due to different malware sets (and possibly incorrect labeling) used in our experiments and the reason for the higher accuracy of dynamic-behavior approaches is also likely due to their high-level generalization of behavior at the cost of longer
running time and limited coverage as discussed in Section 1. Therefore, MutantX-S can provide an alternative way of categorizing malware and is complementary to the behavior-based analysis with better scalability while maintaining reasonably good accuracy. Indeed, Fig. 5 shows that it takes only less than 30 seconds to complete the clustering for the entire reference dataset (we also ran the K-mean and hierarchical clustering on the same dataset which respectively took 32.3 seconds with precision 0.75 and 51.3 seconds with precision 0.82). In addition, we observe that the recall of MutantX-S is around 0.3 and 0.4. However, this low value of recall is not surprising, because there often exists significant diversity across malware variants. For instance, we observed that one variant in Vundo family is 10 times larger in terms of file size than the other Vundo variant. This is possibly due to mislabeled samples, unidentified packers or heavily-obfuscated binaries. Because of the highly diverse variants, MutantX-S often breaks one family into several sub-families, resulting in a low recall, e.g., MutantX-S creates more than 50 clusters for the reference dataset which contains 20 families according to the labels. Albeit less ideal, a breakdown into sub-families is acceptable in practice, e.g., predicting labels for unknown samples as we will show later.

Another observation from these results is that \( P_{\text{max}} \) (the threshold for distances from data points to their nearest prototypes) has a greater influence on the clustering speed, since a smaller \( P_{\text{max}} \) forces the algorithm to find more prototypes to cover all the data points, thus requiring more computation. On the other hand, \( \text{Min}_d \) has a major impact on the clustering accuracy. Increasing \( \text{Min}_d \) reduces the precision, because a smaller inter-cluster distance threshold will stop the prototype-merging process earlier which reduces the probability of combining unrelated prototypes into a larger cluster. However, the price for this is the over-fitting of clustering, i.e., the algorithm tends to create several small clusters. Hence, a trade-off has to be empirically made, as in our later experiments.

### 7.3 Validity of the Hashing Trick

The main concern in using the hashing trick is the possible loss of information due to the compression of high dimensional features into a lower dimensional space. To evaluate the efficacy of hashing trick, we use different number of hash bins to cluster the reference data set. The hash function used in MutantX-S is MurmurHash 2.0 [1], a simple hash implementation with uniform value distribution, high throughput, and good collision resistance. As comparison, we also ran MutantX-S on the original feature vectors without the hashing trick, which serves as the baseline benchmark and best-possible result achievable without information loss.

Figure 6 compares the precision, clustering time and peak memory requirements with different hash sizes (the number of hash bins ranging from \( 2^8 \) to \( 2^{10} \) and no hash). Different bars represent the results generated by different parameter combinations. From the left figure, we find that as the hash size increases, the precision improves because the collision probability reduces. In fact, when the hash size is large enough, the probability of collision becomes so negligible that the hashed features vector perform the same as the original ones. For instance, with more than \( 2^{12} \) hash bins, the clustering achieves almost the same precision, 0.864, as the original features \( P = 0.868 \). However, as the hash size becomes smaller, the impact of collision starts to surface. When the number of hash bins reduces to \( 2^8 = 256 \), the precision drops significantly (less than 0.5) for some parameter combinations, due to collision of many critical features (e.g., features indicative of different families are now mapped to the same hash bin). In this regard, a larger hash size is preferable. On the other hand, the middle and right figures in Figures 6 show that a small hash size is very effective in reducing the algorithm’s running time and memory footprints. This is because smaller number of hash bins means shorter feature vectors which require less memory for storage and fewer CPU cycles to compute the distance. For instance, as the hash size decreases from 16 bits to 8 bits, the required running time drops from almost 2 minutes to less than 10 seconds and memory requirement from 800 Mbytes to less than 100 Mbytes, at
the cost of precision. In practice, a 12-bit hash function is found to be a good compromise, reducing the time and memory requirements by over 80% while still keeping good accuracy. Figure 6 also shows that as the number of malware increases, the hashing trick becomes critical. Without it, the memory requirement could quickly become prohibitively high.

### 7.4 Impact of N-gram on Performance

Intuitively, as N increases, N-gram becomes more descriptive, providing better distinguishability. However, this comes at the cost of exponential increase in the dimensionality of the resulting feature vectors \(m^N\) where \(m\) is total number of different opcodes), as well as the required storage and computation time. Therefore, previous work that uses N-gram based approaches commonly chose small \(N\) (3 or 4). Fortunately, the hashing trick enables us to compress the feature vectors and evaluate the performance of large \(N\). Figure 7 summarizes the result.

From Figure 7, one can observe that use of a larger \(N\) value indeed improves the precision, e.g., 4- and 5-grams achieve better precision than 3-gram since larger grams can better capture the underlying instruction semantics. However, the figure also shows that 6-gram performs the worst. This is because the number different 6-grams (i.e., over \(6.4 \times 10^{12}\)) is too large for the 12-bit hash function (4096 hash bins), leading to a large number of collisions between irrelevant features. In MutantX-S, we have chosen 4-gram, because the improvement provided by 5-gram is not large enough to warrant the additional storage and computation overheads.

### 7.5 Scalability of MutantX-S

In this subsection, we evaluate the scalability and accuracy of MutantX-S on the large malware data set with over 130,000 samples. We ran MutantX-S on the entire set with different parameters and plotted the results in Fig. 8. The right figure shows the amount of time for clustering the entire set. The value \(P_{\max}\) seems to have a more significant impact on the running time. For example, when \(P_{\max}\) is set to 0.5, the clustering takes less than 1 hour which is almost half of the time when \(P_{\max}\) is set to 0.2. As mentioned before, \(P_{\max}\) determines the number of prototypes extracted from the input data which determines the total number of distance computations required for clustering. Although a larger \(P_{\max}\) leads to a shorter running time, the left plot in Fig. 8 illustrates the correlation between a large \(P_{\max}\) and the reduced clustering precision, i.e., increasing \(P_{\max}\) from 0.2 to 0.5 reduces the precision by almost 10%. This can be explained as follows: a large \(P_{\max}\) allows each prototype to cover a large portion of the space, thus increasing the possibility of including samples from irrelevant families. With a reasonable setting (e.g., Min_d = 0.5 and \(P_{\max}\) = 0.4), MutantX-S is able to complete the clustering of over 130K malware in less than 1.5 hours with the precision close to 0.82. The peak memory usage is around 3.6GB. These results indicate that MutantX-S is very efficient in handling a large number of samples and thus has the potential to keep up with the huge influx of malware variants received nowadays.

### 7.6 Predicting Labels of Unknown Malware

So far, we have evaluated MutantX-S using the data set of known malware families. In a realistic scenario, e.g., in AV companies, MutantX-S is more likely to be used to analyze new incoming malware and predict their family labels. In such a scenario, incoming malware...
are analyzed and labeled according to their association with the closest kin in the previously-analyzed samples. To simulate this situation, we need a chronological order of malware samples according to their creation time. We extract the creation time for each malware from their IMAGE_FILE_HEADER. IMAGE_FILE_HEADER is a standard header in the PE file and contains a timestamp field that is set by the compiler at the compilation time. We use this timestamp to bucket malware programs into months and select one year worth of malware (more than 40,000 unique samples). Fig. 9 shows the distribution of the number of new malware samples across all months. Next, we use these malware to simulate the process of determining the labels for new incoming samples.

![Figure 9: Number of new malware samples in each month used to evaluate prediction capability](image)

![Figure 10: Accuracy in predicting family labels for unknown malware](image)

Specifically, we separate the malware program into training set and testing set based on their creation time in order to simulate the scenario where AV companies have analyzed the malware from the training set and try to predict the labels for newly-received malware (test set). The test set consists of malware samples from each month between July and December (these months are “test months”). Then, we choose 3 different training sets. For the first training set, we use samples from all months from January to one month before the test month. For instance, if the test month is September, the training months are January through August. For the second training set, we use 6 months prior to the test month, i.e., if September is the test month, March through August will be the training months. Finally, as a controlled experiment, we keep the first 6 months (i.e., January through June) as the training month regardless of test months. Given any training set, MutantX-S creates a set of clusters $C_i$ ($i = 0, 1, \ldots, n$). Each cluster has a label $L(C_i)$ determined by the majority family labels of the constituent malware samples. Then MutantX-S determines the family label $L(x_j)$ of the new sample $x_j$ in the test month based on the label of the cluster that is closest to $x_j$, i.e., $L(x_j) = L(C_i)$ where $d(x_j, C_i) = \min(d(x_j, C_k)) \forall k = 0, 1, \ldots, n$. We then compare this predicted family label with the original label of $x_j$ and plot the percentage of correctly predicted samples in Fig. 10. The first observation from the figure is that malware are constantly evolving and the information obtained from previous clustering can become obsolete quickly, as shown by the bottom green line where we kept on using the same first 6 months as the training data and the prediction accuracy degraded rapidly from 0.7 in July to below 0.4 in December. In contrast, if we use the full history as the training data, the accuracy stays consistently in the 0.7–0.8 range (the top red line in Fig. 10), thanks to the up-to-date information from the recent malware. However, in reality, due to the resource (e.g., storage) constraints, it may not be possible to keep the entire history of previous malware samples. It is more efficient to use only the most recent history, e.g., 6 months as in the middle blue line. From Fig. 10, one can see that the result is very close to that of using the full history, with only a small decrease, about 2 to 3%. These results imply that there exists a strong temporal correlation among malware variants which can be exploited by MutantX-S in predicting the labels for unknown malware samples.

8 Limitations and Improvements

Here we discuss limitations of the current prototype of MutantX-S that could be exploited by adversaries to degrade its effectiveness in clustering. As a static-analysis approach, MutantX-S is vulnerable to binary/instruction-level obfuscation. First, even with a generic unpacking algorithm, MutantX-S is less effective against advanced packers that employ sophisticated protection mechanisms, e.g., anti-debug, anti-emulation, etc. Specialized unpacking tools [2] have been developed for these packers and they can be incorporated into MutantX-S to combat sophisticated packers. Second, MutantX-S extracts features from disassembled malware code. Unfortunately, producing correct disassembly is often very challenging and many anti-disassembly tricks [31] can be used to confuse a disassembler, such as mixture of code and data, making an infeasible conditional jump to the middle of next instruction, etc. Although the current prototype does not handle these types of obfuscation for simplicity, there are a variety of techniques [16] proposed to mitigate these problems. Third, MutantX-S relies on the similarity of code instructions to cluster malware samples. It is possible to create syntactically distinct but semantically similar variants through heavy instruction-level obfuscation. To address these problems, MutantX-S could incorporate more advanced de-obfuscation techniques [27, 22] and normalize the malware codes before clustering them. Note that dynamic-behavior-based approaches do not suffer from this limitation, but they come with their own deficiencies—limited coverage, scalability and specific evasion techniques. Therefore, MutantX-S’ goal is not to replace the dynamic approaches, but to complement...
them and collaboratively mitigate their weaknesses (e.g. apply dynamic analysis only on representative samples or outliers of static analysis). Finally, MutantX-S cannot handle file injector or parasitic malware types which inject themselves into host executables. This is a limitation for any similarity based clustering, regardless static or dynamic approaches, because most features are from the host executables rather than the malware. Such parasitic malware are a matter of our future inquiry.

9 Conclusion

In this paper, we have presented the design, implementation and evaluation of a malware clustering system based on static features, called MutantX-S. MutantX-S can accurately and efficiently group malware variants according to the similarity in their code instructions. It converts each malware program into a compact but effective op-code representation and performs prototype-based clustering on the corresponding N-gram feature vectors. It also incorporates a generic unpacking technique to maximize the capability of analyzing the malware’s original instructions. To ensure the scalability, MutantX-S uses a combination of a hashing kernel that reduces the dimensionality of feature vectors and a close-to-linear time prototype-based clustering that uses a small set of representative samples for fast data organization. Equipped with these techniques, MutantX-S is experimentally shown to be able to process more than 130,000 malware samples within a few hours. As a static-analysis approach, MutantX-S is expected to be very effective and can be combined with existing dynamic-behavior-based system to provide the level of accuracy and coverage required to pace with the current malware sample submission rate.

References