Unsupervised Detection and Clustering of Malicious TLS Flows

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Malware abuses TLS to encrypt its malicious traffic, preventing examination by content signatures and deep packet inspection. Network detection of malicious TLS flows is an important, but challenging, problem. Prior works have proposed supervised machine learning detectors using TLS features. However, by trying to represent all malicious traffic, supervised binary detectors produce models that are too loose, thus introducing errors. Furthermore, they do not distinguish flows generated by different malware. On the other hand, supervised multi-class detectors produce tighter models and can classify flows by malware family, but require family labels, which are not available for many samples.

To address these limitations, this work proposes a novel unsupervised approach to detect and cluster malicious TLS flows. Our approach takes as input network traces from sandboxes. It clusters similar TLS flows using 90 features that capture properties of the TLS client, TLS server, certificate, and encrypted payload; and uses the clusters to build an unsupervised detector that can assign a malicious flow to the cluster it belongs to, or determine it is benign. We evaluate our approach using 972K traces from a commercial sandbox and 35M TLS flows from a research network. Our clustering shows very high precision and recall with an F1 score of 0.993. We compare our unsupervised detector with two state-of-the-art approaches, showing that it outperforms both. The false detection rate of our detector is 0.032% measured over four months of traffic.

CCS Concepts:
- Security and privacy → Malware and its mitigation.

Additional Key Words and Phrases: Malware; TLS; Network Detection; Clustering

1 INTRODUCTION

Transport Layer Security (TLS) is the most popular cryptographic protocol, widely used to provide confidentiality, integrity, and authentication to applications such as Web browsing, email, and instant messaging [7, 29]. Its security properties and wide availability make TLS also appealing for malware, which can abuse it to hide their malicious traffic among benign traffic of a myriad of applications, while preventing examination of its application payload. In February 2020, 23% of malware were using TLS [25].

Network detection of malicious TLS flows is an important, but challenging, problem. It allows to protect whole networks by monitoring their traffic, regardless of whether endpoint security has been deployed. An important property for scalability and privacy is that the network detection should not require decrypting the content, i.e., should avoid man-in-the-middle (MITM) interception [16]. Another important property is to cluster the detected flows with other similar malicious flows, providing valuable threat intelligence to the analysts that investigate a detection.

Anderson and McGrew have proposed supervised machine learning (ML) detectors for malicious TLS flows [5, 6, 8]. A limitation of binary supervised detectors (e.g., [8]) is that they try to distinguish any malicious TLS flow, regardless of the malware family producing it. This is problematic because different families may exhibit significant differences in TLS
usage (e.g., TLS versions, ciphersuites, extensions, certificates). To cover all those differences, the generated model tends to become too loose, thus introducing errors. In addition, a binary detector does not provide contextual information about similar malicious flows. They have also proposed combining TLS features with HTTP and DNS features to improve the binary detection [5]. However, some families may only use TLS (e.g., HTTPS, but no HTTP) and may connect using IP addresses instead of domain names. Furthermore, HTTP and DNS features may contain sensitive user information, thus lowering user privacy. In their original work, Anderson et al. also evaluated a multi-class supervised classifier, where each class corresponds to a different malware family [8]. This approach better models the TLS traffic of individual families and classifies the detected flows. But, it requires clean family labels to train the classifiers. A common labeling method is a vote on the families present in the AV detection labels of a sample [41]; unfortunately, this approach is ineffective for many samples. As a concrete example, Anderson and McGrew [8] could only label this way 27% of 20.5K samples using TLS; no classifier could be built for the families of the 73% unlabeled samples, and thus their malicious traffic could not be detected. Recent works have proposed anomaly based intrusion detection systems using neural network auto-encoders [12, 33]. These works do not specifically target TLS flows, but can be applied to them as they do not require access to unencrypted payload. Since they build models of benign traffic, they do not require labeled malicious traffic during training. But, they suffer false positives when natural changes affect the benign traffic.

In this paper, we present a novel unsupervised approach to detect and cluster malicious TLS flows. Our approach respects user privacy as it only requires access to the encrypted TLS flows, and not to their unencrypted payload or any other unencrypted traffic. Our approach takes as input traces of network traffic generated by executing suspicious samples in a sandbox. From each TLS flow in the traces, it extracts 90 features that capture characteristics of the TLS client, the TLS server, the server’s certificate, and the encrypted payload. After filtering benign TLS traffic, the remaining vectors are clustered, so that each cluster contains similar traffic belonging to a (potentially unknown) malware family. Since malware families may use different types of traffic (e.g., C&C, updates from download server) multiple clusters can be output for a family. The use of clustering removes the requirement for family labels as it allows detecting any malicious traffic similar to the training flows, even if the training flows could not be annotated with a known family name, i.e., flows from the 73% samples that Anderson and McGrew [8] had to remove from their training. The clusters are input to the unsupervised detector that can be deployed at the boundary of a network to identify malicious TLS flows. The detector measures the distance of a given flow to all clusters and outputs the closest cluster. If no cluster is close, the flow is determined to be benign. If family labels are available for the identified cluster, the analyst also obtains the family of the detected flow. When family labels are not available, the detection is not affected: the flow is associated with the random identifier of its cluster, but still provides contextual information about samples generating similar flows.

To evaluate our approach, we use 972K network traces provided by a commercial sandbox vendor and 35M TLS flows collected at the boundary of a research network over seven months. We identify, for the first time, how the sandbox can significantly impact the collected TLS traffic if it runs old OS versions (e.g., Windows 7, Windows XP). Those OSes use TLS 1.0 by default, instead of the currently dominating TLS 1.2 and 1.3 versions. Thus, training a classifier with malicious traffic from a single sandbox using an old OS could incorrectly capture that TLS 1.0 traffic is malicious and TLS 1.2 and 1.3 benign. This is an important finding because popular sandboxes (e.g., VirusTotal [19]) run decade-old OS versions since a common belief is that the lack of newer OS defenses makes it easier for malware to run and manifest its behaviors. Our results highlight the importance of using a variety of OS versions in malware sandboxes. Furthermore, this issue could have impacted previous work that identified significant differences between malware and benign programs TLS client characteristics (e.g., malware using older ciphersuites and less extensions) [5, 8], as those...
same authors have recently concluded that TLS client features are not enough by themselves [7], in contrast with their earlier claims.

Our clustering achieves a F1 score of 0.993. We observe that 31% of the produced clusters only contain samples for which the state-of-the-art AVClass labeling tool [41] is not able to obtain family names: supervised multi-class approaches would not work for those samples. We also observe that our clustering is able to group TLS 1.3 flows from multiple samples of the same family, even when no Server Name Indication (SNI) header is present. TLS 1.3 is a challenging case, not evaluated in prior work, as certificates are encrypted and client and server features are greatly reduced.

We compare our unsupervised detector with two state-of-the-art approaches. Our comparison with Joy [3], the state-of-the-art supervised binary detector by Anderson et al. [8], shows that when applied to the same dataset, our approach achieves a F1 score of 0.91, compared to 0.82 for Joy. We also compare our approach with Kitsune [33], the state-of-the-art auto-encoder-based anomaly detector. Our approach achieves a F1 score of 0.99 compared to 0.59 for Kitsune. We also evaluate our detector over long windows of time to estimate its false detection ratio (FDR). Over one week of traffic from the research network, our approach achieves an FDR of 0.031%. Over four months, the FDR remains almost the same at 0.032%, highlighting the stability of the detection model.

This paper provides the following contributions:

- We present a novel unsupervised approach to detect and cluster malicious TLS flows. Compared to binary supervised detectors, our clustering approach models separately TLS characteristics from different families. This results in tighter models that improve detection and can provide contextual information about the cluster a detected flow belongs to. Compared to multi-class classifiers, our approach can detect samples for which family labels are not available.
- We observe that training malicious TLS detectors on traces from a single sandbox that uses old OS versions can significantly bias the detector. This highlights the importance of using a variety of OS versions in malware sandboxes.
- We evaluate our approach using 972K network traces from a commercial sandbox and 35M TLS flows from a research network. Our unsupervised detector achieves a F1 score of 0.91, compared to 0.82 for the state-of-the-art supervised detector, and a FDR of 0.032% over four months of traffic.

The remainder of this paper is organized as follows. Section 2 motivates our research problem. Section 3 details our novel unsupervised approach to detect and cluster malicious TLS flows. Section 4 describes the datasets used. Section 5 evaluates our approach and compares it with state-of-the-art approaches. Section 6 presents prior related work. Section 7 discusses limitations and avenues for improvement. Finally, Section 8 concludes. For the reader’s benefit Table 15 in the Appendix details the acronyms used in this work.

2 MOTIVATION

Our goal is to detect malicious TLS flows (TLS sessions) between an infected host in a protected network, e.g., an enterprise or university network, and a remote malicious server. A pre-requisite is that to respect user privacy only TLS flows are accessible from the protected network. This implies that the application payload of the TLS flows should not be accessed, i.e., no MITM, and that unencrypted traffic should not be needed for the detection. Thus, detection features should exclusively come from TLS flows.
Our intuition is that it is possible to capture TLS characteristics of a specific type of malware family traffic (e.g., C&C, updates), but that it is very hard to capture TLS characteristics that distinguish any malware using TLS from any benign application using TLS. For example, certificates and domains in SNI headers are clearly family-specific. Similarly, encrypted payload features such as packet sizes are specific to the protocols (e.g., C&C, update) used by each family [20].

Thus, rather than building a supervised binary classifier, we propose an unsupervised detector that clusters similar malicious TLS flows and then detects new TLS flows by measuring the distance to the clusters. A benefit of our clustering approach is that the model can assign detected flows to the cluster that led to the detection. Some clusters will be labeled with a recognizable family name such as upatre, zbot, or bublik. For others, the family may be unknown, but the cluster still provides important contextual information in the form of samples that generate similar TLS flows. In contrast with multi-class supervised classifiers (e.g., [8]) family labels are not required for the input samples, so that the detection still works for the large fraction of samples that may miss them.

**Ethical considerations.** The passive data collection performed at the research network was approved and performed according to the institutional policies. To protect user privacy, it covers only the collection of encrypted TLS flows and excludes personally identifiable information such as client IP addresses. Access to the data is limited to employees of the Institution. This research made no attempt to decrypt the TLS flows. Our goal is to enable the detection of malicious TLS traffic, while maintaining user privacy.

### 3 APPROACH

Our approach takes as input network traces produced by running suspicious executables in a sandbox. It outputs an unsupervised detector that can be deployed on a network to detect malicious TLS flows. The input network traces are annotated with the hash of the sample whose execution produced it. Our approach comprises four steps, illustrated in Figure 1. Section 3.1 describes the feature extraction that produces a feature vector for each TLS flow in the input network traces. Section 3.2 presents the filtering that removes feature vectors corresponding to benign traffic. Section 3.3 details the clustering, which groups similar feature vectors together. Finally, Section 3.4 describes the unsupervised detector, which given the feature vector of a previously unseen TLS flow classifies it as malicious (with its corresponding cluster) or benign.

#### 3.1 Feature Extraction

TLS fingerprints are applied to the first payload bytes of each TCP connection to identify TLS flows [21], regardless of the ports used for the communication. For the identified TLS flows, the TCP connection is reassembled, the full TCP
payload extracted, and then the early part of the TCP payload corresponding to the TLS handshake is separated from the application data using the value of the content type field of the TLS records. TLS flows that have no application data in either direction are removed.

We extract 90 features from the remaining TLS flows. Of those, 67 features are new, while the other 23 features have been used in prior works. The features can be grouped into four categories. Client, server, and certificate features are extracted from the TLS handshake, while encrypted payload features are instead extracted from the encrypted application data. Features are either numerical or categorical. To build the feature vectors, numerical features are normalized using their z-score, i.e., by subtracting the mean and dividing by the standard deviation. Categorical features are first applied one-hot encoding and the result is multiplied by the term-frequency inverse document-frequency (TF-IDF) of the values.

### Client features
These 11 features, summarized in Table 1, are extracted from the Client Hello message. They capture the functionality supported by the TLS client software. Programs either use the default configuration of a cryptographic library or OS API, or configure them with their preferences. Client features identify programs whose TLS functionality is configured similarly. The features correspond to the highest supported TLS and record versions, the list of supported TLS versions (extension added in TLS 1.3), the list of supported ciphers, compression methods, elliptic curves and point formats, the list of extensions included in the message, the domain name in the SNI extension, and the list of supported application protocols in the Application Layer Protocol Negotiation (ALPN) extension (e.g., HTTP/0.9, SPDY/1). The fake resumption feature is explained later in the resumed sessions paragraph.

### Server features
The 9 server features in Table 2 correspond to the destination port and features extracted from the Server Hello message. Server features capture the TLS functionality of the server software, i.e., the parameters the
server selects for the TLS session after intersecting the client TLS support with its own TLS support. Server features identify servers configured similarly. The Server Hello features are the selected TLS version, record versions, cipher, and compression method; the list of extensions in the message, the selected application protocol in the ALPN extension, and the lifetime in the SessionTicket extension. The last feature captures the signature in the SignedCertificateTimestamp extension that a server may use to transmit signed proofs of the server’s certificate presence in the Certificate Transparency (CT) logs [9].

**Certificate features.** These 24 features, summarized in Table 3, are extracted from the certificate chain sent by the server. These features capture the number of certificates in the chain and fields of the leaf certificate. The focus is on the leaf certificate because that certificate is specific to the service, while other certificates in the chain belong to the certification authorities (CAs) used, and thus may be common to many unrelated services. Nine leaf certificate features correspond to certificate parameters, namely the version, its validity period, the number of Subject Alternative Names (SAN) and extensions included, the validation status on the day we first process a flow, whether the certificate is self-signed, the signature algorithm, public key length, and public key hash. Another seven features correspond to fields of the Subject Distinguished Name (DN), and the remaining seven to the same fields in the Issuer DN. In the rare case where client certificates are used an extra 22 analogous features are extracted from the client’s certificate chain.

**Encrypted payload features.** Another 24 features are extracted from the encrypted application data transferred after the TLS handshake has completed. These features capture the application protocol used for communication. The intuition is that the protocol changes infrequently because protocol updates require both client and server software updates and need to be thoroughly debugged to maintain compatibility. In particular, prior work has shown that the command and control (C&C) protocol used by malware changes much slower than its communication endpoints (i.e., domains, IP addresses, ports) [15]. Similarly, we expect the protocol to also change less frequently than the TLS configuration parameters.

| Feature                        | Type  | PriorWork | TLS 1.2 | TLS 1.3 |
|--------------------------------|-------|-----------|---------|---------|
| (c|s)_num_certs                  | Cat   | ✓         | ✓       | ✗       |
| (c|s)_leaf_cert_version          | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_validity         | Cat   | ✓         | ✓       | ✗       |
| (c|s)_leaf_cert_num_SAN          | Cat   | ✓         | ✓       | ✗       |
| (c|s)_leaf_cert_ext_num          | Cat   | ✗         | ✓       | ✗       |
| s_leaf_cert_validity_status    | Cat   | ✗         | ✓       | ✗       |
| s_leaf_cert_self_signed        | Cat   | [8]       | ✓       | ✗       |
| (c|s)_leaf_cert_sign_alg         | Cat   | [8]       | ✓       | ✗       |
| (c|s)_leaf_cert_pubkey_hash      | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_pubkey_size      | Cat   | [8]       | ✓       | ✗       |
| (c|s)_leaf_cert_subj_cn          | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_subj_o           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_subj_c           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_subj_st          | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_subj_l           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_subj_email       | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_cn           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_o            | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_ou           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_c            | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_st           | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_l            | Cat   | ✗         | ✓       | ✗       |
| (c|s)_leaf_cert_iss_email        | Cat   | ✗         | ✓       | ✗       |

Table 3. Certificate features.
Table 4. Payload features.

| Feature       | Type | PriorWork | TLS 1.2 | TLS 1.3 |
|---------------|------|-----------|---------|---------|
| enc_data_size | Num  | ×         | ✓       | ✓       |
| enc_sent_size | Num  | ×         | ✓       | ✓       |
| enc_recv_size | Num  | ×         | ✓       | ✓       |
| enc_num_pkts  | Num  | ×         | ✓       | ✓       |
| enc_sent_pkts | Num  | ×         | ✓       | ✓       |
| c_max_seq     | Num  | ×         | ✓       | ✓       |
| c_max_length  | Num  | ×         | ✓       | ✓       |
| s_max_seq     | Num  | ×         | ✓       | ✓       |
| s_max_length  | Num  | ×         | ✓       | ✓       |
| sent_recv_pkts_ratio | Num   | ×      | ✓       | ✓       |
| sent_recv_size_ratio | Num   | ×      | ✓       | ✓       |
| msg_pkts_c_0  | Num  | [20]     | ✓       | ✓       |
| msg_size_c_0  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_c_0  | Num  | [20]     | ✓       | ✓       |
| msg_size_c_0  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_s_0  | Num  | [20]     | ✓       | ✓       |
| msg_size_s_0  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_c_1  | Num  | [20]     | ✓       | ✓       |
| msg_size_c_1  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_s_1  | Num  | [20]     | ✓       | ✓       |
| msg_size_s_1  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_c_2  | Num  | [20]     | ✓       | ✓       |
| msg_size_c_2  | Num  | [20]     | ✓       | ✓       |
| msg_pkts_s_2  | Num  | [20]     | ✓       | ✓       |
| msg_size_s_2  | Num  | [20]     | ✓       | ✓       |

Traffic analysis approaches often leverage the number, direction (i.e., client-to-server or server-to-client) and sizes of packets as features to identify encrypted content (e.g., [18, 42]). However, packets do not always accurately capture the underlying protocol because application messages can be fragmented into multiple packets by the transport and IP protocols. To address this issue, we define a **sequence** as all consecutive packets sent in one direction until another packet is seen in the opposite direction. The concatenation of the payload of all packets in a sequence is a good approximation of an application message [20]. The use of variable-length sequences avoids the need to select a threshold.

We call two consecutive sequences in opposite direction a **request-response pair** (RRP). The number of RRPs to consider is a hyper-parameter of the payload features. The intuition to select this parameter is that the initial part of the communication is more commonly related to the protocol, while later parts may be more related to the transferred content (e.g., files sent). In this work, we consider the first three RRPs, analyzing a total of six sequences. In our sandbox traces we observe that 95% of TLS flows have a single RRP, 3% have two, and 2% have at least three RRPs.

For each sequence, two features are extracted: the size of the concatenated payload (e.g., msg_size_c_0) and the number of packets in the sequence (e.g., msg_pkts_c_0). These sequence features correspond to half of the 24 payload features. The other payload features correspond to the total byte size of the encrypted payload (and its split in sent and received bytes); the total number of packets (and its split in sent and received packets); the size of the larger sequence in each direction; the maximum number of packets in a sequence in each direction; the ratio of packets sent over packets received; and the ratio of bytes sent over bytes received.

In conclusion, payload features identify TLS flows with similar content, despite domain and IP address polymorphism. We have also experimented with timing features, but have found them too sensitive to the network setup (e.g., server location, congestion) and thus we do not use them.

**Resumed sessions.** TLS resumption allows to quickly re-establish a prior TLS session using a shorter handshake [39]. The server encapsulates the session state into a ticket sent to the client. Later, the client can resume the previous session
by sending the corresponding ticket to the server. The shorter handshake does not include client or server certificates. To avoid leaving the certificate features empty (which may make resumed sessions look alike), feature extraction tracks session tickets sent from servers. When a TLS session is resumed, it uses the ticket sent by the client to identify the original TLS session (containing the same ticket in the opposite direction) and extracts the missing certificate features from the original session. If the original session cannot be identified, the fake resumption client feature is set to indicate that it may not be a real resumed session. Fake resumptions are used to avoid confusing middleboxes that do not support TLS 1.3 [24]. We also observe them used by Ultrasurf, an Internet censorship circumvention tool, which establishes TLS 1.2 flows without certificates.

**TLS 1.3.** Most features presented so far are available up to TLS 1.2. However, TLS 1.3 changes the protocol to reduce the information available in the TLS handshake. In particular, some fields become encrypted and other fields have fewer values to choose from. These changes are captured in the TLS 1.3 columns in Tables 1–4. In particular, client features such as the list of ciphers, elliptic curves, and point formats provide less information in TLS 1.3, as many values have been removed for increased protection, e.g., against downgrade attacks. However, as long as clients still support TLS 1.2, we expect the removal of those values to happen slowly over time. Furthermore, certificates are encrypted so their features cannot be extracted directly from the network trace. On the other hand, payload features are not affected. Despite these changes, our approach is able to produce accurate TLS 1.3 clusters.

### 3.2 Filtering

Sandbox traces may include benign traffic from different sources. One source is background traffic generated by the OS and other benign programs installed in the virtual machine. Another source are benign samples executed in the sandbox. Yet another source are flows to benign services performed by malicious samples such as those to test Internet connectivity. Some of that benign traffic may use TLS. To identify benign traffic in the network traces we use the Tranco list of the top 1M popular domains [2, 30]. Removing benign TLS flows is important to avoid generating clusters of benign traffic and for scalability. We also filter vanilla Tor traffic used by some malware samples, which we identify using a previously proposed fingerprint [32]. Note that for better scalability, flows without application data in either direction were already removed prior to feature extraction. Of course, any filtering can be incomplete, e.g., some unpopular benign domains could remain. An advantage of an unsupervised model is that any remaining benign traffic would produce its own cluster. Once that benign traffic is identified, the cluster can be removed, without requiring a retraining of the whole model, which would be needed by supervised approaches.

### 3.3 Clustering

The goal of the clustering is to group together similar feature vectors that correspond to the same type of malicious TLS traffic. Each cluster comprises of feature vectors generated by the same or different samples. Feature vectors from the same sample may end up in different clusters if the sample produces different types of communication such as C&C communication or communication with an update server. When a cluster contains TLS flows from different samples, those samples should belong to the same malware family. However, samples from the same family could end up in different clusters, e.g., when a subset of samples of the family exhibit some type of traffic and a different subset of family samples exhibit different traffic.

We use a hierarchical density-based clustering algorithm based on HDBSCAN [17]. It does not require the number of clusters to be specified, recognizes clusters of arbitrary shape and variable density, scales to large datasets, and allows
Unsupervised Detection and Clustering of Malicious TLS Flows

working with any kind of data by defining arbitrary distance functions. It distinguishes between clusters and noise, i.e., scattered data points that shouldn’t be considered part of any cluster. It has three hyper-parameters: the number of elements that should be close to a central one to define a dense zone ($m_{pts}$), the minimum cluster size ($m_{c}$), and a parameter ($m$) that tunes the density of linkage in the data structure it uses for neighbor search. Our evaluation searches for the best values for these parameters. The distance function used divides the features in two sets: numerical and categorical. First, it calculates the Euclidean distance of the numerical features, and multiplies it by the fraction of numerical over all features. Then, it computes the cosine distance between the categorical features, multiplying it by the fraction of categorical features. The final distance is the sum of these two values.

For each produced cluster, the domains in the SNI header and the leaf certificates of the flows in the cluster are collected, so that they can be added to blacklists. In addition, our approach tries to assign a human-interpretable label to each cluster by applying the AVClass [41] labeling tool to the samples that produced the flows in the cluster. We detail the labeling in Section 4.2. The cluster label corresponds to the family that has a majority in the cluster followed by a suffix to differentiate multiple clusters from the same family. For 31% of the clusters AVClass cannot obtain a family for any sample, but, in contrast to multi-class supervised classifiers, this does not affect our unsupervised detector, affecting only the availability of human readable family names to identify the clusters.

3.4 Detection

The unsupervised detector leverages the produced clustering model to decide whether a previously unseen flow belongs to a known cluster. Detection consists in searching for the closest node to a given flow, if any. Otherwise the flow is considered an outlier (i.e. benign). For this, we evaluate two different methods. The variable threshold method determines the density of a cluster as the largest distance of a node in that cluster from its closest neighbor; if the distance of the vector to a node in a cluster is below this threshold, the vector is considered to belong to that cluster. The fixed threshold method instead defines a fixed threshold for all clusters, so that the unseen element should be close enough to a cluster’s node to be part of it. Regardless of the method, if the given flow is assigned to a cluster, then it is labeled as malicious and the cluster identifier is output. If no cluster is close enough, the flow is labeled as benign. The detection threshold is the main parameter that controls false positives (FPs) and false negatives (FNs). If set very tight, then false positives are minimized, at the expense of increasing false negatives. When relaxed, false positives increase, while false negatives reduce. We evaluate this effect in Section 5.2.

4 DATASETS

To perform the clustering and build the detectors, we use 972K sandbox network traces provided to us by a security vendor, summarized in Table 5. To evaluate the produced detector, we use seven months of TLS traffic collected at the boundary of a research network, summarized in Table 6.
The table below shows the summary of collected research network traffic.

| Dataset       | Start       | End         | SRC | TLS Destinations | TLS Flows | TLS Version |
|---------------|-------------|-------------|-----|------------------|-----------|-------------|
|               |             |             |     | SNI IP Ports     | All       | L0          |
|               |             |             |     | All Filtered     | Resumed   | L2 L3 Other |
| Benign01      | 2019-10-08  | 2019-11-24  | 1.0K| 108.8K 85.3K 824 | 9.6M      | 0.9% 12.2% |
| Benign02      | 2019-12-10  | 2020-01-31  | 1.0K| 127.2K 100.3K 1.3K | 13.5M     | 0.8% 18.4% |
| Benign03      | 2020-02-01  | 2020-04-30  | 1.0K| 120.9K 98.4K 2.9K | 11.6M     | 0.9% 17.4% |
| Comp.Train    | 2020-10-23  | 2020-10-25  | 843 | 6,257 8,409 37  | 879.9k    | 0.7% 65.5% |
| Comp.Test     | 2020-10-28  | 2020-10-28  | 496 | 7,277 9,003 1.0k | 396.2k    | 0.7% 33.7% |

Table 6. Summary of collected research network traffic.

**Sandbox network traces.** We use two datasets (SB-small, SB-medium) of network traces obtained by a security vendor from the execution of suspicious samples in their sandbox. Each sample was run for one minute and sleeps introduced by the sample were skipped. The network trace contains all the traffic produced by the sample. Each sample has a single network trace. All traces contain TLS flows because that was the selection criteria used by the security vendor to share executions with us.

The union of the SB-small and SB-medium datasets produces the SB-all dataset. SB-all contains before filtering 12.9M flows on 527 destination ports, with the top three being 443/tcp (93.6%), 9001/tcp (2.67%), and 80/tcp (1.87%). Of the 12.9M TLS flows, 24.5% have a payload and 8.2% (1M) remain after filtering and are used in the clustering. We explain the reasons for this significant drop in Section 4.1. Those 1M TLS flows are almost exclusively for 443/tcp (99.8%) and are originated by 28% of the 972K samples. Of all samples, 9% exclusively communicate through TLS (excluding DNS and DHCP) while 91% use HTTP in addition to TLS. Thus, HTTP traffic could not be used for detecting 9% of the samples, even if user privacy was not a concern. We also observe three times more effective second-level domains (e2LDs) contacted through TLS compared to HTTP. 6% of the e2LDs are contacted both via HTTP and HTTPS, likely due to HTTP redirections towards HTTPS URLs.

**Research network traffic.** To evaluate false positives (FPs), we use logs of TLS flows collected at the boundary of a research network. Since no infections were detected in this network during the monitoring period we assume that the traffic is benign. For privacy reasons, the logs consist exclusively of TLS flows. The traffic is split into five datasets, summarized in Table 6. The first three comprise over seven months of traffic originated by 1,216 source IP addresses that produce 34M TLS flows. For the comparison with Joy [3], we collected two additional short captures, where we run Joy in parallel with our TLS log collection.

### 4.1 TLS Versions

There exist two significant differences between the SB-all sandbox traffic and the benign traffic from the research network. First, in SB-all only 24% of the TLS flows exchanged any application data. This is in stark contrast with 96% of the research network flows having application data. Second, 93% of the sandbox flows after filtering use TLS 1.0, 5.6% TLS 1.2 and less than 1% use TLS 1.3. This TLS 1.0 dominance is in stark contrast with the traffic from the research network where 80-86% of the flows after filtering use TLS 1.2, 12%-18% TLS 1.3, and less than 1% TLS 1.0. These differences cannot be due to the different dataset time frames as SB-medium and Benign01 partially overlap in the second half of 2019.

We believe both differences are rooted in the sandbox using almost exclusively Windows 7 virtual machines, which we have verified by applying the p0f passive fingerprinting tool on the network traces [4]. Windows 7 system libraries by default use TLS 1.0. TLS 1.1 and 1.2 are supported, but have to be manually enabled by the user [31]. We believe the two differences are caused by the majority of the malware using the default Windows TLS functionality, rather than a
cryptographic library statically linked in the executable. If the malware was using a statically linked cryptographic library, then, in 2017-2018, the default would be to use TLS 1.2. To use TLS 1.0, the malware developers would have to configure the used cryptographic library to specifically use TLS 1.0, which seems unlikely as this happens for samples from many families. The 6.5% of flows using TLS 1.2 and 1.3 likely correspond to malware using a statically linked TLS library or invoking the default browser in the sandbox to open a webpage.

The low fraction of TLS flows with application data is also likely due to the use of the default TLS functionality in Windows 7. The malware tries to connect to the servers using TLS 1.0, but many servers no longer support TLS 1.0, or the offered ciphersuites, and reject it. Note that the PCI Council suggested that organizations migrate from TLS 1.0 to TLS 1.1 or higher before June 30, 2018 [1]. This conclusion is supported by 37% of the TLS flows having a protocol_version alert, i.e., no TLS version can be agreed, and another 16% a handshake_failure alert, i.e., no ciphersuite can be agreed.

This analysis highlights the impact sandbox configuration can have on the collected data. Configuring the sandbox with old software may be beneficial to observe some behaviors like exploitation, but it can negatively impact other aspects such as TLS behavior. Running the sample on multiple OSes is arguably the best alternative, but it impacts scalability. Note that we do not control the sandbox and thus cannot configure it with newer OSes. This is a common scenario where data collection and analysis are performed by different teams. The main impact of the sandbox in our work is that flows with no application data are filtered, and eventually some network traces may be removed because they do not contain any flows with application data. Thanks to the large size of our dataset, even after filtering, we are still left with 1M TLS flows from 272K malicious samples. We do not think other selection biases are introduced as the TLS version has little influence in the clustering results according to the feature analysis process.

**TLS 1.3.** Since its release on August 2018 TLS 1.3 has seen fast adoption [28, 29]. Holtz et al. measured that by April 2019, it was used in 4.6% of TLS flows [28]. In our research network, one year later we observe 17.4% TLS 1.3 flows, nearly a fourfold increase. In the sandbox dataset, after filtering a modest 0.9% flows from 6.8K samples use TLS 1.3. This shows that a minority of malware authors try to keep their TLS traffic as secure as possible, avoiding the default TLS versions offered by the OS and using instead a statically linked cryptographic library they can customize. Most TLS 1.3 flows belong to three malware families: sofacy, an alias for the Fancy Bear (APT28) Russian cyber espionage group, lockyc, an imitator of the locky ransomware, and razy that steals cryptocurrency wallets [40]. The main impact of TLS 1.3 is that certificates are not observable. Additionally, the SNI can be transmitted encrypted by using new extensions. We also expected a reduced number of ciphersuites, but due to backwards compatibility we observe 14–78 ciphersuites being offered, much higher than the five standard TLS 1.3 ciphersuites. Despite the reduced feature set, our evaluation shows our approach successfully handles TLS 1.3.

### 4.2 Family Labeling

We query the hashes of all 972K sandbox samples to VirusTotal (VT) to collect their AV labels. Among those, 64% (623K) were known to VT. We feed the VT reports to the AVClass malware labeling tool [41]. AVClass outputs the most likely family name for each sample and also classifies it as malware or PUP based on the presence of PUP-related keywords in the AV labels (e.g., adware, unwanted). Overall, AVClass labels 59% (574K) of the samples. For the remaining samples no family was identified because their labels were generic. The 272K samples in the filtered SB-all dataset are grouped in 738 families, 545 malware and 193 PUP. For the interested reader, Table 14 in the Appendix shows the top 20 families.
Table 7. Manually generated ground truth.

| Family   | Total flows | Samples | Clusters |
|----------|-------------|---------|----------|
| clipbanker | 10,183      | 9,718   | 3        |
| shiz     | 10,105      | 9,250   | 4        |
| upatre   | 20,352      | 8,738   | 3        |
| bublik   | 140         | 57      | 5        |
| —        | 185         | 170     | 12       |
| ekstak   | 20          | 20      | 1        |
| miancha  | 9           | 9       | 1        |
| Total    | 40,994      | 27,962  | 29       |

Table 8. Clustering results on the ground truth. “Singl.” refers to singleton clusters (i.e., only one element).

| ID   | Features | Param. | ZS | Clusters | All | Singl. | Min | Max | Med. | Mean | PSTD | Prec. | Recall | F1   | Time |
|------|----------|--------|----|----------|-----|--------|-----|-----|------|------|------|-------|-------|------|------|
| FD1  | all      | default | ✓  | 27       | 0   | 2      | 9.978 | 65  | 1,518.3 | 3,121.6 | 0.993 | 0.872 | 0.928 | 18.0 |
| FD2  | no-client | default | ✓  | 25       | 0   | 2      | 9.990 | 65  | 1,639.8 | 3,257.3 | 0.992 | 0.877 | 0.931 | 16.9 |
| FD3  | no-server | default | ✓  | 10       | 0   | 21     | 20,213 | 354 | 4,099.4 | 6,274.6 | 0.747 | 0.905 | 0.819 | 16.6 |
| FD4  | no-cert   | default | ✓  | 27       | 0   | 2      | 10,003 | 26  | 1,518.3 | 3,503.6 | 0.986 | 0.990 | 0.993 | 13.6 |
| FD5  | no-payload | default | ✓  | 9        | 0   | 51     | 10,290 | 4,971 | 4,554.9 | 6,196.0 | 0.982 | 0.855 | 0.914 | 13.1 |
| FD6  | payload   | default | ✓  | 20       | 0   | 4      | 10,008 | 78  | 2,049.7 | 3,940.1 | 0.994 | 0.990 | 0.992 | 10.6 |
| FD7  | prior     | default | ✓  | 24       | 1   | 1      | 10,065 | 51  | 1,708.1 | 3,575.9 | 0.989 | 0.958 | 0.973 | 19.2 |
| FD8  | no-cert   | default | ✓  | 27       | 0   | 2      | 9,991  | 21  | 1,518.3 | 3,467.4 | 0.995 | 0.982 | 0.988 | 12.8 |
| FD9  | no-vert   | best    | ✓  | 27       | 0   | 2      | 10,003 | 26  | 1,518.3 | 3,503.6 | 0.996 | 0.990 | 0.993 | 13.6 |

To establish the malware family responsible for a cluster, we apply a majority vote on the AVClass labels of the samples in the cluster. However, for 35% of clusters, AVClass does not assign a family to any of the samples in the cluster (i.e., they only have generic labels), and thus the cluster cannot be labeled. Note that, in contrast to multi-class supervised classifiers, our unsupervised detector does not use family labels and thus can still detect flows for the 41% of samples and 35% of clusters that AVClass cannot label. In a detection, even when the cluster to which the detected flow belongs does not have an associated family name, it still provides important contextual information to the analysts by capturing other malicious samples that generate similar traffic.

4.3 Ground Truth

To evaluate the clustering results, we use a manually labeled subset of flows from SB-all, summarized in Table 7. AVClass results were used to randomly select samples from four of the largest families (clipbanker, upatre, shiz, bublik), a couple of small families (ekstak, miancha), and a variety of samples that AVClass cannot classify. Note that the AVClass family is not used as ground truth by itself, as it is not available for all samples, it may be incorrect for some samples, and does not separate different types of traffic from the same sample. Still, the family labels help ensure a variety of malware is included. Then, the benign traffic was filtered and features were extracted (e.g., certificates, domains in SNI headers, payload sequences). In addition, additional information was obtained that is not available to our detector such as VT reports that contain file properties and behavioral information, other features in the network traces not used by our approach (e.g., non-TLS traffic, destination IP addresses), and the AVClass family. By examining static, dynamic, and shared indicators in the reports and the network traffic, 29 clusters were identified.

5 EVALUATION

This section first presents the clustering results in Section 5.1 and then the detection results in Section 5.2.
5.1 Clustering Results

We leverage the ground truth to assess the clustering accuracy along three dimensions: features, clustering algorithm parameters, and z-score normalization for numerical features. To evaluate clustering accuracy we use precision, recall, and F1 score, common metrics for evaluating malware clustering results [11]. These metrics do not require or use cluster labels. They measure structural similarity between the obtained clustering and the ground truth clustering.

Table 8 summarizes the results obtained for 9 clustering configurations. First, we evaluate how different sets of features affect the results, using default parameters for the clustering and z-score normalization. We evaluate 7 sets of features. FD1 corresponds to using all features and acts as a baseline. The other feature sets correspond to an ablation study where we remove some features and measure how much the accuracy metrics are reduced with respect to the FD1 baseline. To evaluate the impact of each feature category, we build four feature sets (FD2–FD5), each excluding the features in one feature category (e.g., excluding client features in FD2). To evaluate the impact of payload features, we exclude features from the other three categories (client, server, certificate) in FD6. To evaluate the impact of our novel features, we exclude them in FD7, leaving only those already present in prior works. This search shows that server and payload features provide most information (largest drop when excluded) and client features also provide some information. However, certificate features are not useful (excluding them achieves best results) because they make the clustering split true clusters into subclusters due to the prevalence of certificate polymorphism and certificates from free CAs. The only useful information in free certificates is the domain name, which often overlaps the SNI feature. In addition, some CDNs like CloudFlare are abused by multiple families and the similarity of their certificates does not capture a real relationship. Based on these results, when exploring the other dimensions, we exclude the certificate features. The results from FD7 show that the new features proposed in this work increase the clustering accuracy raising the F1 score to 0.993, compared to 0.973 when using only the features proposed by prior work. Next, we evaluate the z-score normalization of the numerical features observing that normalization improves results. Finally, we perform another search to optimize the clustering hyper-parameters. The table does not show every parameter value configuration evaluated. It only shows the results with the best parameter configuration, which turns out to be the default parameters. The best clustering is FD9, which does not use certificate features, applies z-score normalization for numerical features, and uses hyper-parameters $mpts = 2$, $mcs = 2$, and $m = 10$. It achieves a precision of 0.996, a recall of 0.990, and a F1 score of 0.993.

**SB-All clusters.** Table 9 shows the clustering results on the 1M flows in SB-all using the best clustering (FD9). It produces 18,569 clusters of which 49% contain multiple flows and the rest are singletons. 36% of the clusters contain flows from multiple samples, 12% more than one server leaf certificate, and 3% more than one SNI. These results show that the clustering is able to group multiple samples that belong to the same family in the same cluster, despite domain and certificate polymorphism that malware authors may apply to avoid blacklists. We also observe that 31% (5,847) of the clusters (2,076 non-singleton clusters) only contain samples without an AVClass family label. Samples in those families could not be detected using supervised multi-class classifiers since no labels exist for training their model.
We manually analyze the clusters and report below some observations and example clusters. The largest cluster has 335,026 flows from the *clipbanker* family. There are 1,118 clusters without domain information, i.e., all flows lack an SNI header. One such cluster has 8 flows, each from a different sample. The flows connect to three servers (i.e., destination IP addresses) that use two certificates, one for ".zohoassist.com" and the other for ".zoho.com". There are 8 content sequences, all with RRPs with similar sizes. AVClass fails to provide a family label for all eight samples. This is an example of the clustering being able to group multiple samples despite the absence of domain information and the malware using multiple certificates. It is also an example of a cluster where AVClass fails to label samples and supervised multi-class classifiers do not work.

A total of 50 clusters (33 non-singletons) have TLS 1.3 flows, which lack certificates, and may also lack a SNI header, making them challenging to detect and label. Of the 33 non-singleton clusters, 30 contain only TLS 1.3 flows and three contain multiple TLS versions. Further examination shows that these 33 clusters likely belong to two families. According to AVClass, four TLS 1.3 clusters correspond to the *sofacy* family. Each sample of this family produces a single TLS flow to domains huikin.host or w.huikin.host, both hosted at IP address 18.197.147.148, but the clustering splits the traffic into subclusters with different encrypted payload sequences. Of the 3,418 samples in these clusters, 37 have no AVClass family, but still are correctly clustered with their family peers. For the other 29 non-singleton TLS 1.3 clusters, we observe that all flows lack a SNI header, but go to the same destination IP address 3.123.117.231. Note that the destination IP address is not a feature in our clustering. This indicates that the grouping is correct although multiple clusters are obtained based on differences on the encrypted payload. In the future, we plan to evaluate the destination IP address as a feature, which we originally thought was problematic due to IP reuse. Many samples in these clusters have an AVClass family label, but those labels correspond to 17 families, so it is not possible to identify the correct family. This highlights how our clustering can group samples not only with missing labels, but also with conflicting ones, which would be problematic for supervised approaches.

We observe multiple families abusing free certificates such as Let’s Encrypt and Tencent Cloud’s TrustAsia certificates. One such cluster consists of 12 flows, each from a different sample. It contains three domains: atendimentostore-al.com, atendimentostore-ac.com, and buricamiudos-al.com. The similarity between the domain names indicates that the cluster is correct. Each domain resolves to a different server and has its own Let’s Encrypt certificate. All samples have generic detection labels, so AVClass does not output a family for any of them. The payload consists of four content sequences, all of them with two RRPs. The first RRP has a 160 bytes request and a 7088–7280 bytes response. The second has a request 96–112 bytes request and a 5.18MB–5.38MB response, potentially corresponding to a downloaded file. The clustering is able to group the 12 samples despite the use of different domains and certificates.

We also observe CloudFlare being abused by many families. One such cluster consists of five flows from three samples. Each flow is for a different domain and goes to a different CloudFlare server using different CloudFlare-issued certificates. The similarity in this case comes from the client and payload features. Overall, we observe that the clustering is able to split different families abusing CloudFlare infrastructure into their own clusters.

### 5.2 Detection Results

This section evaluates our unsupervised detector. First, we select the best configuration. Then, we measure the false detection rate (FDR) of the selected configuration using benign traffic from the research network. Finally, we evaluate false negatives (FNs).
Unsupervised Detection and Clustering of Malicious TLS Flows

Table 10. Comparison of unsupervised detector configurations on 95K flows from one day of benign traffic.

| Model | Thres. sel. | Thres. | MCS | FDR   | Alarms |
|-------|-------------|--------|-----|-------|--------|
| FD9   | var         | -      | -   | 1.8%  | 1,698  |
| FD9   | var         | -      | 50  | 0.11% | 109    |
| FD9   | fixed       | 0.20   | -   | 0.4%  | 389    |
| FD9   | fixed       | 0.10   | -   | 0.08% | 73     |
| FD9   | fixed       | 0.05   | -   | 0.002%| 2      |

Unsupervised detector configuration. For selecting the best unsupervised detector configuration, we examine which threshold selection method produces a lower FDR with the best clustering configuration (FD9), and whether removing small clusters with few flows can significantly improve the FDR. Table 10 captures the results of applying each detector configuration on 95K flows from one day of benign traffic. We first evaluate the variable threshold selection method. We compare results when keeping and removing clusters with less than 50 flows. Removing them reduces the FDR from 1.8% to 0.11%, but at the cost of not being able to detect traffic that matches those clusters. Then, we evaluate the fixed threshold selection method using different threshold values. We start with threshold 0.2 because the vast majority of false alarms occur at that or greater distances in the variable method. Then, we halve that threshold a couple of times to observe the effects. The results show that the fixed threshold achieves the lowest FDR and that smaller thresholds make the detection stricter and thus reduce FPs. In the limit, a threshold of zero would make the detector flag only flows with identical feature vectors to those in the cluster. So, we select 0.05 as the best threshold as it still detects small modifications, as shown later in the FN evaluation.

FDR. To determine the real FDR of the unsupervised detector, we first apply the selected configuration (0.05 fixed threshold) on one week of traffic from the Benign02 dataset, observing a total of 119 alarms, for a FDR of 0.031%. To evaluate degradation over time, we then apply the detector again on almost four months of benign traffic (111 days corresponding to union of the Benign02 and Benign03 datasets in Table 6), observing 708 alarms produced by 5 clusters, corresponding to a measured FDR of 0.032%. Thus, the FDR remains stable even after several months.

False negative evaluation. We also perform an experiment to validate that the chosen configuration of the unsupervised detector is not too strict and still detects variations of flows in the clusters. For this experiment, we apply the clustering, using the same configuration as FD9, on 90% randomly sampled flows of each cluster in the ground truth, reserving the other 10% as testing data never seen by the model. We build an unsupervised detector using the previously selected configuration of a fixed 0.05 threshold. We use the produced model to make predictions on the 10% unseen flows. In this scenario, true positives (TPs) are flows assigned to a cluster by a closest neighbor that shares the same manually assigned cluster in the ground truth. If a flow is not assigned to any cluster (no nearest neighbor) it is a FN, as we know it is malicious. When the nearest neighbor of the flow is in a different ground truth cluster than the evaluated flow, we consider it a FP since the output cluster is wrong. We perform a 10-fold cross-validation, sampling different testing data each time. Five runs have 100% TPs, and there are a total of 12 FNs on all 10 runs, for a FN rate of 0.029%. No FPs are observed. This experiment confirms that the unsupervised detector is capable of detecting previously unseen flows with low FNs, and that the selected clustering configuration is not too strict.
5.3 Comparison with Prior Work

This section compares our approach with two state-of-the-art publicly available detection tools: the Joy [3] binary supervised classifier and Kitsune [33], an auto-encoder (AE) based anomaly detector. Both tools can detect malicious traffic, but do not classify the detected traffic into families. Thus, the comparison focuses on the detection goal.

**Joy.** We compare our unsupervised detector with Joy [3], the publicly available implementation of the binary supervised detector from Blake and McGrew [5, 6]. We focus the comparison on the malicious flow detection since the implementation of the multi-class supervised classifier by the same authors [8] is not publicly available. One limitation of Joy is that it considers all network flows in the input network traces as malicious. However, as shown in Section 4, much traffic in sandbox traces is benign. To understand the impact of this choice by Joy, as well as to make a fair comparison between Joy and our unsupervised detector, we build three different Joy logistic regression models. The joy-polluted model applies Joy without any modifications. Thus, all flows in the sandbox network traces are considered malicious. The joy-unpolluted-exc model excludes from the training benign flows identified by our filtering step. The joy-unpolluted-inc model labels the benign flows identified by our filtering step as negative. This last model explicitly tells Joy that the sandbox traces indeed contain benign traffic. Finally, unsupervised corresponds to our unsupervised detector using filtering and the best configuration identified in Section 5.2.

For the training, we use 90% of the network traces from the SB-small dataset as positive class (minus benign flows for models with filtering) and three days of traffic from the research network as the negative class. For the research network traffic, we run Joy in parallel with the TLS log collection since Joy requires network traces as input and cannot process directly our TLS logs. For the testing, we use the remaining 10% traces of SB-small and an extra day of traffic from the research network. Two small differences in feature extraction between Joy and our approach are that Joy is not able to process a portion of SSLv2 flows and that it classifies any flow, even those that do not complete the TLS handshake. To make the comparison as fair as possible, we exclude both cases so that the comparison happens on the same flows.

Table 11 summarizes the comparison. Using Joy without modifications (joy-polluted) produces a very large number of FPs and overall a low 0.22 F1-score. This indicates that Joy is learning to differentiate sandbox traffic (mostly TLS 1.0) from traffic from the research network (mostly TLS 1.2 and 1.3). This is confirmed by the difference between joy-unpolluted-exc and joy-unpolluted-inc. When, during training, Joy is told that benign traffic in the sandbox is not necessarily malicious (joy-unpolluted-inc), the accuracy greatly improves as many FPs are removed pushing the F1 score from 0.22 up to 0.82. However, FNs increase significantly because Joy is forced to relax its model that now has to account for some sandbox traffic not being malicious. In contrast, our unsupervised approach captures different types of traffic from a family in their own clusters, producing a tighter model. Our unsupervised detector outperforms all Joy models, achieving a F1 score of 0.91, compared to 0.82 for Joy’s best model.
Kitsune. We also compare our approach with Kitsune [33], a state-of-the-art AE-based anomaly detector. Kitsune’s approach does not require malicious traffic during training. It builds an ensemble of neural network AEs from input benign traffic and derives a detection threshold by examining the maximum root-mean-square error (RMSE) observed in the input benign traffic. Given test traffic, Kitsune computes the RMSE value. If the value is larger than the inferred threshold, then the traffic is considered anomalous and an intrusion is flagged. Similar to Joy, Kitsune takes as input network traces in PCAP format and thus we cannot use our TLS logs from the research network for this evaluation. Unlike with Joy, we could not run Kitsune in parallel with our TLS log collection, since our collection had been discontinued by the time we performed this evaluation. To evaluate both tools on the same inputs, we leverage the sandbox traces. We first filter out all non-TLS traffic from the traces by selecting the packets to/from port tcp/443, and then separate benign traffic from malicious traffic using our filtering (Section 3.2).

At first, we tried to produce a Kitsune model using all the benign traffic in the SB-small dataset, but after one week running, the model had not finished and we stopped it. Kitsune was designed to run in low-resource network devices and its design minimizes the amount of memory used. However, it runs on a single thread making runtime the bottleneck. Thus, its model training does not scale to large amounts of traffic. Because of this, we use a small set of ground truth traces to train and test both tools. More concretely, we use 4,125 ground truth traces to train each model. Then, we test both tools on the same traffic that was not part of the training of neither of the two approaches. In particular, we use the benign traffic along with the malicious traffic of 5,156 traces to build the testing dataset. We use the Kitsune configuration suggested by its authors [33]: the detection threshold is the maximum RMSE value seen during the training phase and the maximum number of features allowed per AE is 10.

Another key difference is that Kitsune operates at the packet level, while our approach operates at the flow level. To compare the results of both approaches, we first create a mapping from each packet to the flow it belongs. When Kitsune flags a packet as an intrusion, we use the mapping to identify the flow to which the packet belongs and mark the whole flow as malicious. Flows where no packet has been flagged as an intrusion are considered benign. To build the packet-to-flow mapping, we produce a flow identifier for each packet using a set of six values: hash of the trace where the packet appears, source IP, source port, destination IP, destination port, and protocol. To assign the same identifier to both directions of the flow we first sort the six values lexicographically and then hash them to produce the flow identifier. After applying Kitsune’s feature extractor to the ground truth traces, we add two additional fields to the Kitsune vectors: the flow identifier and the SNI field for the flow. The SNI is used by the filtering to determine if a flow is benign or malicious. We also modify the feature extraction of our approach to include the flow identifier.

Table 12 shows the results of both models. Kitsune achieved a precision of 0.54, a recall of 0.65, and an F1 of 0.59. On the same dataset, our approach achieves a precision of 0.99 and a recall of 0.99, for an F1 of 0.99. The low precision of Kitsune is due to a large number of FPs (13,137). False positives are a common problem with anomaly detectors since any significant deviation from the profiled benign traffic is flagged as an intrusion, while the benign testing traffic may contain natural changes that are not related to malicious behavior. Kitsune also introduces 8,323 FNs, likely due to malicious traffic with similar packet sizes and inter-arrival times to benign traffic, which cannot be easily distinguished.

| Model                | TP    | FP    | TN    | FN    | Prec. | Recall | F1   |
|----------------------|-------|-------|-------|-------|-------|--------|------|
| kitsune (flow-level)| 15,681| 13,137| 3,527 | 8,323 | 0.54  | 0.65   | 0.59 |
| unsupervised         | 30,297| 1     | 22,317| 94    | 0.99  | 0.99   | 0.99 |

Table 12. Comparison with Kitsune on ground truth TLS traffic.
using the benign traffic model. Our approach can ameliorate that problem by using three additional categories of TLS-specific features (client, server, certificate).

6 RELATED WORK

Table 13 summarizes the most related work. It includes three works that specifically explore the detection and classification of TLS flows [5, 6, 8] and two general anomaly-based intrusion detection systems that do not specifically target TLS flows, but can be applied to them as they do not require access to unencrypted payload data [12, 33]. The bottom row captures the approach presented in this paper. The table characterizes each work according to its goal, approach, and features used. The goal can be detecting malicious flows, as well as classifying those malicious flows by originating family. The approach captures whether the work uses supervised ML models, unsupervised clustering, and anomaly detection based on auto-encoders. It also captures the approach granularity, i.e., whether it works at the flow (F) or packet (P) level. The features used can be TLS-specific (client, server, certificate), specific to other protocols such as DNS and HTTP, or examine the payload and inter-arrival times of packets in a flow in a protocol-agnostic manner.

Next, we compare these 5 works with our approach.

Anderson et al. [8] first propose a binary (logistic regression) supervised detector using features from TLS flows. In addition, they train a logistic regression multi-class classifier for 18 malware families, but fail to generate a classifier for 73% of their input samples for which they cannot obtain a family label. We compare our unsupervised detector with the public implementation of their binary supervised classifier. Their implementation assumes all TLS flows in the input network traces are malicious leading to a very low F1 score. After fixing that issue, the F1 score raises to 0.82, compared to 0.91 for our unsupervised detector on the same data. Compared to their multi-class classifier, our unsupervised detector does not require family labels and detects flows from samples without a family, while still assigning a family to the detected flows if available.

In follow-up work, Anderson and McGrew [5] add to their TLS detector features from DNS responses and HTTP flows. In contrast, our approach operates solely on TLS flows and does not require plain-text protocols, increasing user privacy. Furthermore, our unsupervised approach can assign detected flows to their family clusters, and handles samples that do not use HTTP or connect to their C&C servers using IP addresses.

Anderson and McGrew [6] also evaluate six supervised learning classifiers for detecting malicious TLS flows despite inaccurate ground truth and non-stationarity of network data. In their experiments, random forest performed best, but
the quality of its results decreased significantly over time. In comparison, the FDR of our unsupervised detector does not degrade over a four-month period.

Mirsky et al. [33] present Kitsune, an anomaly detection approach that takes as input benign traffic and uses an ensemble of auto-encoders to detect anomalies that indicate intrusions. Using an anomaly-based approach removes the need for a malicious training dataset, but prevents it from addressing the classification goal. Kitsune uses packet sizes and inter-arrival times as features, so it can be applied to any protocol including TLS flows. It is designed to be efficient, so that it can run on network devices that have limited resources (e.g., a Raspberry PI). We compare our approach with the publicly available implementation of Kitsune showing that our approach significantly improves the accuracy.

Bovenzi et al. [12] present H2ID, an intrusion detection system that addresses both the detection and classification goals. Similar to Kitsune, it first uses an auto-encoder approach to detect anomalies as intrusions and uses payload size and inter-arrival timing as features, so it can be applied to different protocols, including TLS flows. But, it adds a second phase where it applies a supervised ML model to classify the detected anomalies into known attacks, or unknown if they do not match the model. In contrast, our approach does not require a labeled training dataset and can cluster similar malicious flows even when their family is unknown.

**TLS fingerprints.** A large body of work has built TLS fingerprints to identify the applications that initiate TLS flows. Fingerprints have been used to analyze several aspects of the TLS ecosystem, including the impact of HTTPS interception by middleboxes and antivirus products [22], the evolution of TLS clients over time [7, 29], and the TLS implementations of popular censorship circumvention tools [23]. Prior works also build TLS fingerprints for detecting malware and PUP families [13, 38]. However, recent work shows that malware TLS fingerprints generate high FPs in real networks [7]. All these approaches build TLS fingerprints using solely features extracted from the Client Hello message such as TLS version, supported ciphersuites and extensions, and elliptic curves point formats. Van Ede et al. [43] proposed FlowPrint, a semi-supervised approach for fingerprinting mobile apps from their TLS traffic using also destination features such as the server certificate, IP address, and port. In comparison, our clustering also uses client and certificate features, but enhances the detection by further including server and encrypted payload features.

**Malware clustering.** There has been extensive work on malware clustering techniques using a variety of features such as system calls, system changes, and network traffic [10, 11, 14, 20, 27, 34, 36, 37]. Most similar to our approach are clustering approaches based on network traffic, which may build detection signatures [27, 34, 36] or unsupervised detectors [20] using the produced clusters. Some of these works propose generic payload features that capture message sizes [20, 36], but none of these works uses TLS-specific features. In future work, we would like to combine our TLS features with other network and behavioral features to build a malware family classifier for samples executed in a sandbox.

7 DISCUSSION

This section discusses limitations and avenues for improvement.

**Potential biases.** We identify two potential sources of bias in our methodology. First, we discard almost 64% of the sandbox TLS flows in our malware dataset because they try to use TLS 1.0, which was already deprecated by many servers at the time of the execution. This happens because most malware uses the Windows TLS functionality, and Windows 7, the sandbox OS version, uses by default TLS 1.0. Of the 9.3M discarded connections, 23% would have been anyway removed later by the filtering. Second, we filter out benign domains, which may result in excluding some malware families from our study. For example, click-fraud malware generates revenue by falsifying clicks on
pay-per-click campaigns and typically contacts numerous benign destinations. Other malware families may abuse benign content hosting services such as code repositories (e.g., Github and Bitbucket), document editors (e.g., Google Docs, Pastebin), cloud storage services (e.g., Dropbox, Google Drive), or even social media (e.g., Twitter). Despite excluding some malware families, our dataset still encompasses a large part of the malware ecosystem, containing 738 different families (see Section 4.2). A third bias could be introduced by our ground truth not being representative of the whole SB-all dataset. We try to ameliorate this by including multiple families, limiting the number of samples of each family, and including samples without a known family.

**Detection through other protocols.** Usage of TLS by malware keeps increasing, having more than doubled from 10% in 2016 [8] up to 23% in 2020 [25]. However, malware may still use unencrypted traffic or mix unencrypted and encrypted protocols, as illustrated by 91% of samples using plain HTTP in addition to TLS. Prior work suggested using unencrypted protocols such as HTTP and DNS to assist in the detection of TLS malware [5]. However, we already observe 9% of the samples using TLS, but not other unencrypted traffic beyond DNS; we expect this ratio to keep increasing over time. Moreover, samples not using (or encrypting) a TLS SNI header (the one case where DNS helps) could also connect to their C&C using IP addresses. Furthermore, a purely TLS-based detection improves user privacy, and technologies such as DNS over HTTPS could further hamper DNS utility. While detection via other protocols is still a possibility for a significant fraction of samples, that is not the case for all samples and the situation is likely to get worse.

8 CONCLUSION

Detecting malicious TLS traffic is an important, but challenging, problem. Binary supervised detectors are limited in that they try to distinguish any malicious TLS flow, regardless of the malware family producing it. This produces models that are too loose, introducing errors. In addition, they do not provide contextual information about the detected flows. Multi-class supervised classifiers produce tighter models for specific malware families, and can classify the detected flows. But, they require family labels to train the classifiers, which are not available for a large fraction of samples.

We have proposed a novel unsupervised approach for detecting and clustering malicious TLS flows. It first clusters similar malicious TLS flows without requiring family labels. Then, it builds an unsupervised detector that measures distance to the clusters to determine if a given flow is malicious (belongs to a cluster) or benign (no cluster is close enough). We have evaluated our approach using 972K traces from a commercial sandbox and 35M TLS flows from a research network. Our unsupervised detector achieves a F1 score of 0.91, compared to 0.82 for the state-of-the-art supervised detector, and a FDR of 0.032% over four months of traffic.

In future work, we plan to evaluate additional features such as the destination IP address and timing-related features. For example, the IP address we originally thought was problematic due to IP reuse, but our evaluation shows there are cases where it can be useful. Timing-related features have been used by prior work (e.g., [8, 12, 33]), but our examination found them too sensitive to the specific network setup, so we believe there is a need for a systematic evaluation on their usefulness. Furthermore, we would like to explore how to generalize our approach to handle other types of network traffic beyond TLS.

9 DATA AVAILABILITY STATEMENT

This work uses two data types: [MALWARE-TRACES] are network traces from likely malicious samples executed in a sandbox. [BENIGN-TRACES] are network traces from a research network containing traffic considered benign.
MALWARE-TRACES data used to support the findings of this study have not been made available because they come from a commercial sandbox and are considered proprietary data for the commercial service. BENIGN-TRACES data used to support the findings of this study have not been made available because they contain sensitive user data that cannot be made publicly available by the research institution.

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This submission is also available as an Arxiv preprint [26].

A APPENDIX

| Family       | Type    | SNI | IP  | TLS flows | Samples |
|--------------|---------|-----|-----|-----------|---------|
| clipbanker   | Malware | 7   | 10  | 319,185   | 88,680  |
| upatre       | Malware | 251 | 347 | 311,687   | 64,860  |
| shin         | Malware | 12  | 18  | 41,578    | 19,959  |
| zbot         | Malware | 120 | 116 | 46,437    | 5,502   |
| pcchist      | Malware | 1   | 1   | 4,713     | 4,653   |
| installmonster| PUP    | 61  | 75  | 4,537     | 4,163   |
| sofacy       | Malware | 1   | 1   | 3,381     | 3,381   |
| xetapp       | PUP     | 2   | 2   | 3,908     | 2,828   |
| oxypumper    | PUP     | 7   | 502 | 3,051     | 2,431   |
| bublik       | Malware | 36  | 33  | 30,741    | 2,240   |
| vkontaktejd  | PUP     | 2   | 12  | 2,060     | 1,599   |
| khalesi      | PUP     | 8   | 7   | 1,787     | 1,591   |
| playtech     | PUP     | 8   | 17  | 2,912     | 1,497   |
| multiplug    | PUP     | 2   | 2   | 9,223     | 1,055   |
| adposhel     | PUP     | 2   | 28  | 958       | 958     |
| rary         | Malware | 88  | 120 | 10,579    | 945     |
| lockyc       | Malware | 2   | 3   | 724       | 709     |
| noobyprotect | Malware | 12  | 22  | 1,133     | 632     |
| downloadassistant | PUP | 50  | 63  | 574       | 573     |
| defl         | Malware | 76  | 114 | 1,127     | 542     |

Table 14. Top 20 families by samples after filtering.

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### Table 15. Acronyms used in the paper.

| Acronym | Full name |
|---------|-----------|
| AE      | Auto-Encoder |
| ALPN   | Application Layer Protocol Negotiation TLS extension |
| API     | Application Programming Interface |
| APT28   | Fancy Bear Russian cyber espionage group |
| C&C     | Command-and-Control |
| CA      | Certification Authority |
| CDN     | Content Delivery Network |
| CT      | Certificate Transparency |
| DHCP    | Dynamic Host Configuration Protocol |
| DN      | Distinguished Name |
| DNS     | Domain Name System |
| eLD     | Effective Second-Level Domain |
| FDR     | False Detection Ratio |
| FN      | False Negative |
| FP      | False Positive |
| HDBSCAN | Hierarchical Density-Based Spatial Clustering of Applications with Noise |
| HTTP    | Hypertext Transfer Protocol |
| HTTPS   | Hypertext Transfer Protocol Secure |
| IP      | Internet Protocol |
| mcs     | minimum cluster size |
| MITM    | Man-in-the-Middle |
| ML      | Machine learning |
| OS      | Operating System |
| PUP     | Potentially Unwanted Programs |
| RMSE    | Root-mean-square Error |
| RRP     | Request-Response Pair |
| SB      | sandbox |
| SAN     | Subject Alternative Name TLS extension |
| SNI     | Server Name Indication TLS extension |
| SSL     | Secure Sockets Layer |
| TF-IDF  | Term-Frequency Inverse Document-Frequency |
| TCP     | Transmission Control Protocol |
| TLS     | Transport Layer Security protocol |
| TP      | True Positive |
| URI     | Uniform Resource Identifier |
| VT      | VirusTotal |

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Unsupervised Detection and Clustering of Malicious TLS Flows 23

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