Dos and Don'ts of Machine Learning in Computer Security

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Abstract

With the growing processing power of computing systems and the increasing availability of massive datasets, machine learning algorithms have led to major breakthroughs in many different areas. This development has influenced computer security, spawning a series of work on learning-based security systems, such as for malware detection, vulnerability discovery, and binary code analysis. Despite great potential, machine learning in security is prone to subtle pitfalls that undermine its performance and render learning-based systems potentially unsuitable for security tasks and practical deployment.

In this paper, we look at this problem with critical eyes. First, we identify common pitfalls in the design, implementation, and evaluation of learning-based security systems. We conduct a longitudinal study of 30 papers from top-tier security conferences within the past 10 years, confirming that these pitfalls are widespread in the current security literature. In an empirical analysis, we further demonstrate how individual pitfalls can lead to unrealistic performance and interpretations, obstructing the understanding of the security problem at hand. As a remedy, we derive a list of actionable recommendations to support researchers and our community in avoiding pitfalls, promoting a sound design, development, evaluation, and deployment of learning-based systems for computer security.

1 Introduction

No day goes by without reading machine learning success stories. The widespread access to specialized computational resources and large datasets, along with novel concepts and architectures for deep learning, have paved the way for machine learning breakthroughs in several areas, such as the translation of natural languages [13, 31, 120] and the recognition of image content [64, 77, 113]. This development has naturally influenced security research: although mostly confined to specific applications in the past [54, 55, 128], machine learning has now become one of the key enablers to studying

and addressing security-relevant problems at large in several application domains, including intrusion detection [43, 92], malware analysis [68, 86], vulnerability discovery [82, 138], and binary code analysis [42, 109, 136].

Machine learning, however, has no clairvoyant abilities and requires reasoning about statistical properties of data across a fairly delicate workflow: incorrect assumptions and experimental biases may cast doubts on this process to the extent that it becomes unclear whether we can trust scientific discoveries made using learning algorithms at all [57]. Attempts to identify such challenges and limitations in specific security domains, such as network intrusion detection, started two decades ago [11, 115, 121] and were extended more recently to other domains, such as malware analysis and website fingerprinting [3, 71, 101, 107]. Orthogonal to this line of work, however, we argue that there exist *generic pitfalls* related to machine learning that affect all security domains and have received little attention so far.

These pitfalls not only lead to over-optimistic results, but more importantly, affect the entire machine learning workflow, often invalidating assumptions, conclusions, and lessons learned. As a consequence, a false sense of achievement is felt that hinders the adoption of research advances in academia and industry. A sound scientific methodology is fundamental to support intuitions and draw conclusions. We argue that this need is especially relevant in security, where processes are often undermined by adversaries that actively aim to bypass analysis and break systems.

In this paper, we identify ten common—yet subtle—pitfalls that pose a threat to validity and may hinder interpretation of research results. To support this claim, we conduct a longitudinal study on a sample of 30 top-tier security papers from the past decade that rely on machine learning for tackling different problems. To our surprise, each paper suffers from at least three pitfalls; even worse, several pitfalls affect most of the papers, which shows how endemic and subtle the problem is. Although pitfalls are widespread, it is perhaps more important to understand the extent to which they undermine the validity of research. To this end, we

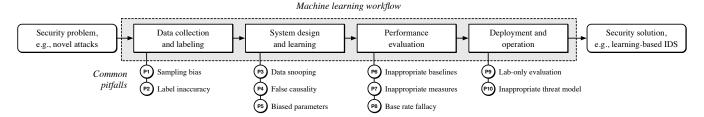


Figure 1: Common pitfalls of machine learning in computer security.

perform an impact analysis of these pitfalls in four different security fields. The findings support our premise echoing the broader concerns of the community.

In summary, we make the following contributions:

- 1. **Pitfall Identification.** We identify ten pitfalls as *don'ts* for machine learning in security that affect the entire workflow (§2), and analyze their prevalence through a longitudinal analysis of 30 representative top-tier security papers published in the past decade (§3).
- 2. **Impact Analysis.** In four different security domains, we experimentally analyze the extent to which such pitfalls introduce experimental bias, inflate results, and lead to misinterpretations, undermining the overall understanding of the problem at hand (§4).
- 3. **Recommendations.** As a constructive step forward, we propose a set of *dos* as actionable recommendations for researchers and practitioners towards the sound development and use of machine learning in security (§5).

Remark. This work should not be interpreted as a fingerpointing exercise. On the contrary, it is a reflective effort that shows how subtle pitfalls, affecting the authors' research also, have a negative impact on actual progress, and how we—as a community—can mitigate them adequately.

2 Pitfalls in Machine Learning

Despite its great success, machine learning is unfortunately prone to several pitfalls during practical application. Overlooking these issues may result in severe experimental bias or incorrect conclusions, especially in computer security. In this section, we present ten common pitfalls that occur frequently in security research. Although some of these pitfalls may seem obvious at first glance, they are rooted in subtle mistakes that are widespread in security research—even in papers presented at top conferences (see §3 and §4).

We group these pitfalls with respect to the stages of a typical machine learning workflow, as depicted in Figure 1. For each pitfall, we provide a short description and discuss its impact on the security domain. Moreover, a colored bar depicts the proportion of papers in our analysis that suffer from

the pitfall, with warmer colors indicating the presence of the pitfall (see Figure 3 for full details and legend).

2.1 Data Collection and Labeling

The design and development of learning-based systems typically starts with the acquisition of a representative dataset. As learning algorithms are supposed to automatically identify inherent patterns and relations from data, having a representative dataset is essential for obtaining accurate results. It is clear that conducting experiments using flawed data leads to the misestimation of an approach's capabilities. The following two pitfalls frequently induce such errors and thus require special attention when developing learning-based systems in computer security.

P1 – Sampling Bias. The collected data does not sufficiently represent the true data distribution of the underlying security problem [1, 30, 33].

Description. With a few rare exceptions, researchers develop their learning-based approaches without exact knowledge of the true underlying distribution of the input space. Instead, they need to rely on a dataset containing a fixed number of samples that aim to resemble the actual distribution. While it is inevitable that some bias exists in most cases, understanding the specific bias inherent to a particular problem is crucial to limit its impact in practice. No meaningful conclusions can be drawn from the training data, if it does not effectively represent the input space or even follows a different distribution.

Security implications. Sampling bias is highly relevant to security, as the acquisition of data is particularly challenging and often requires using multiple sources of varying quality. As an example, for the collection of suitable datasets for Android malware detection only a few public sources exist from which to obtain such data [6, 130]. As a result, it is common practice to combine data from different sources, which can introduce severe biases, as we demonstrate in §4.1. Similarly, in §4.4, we show that approaches for network intrusion detection are often evaluated using synthetic attacks that appear at a much higher frequency in the evaluation datasets than in realistic environments [88, 115].

P2 – Label Inaccuracy. The ground-truth labels required for classification tasks are inaccurate, unstable, or erroneous, affecting the overall performance of a learning-based system [84, 139].

Description. Many learning-based security systems are built for classification tasks. To train these systems, a ground-truth label is required for each observation. Unfortunately, the ground truth is rarely perfect and researchers must account for uncertainty and noise to prevent their models from suffering from inherent bias.

Security implications. For many relevant security problems, such as detecting network attacks or malware, proper labels are typically not available, resulting in a chicken-and-egg problem. As a remedy, researchers often revert to heuristics, such as using external sources that do not provide a reliable ground truth. For example, services like *VirusTotal* are commonly used for acquiring label information for malware. Additionally, changes in adversary behavior may alter the ratio between different classes over time [3, 91, 139], introducing another type of bias known as *label shift* [84]. A system that cannot adapt to these changes will experience performance decay once deployed.

2.2 System Design and Learning

Once enough data has been collected, a learning-based security system can be trained. This process ranges from data preprocessing to extracting meaningful features and building an effective learning model. At each of these steps it is possible to introduce defects or bias.

P3 – Data Snooping. A learning model is trained with data that is typically not available in practice. Data snooping can occur in many ways, some of which are very subtle and hard to identify [1].

Description. It is common practice to split collected data into separate training and test sets prior to generating a learning model. Although splitting the data seems straightforward, there are many subtle ways in which test data (or other background information that is not usually available) can affect the training process, leading to data snooping. While a detailed list of data snooping examples is provided in the appendix (see Table 6), we broadly distinguish between three types of data snooping: test, temporal, and selective snooping.

Test snooping occurs when the test set is used for experiments before the final evaluation. This includes preparatory work to identify useful features, parameters, and learning algorithms. Temporal snooping occurs if time dependencies within the data are ignored. This is a common pitfall, as the underlying distributions in many security-related problems are under continuous change [e.g. 85, 101]. Finally, selective

snooping describes the cleansing of data based on information not available in practice. An example is the removal of outliers based on statistics of the complete dataset (i.e., training and test) that are usually not available at training time.

Security implications. In security, data distributions are often non-stationary and continuously changing due to new attacks or technologies. Because of this, snooping on data from the future or from external data sources is a prevalent pitfall that leads to over-optimistic results. For instance, several researchers have identified temporal snooping in learning-based malware detection systems [e.g., 4, 8, 101]. In all these cases, the capabilities of the methods are overestimated due to mixing samples from past and present. Similarly, there are incidents of test and selective snooping in security research that lead to unintentionally biased results (see §3).

P4 – False Causality. Artifacts unrelated to the security problem create shortcut patterns for separating classes. Consequently, the learning model adapts to these artifacts instead of solving the actual task.

Description. Data can contain artifacts that may loosely correlate with the task to solve but are not actually related to it. Consider the example of a network intrusion detection system, where a large fraction of the attacks in the dataset originate from a certain network region. The model may learn to detect a specific IP range instead of generic attack patterns. Similarly, a detection system might pick up artifacts from synthetic attacks that are unrelated to malicious activity, as in the classic case of the "why six?" issue [121].

Security implications. Complex learning models with non-interpretable feature spaces are often at the core of security tasks. Difficulties in explaining models and results leads to false causality, which often remains an unidentified issue. As an example, §4.2 reports our analysis on a vulnerability discovery system indicating the presence of false causality. Similarly, §4.3 shows that learning-based approaches for source code authorship attribution rely on the identification of unused code fragments, instead of learning the semantically relevant programming patterns used by the developers.

P5 – Biased Parameter Selection. The final parameters of a learning-based method are not entirely fixed at training time. Instead, they indirectly depend on the test set.

Description. Throughout the learning procedure, it is common practice to generate different models by varying hyperparameters. The best-performing model is picked and its performance on the test set is presented. While this setup may appear sound, it can still suffer from bias. For example, misleading results may be produced by using uncalibrated metrics or by investigating the influence of hyperparameters on the test data.

Security implications. A security system whose parameters have not been fully calibrated at training time can perform very differently in a realistic setting. While the detection threshold for a network intrusion detection system may be chosen using a ROC curve obtained on the test set, it can be hard to select the same operational point in practice due the diversity of real-world traffic [115]. This may lead to decreased performance in comparison to the experimental setting. Note that this pitfall is related to data snooping (P3), but should be considered explicitly as it can easily lead to inflated results.

2.3 Performance Evaluation

The next stage in a typical machine-learning workflow is the evaluation of the system's performance. In the following, we show how different pitfalls can lead to unfair comparisons and biased results in the evaluation of such systems.

P6 – Inappropriate Baseline. The evaluation is conducted without, or with limited, baseline methods. As a result, it is impossible to demonstrate improvements against the state of the art and other security mechanisms.

Description. At the core of scientific progress lies the ability to show that a novel approach outperforms the state of the art, for a given metric of interest. When choosing baselines, it is important to remember that, despite great leaps forward in other fields, there exists no universal algorithm in machine learning that dominates all other approaches in general [132]. Consequently, providing only results for the proposed approach or comparing it only with closely related methods, does not give enough context to assess its impact. For example, shallow and deep learning models should be compared side by side, as they provide different advantages and disadvantages [1, 45]; Similarly, machine learning might not be the only strategy for solving a security problem [e.g., 8].

Security implications. An overly complex learning method does not only increase the chances of overfitting, but it also increases the runtime overhead, the attack surface, and the time and costs for deployment. In §4.2 and §4.4, we show two examples in which simple classifiers outperform state-of-the-art deep learning models for vulnerability and network intrusion detection tasks, respectively. Our results demonstrate that by picking appropriate baselines, we achieve a fair comparison to the state of the art and gain a better understanding of the security problem at hand.

P7 – Inappropriate Performance Measures. The chosen performance measures do not account for the constraints of the application scenario, such as imbalanced data or the need to keep a low false-positive rate.

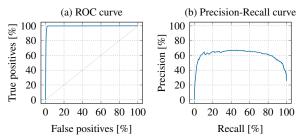


Figure 2: ROC and precision-recall curve as two performance measures for the same scores, created on an artificial dataset with an imbalanced class ratio. Only the precision-recall curve conveys the true performance.

Description. A wide range of performance measures are available and not all of them are suitable in the context of security. For example, when evaluating a detection system, it is insufficient to report just a single performance value, such as the accuracy, because true-positive and false-positive decisions are not observable. However, even more advanced measures, such as ROC curves, may obscure experimental results. Figure 2 shows an ROC curve and a precision-recall curve on an imbalanced dataset (class ratio 1:100). Given the ROC curve alone, the performance appears excellent, yet the low precision reveals the true performance of the classifier.

Furthermore, various security-related problems deal with more than two classes, requiring *multi-class metrics*. This setting can introduce further subtle pitfalls. Common strategies, such as *macro-averaging* or *micro-averaging* are known to overestimate and underestimate small classes [52].

Security implications. Inappropriate metrics are a long-standing problem in security research, particularly in detection tasks. While true and false positives provide a more detailed picture of a system's performance, they can also disguise the actual precision when the prevalence of attacks is low. In §4.1, we show how using different metrics to assess the same Android malware classifier leads to contradicting interpretations of its detection capabilities.

P8 – Base Rate Fallacy. A large class imbalance is ignored when interpreting the performance measures leading to an overestimation of performance.

Description. Class imbalance can easily lead to a misinterpretation of performance if the base rate of the negative class is not considered. If this class is predominant, even a very low false-positive rate can result in surprisingly high numbers of false positives. Note the difference to the previous pitfall: while P7 refers to the inappropriate description of performance, the base-rate fallacy is about the misleading interpretation of results. This special case is easily overlooked in practice (see §3). Consider the example in Figure 2 where 99 % true positives are possible at 1 % false positives. Yet, if we consider the class ratio of 1:100, this actually corresponds to 100 false positives for every 99 true positives.

Security implications. The base rate fallacy is relevant in a variety of security problems, such as intrusion detection and website fingerprinting [e.g., 11, 71, 98]. In website fingerprinting, users can visit billions of web pages, but only a tiny fraction of these web pages are available for evaluation. As a result, it is challenging to provide realistic numbers on the privacy threat posed by attackers. Similarly, the probability of installing malware is usually much lower than is considered in experiments on malware detection [101].

2.4 Deployment and Operation

In the last stage of a typical machine-learning workflow, the developed system is deployed to tackle the underlying security problem in practice. Deployment environments differ considerably from typical laboratory setups and there are further issues to consider when evaluating a learning-based system's practical capabilities.

P9 – Lab-Only Evaluation. A learning-based system is solely evaluated in a laboratory setting, without discussing its practical limitations.

Description. As in all empirical disciplines, it is common to perform experiments under certain assumptions to demonstrate a method's efficacy. While performing controlled experiments is a legitimate way to examine specific aspects of an approach, it should ultimately be evaluated in a realistic setting to transparently assess its capabilities and showcase the open challenges which will foster further research.

Security implications. Many learning-based systems in security are evaluated solely in laboratory settings, overstating their practical impact. A common example are detection methods evaluated only in a *closed-world setting* with limited diversity and no consideration of non-stationarity [15, 70]. For example, a large number of website fingerprinting attacks are evaluated only in closed-world settings spanning a limited time period [71]. Similarly, most learning-based malware detection systems have been insufficiently examined in realistic settings [see 5, 101].

P10 – Inappropriate Threat Model. The security of machine learning is not considered, exposing the system to a variety of attacks, such as poisoning and evasion attacks.

Description. Learning-based security systems operate in an hostile environment. Prior work in adversarial learning has revealed a considerable attack surface introduced by machine learning itself at all stages of the workflow [see 17, 99]. First, membership inference attacks undermine models' privacy, allowing an adversary to leak information of training examples by exploiting overfitting in deep neural networks [110]. Next, preprocessing attacks target the feature extraction step

to inject arbitrary inputs to the system which affect all further steps in the pipeline [135]. *Poisoning and backdoor attacks* tamper with the data to modify a model's behavior [18, 60]. *Model stealing* allows for a model to be approximated, leaking intellectual property and accelerating further attacks [123]. Finally, *adversarial examples* are inputs that allow an adversary to control the final prediction [19, 25].

Security implications. Neglecting to include adversarial influence in the threat model and evaluation is fatal as a system deployed in an adversarial environment which is not robust to adversaries will not be able to provide trustworthy, meaningful results. Additionally, failing to consider machine-learning related attacks will expose the system to an additional attack surface—aside from traditional security issues. For instance, an attacker can more easily evade a model that relies on only a few features than a properly regularized model that has been designed with security considerations in mind [40]. Furthermore, the *semantic gap* describes the discrepancy between extracted features and the corresponding object [127]. For example, an adversary can create adversarial examples of PDFs by injecting content into areas that a regular PDF reader ignores but that a PDF malware detector examines. It becomes thus easy to manipulate the PDF feature vector while ensuring the inconspicuousness of the corresponding object.

3 Prevalence Analysis

Once we understand the pitfalls faced by learning-based security systems, it becomes necessary to assess their prevalence and investigate their impact on scientific advances. To this end, we conduct a ten-year longitudinal study, with a strong focus on the past 6 years, on 30 representative papers published at ACM CCS, IEEE S&P, USENIX Security, and NDSS, the top-4 conferences for security-related research in our community. All papers apply machine learning to different security tasks, encompassing a broad variety of topics. Note that research focusing on the security of machine learning or that does not apply machine learning at all is considered out of scope.

In particular, our sample of top-tier papers includes the following topics: malware detection [9, 34, 86, 101, 117, 134]; network intrusion detection [44, 92, 108, 111]; vulnerability discovery [42, 50, 51, 82]; website fingerprinting attacks [46, 98, 105, 112]; social network abuse [21, 94, 116]; binary code analysis [14, 32, 109]; code attribution [2, 23]; steganography [16]; online scams [73]; game bots [79]; and ad blocking [67]. Figure 4 shows a breakdown of the papers by year of publication.

Review process. Each paper is assigned two independent reviewers who assess the article and identify instances of the described pitfalls. The pool of reviewers consists of six researchers who have all previously published work on the topic of machine learning and security in at least one of the considered security conferences. Reviewers do *not* consider any

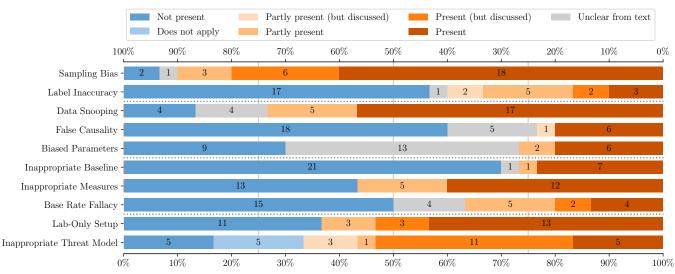


Figure 3: Stacked bar chart showing the pitfalls suffered by each of the 30 papers analyzed. The colors of each bar show the degree to which a pitfall was present, and the width shows the proportion of papers in that group. The number at the center of each bar shows the cardinality of each group.

material presented outside the papers under analysis (other than their associated artifacts such as datasets or source code), and do *not* contact the authors for more information. Once both reviewers have completed their assignments, they discuss the paper in the presence of a third reviewer that may resolve any disputes. In case of uncertainty, the authors are given the benefit of the doubt (e.g., in case of a dispute between *partly present* and *present*, we assign *partly present*).

Throughout the process, all reviewers meet regularly in order to discuss their findings and ensure consistency between the pitfalls' criteria. Moreover, these meetings have been used to refine the definitions and scope of pitfalls based on the reviewers' experience. Following any adaptation of the criteria, all completed reviews have been re-evaluated by the original reviewers—this occurred twice during our analysis. While cumbersome, this adaptive process of incorporating reviewer feedback ensures that the pitfalls are comprehensive in describing the core issues across the state of the art.

We note that the inter-rater reliability of reviews prior to dispute resolution is $\alpha = 0.832$ using Krippendorff's alpha, where $\alpha > 0.800$ indicates confidently reliable ratings [76].

Assessment criteria. For each paper, pitfalls are coarsely classified as either *present*, *not present*, *unclear from text*, or *does not apply*. A pitfall may be wholly present throughout the experiments without remediation (*present*), or it may not (*not present*). If the authors have corrected any bias or have narrowed down their claims to accommodate the pitfall, this

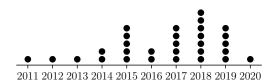


Figure 4: Distribution of papers per year for the 30 papers in our analysis.

is also counted as *not present*. Additionally, we introduce *partly present* as a category to account for experiments that do suffer from a pitfall, but where the impact has been partially addressed. If a pitfall is *present* or *partly present* but acknowledged in the text, we moderate the classification as *discussed*. If the reviewers are unable to rule out the presence of a pitfall due to missing information, we mark the publication as *unclear from text*. Finally, in the special case of P10, if the pitfall *does not apply* to a paper's setting, this is considered as a separate category.

Observations. The aggregated results from the prevalence analysis are shown in Figure 3. A bar's color indicates the degree to which a pitfall is present, and its width shows the proportion of papers with that classification. The number of affected papers is noted at the center of the bars. The most prevalent pitfalls are sampling bias (P1) and data snooping (P3), which are at least partly present in over 73 % of the papers. In more than 50 % of the papers, we identify inappropriate threat models (P10), lab-only evaluations (P9), and inappropriate baselines (P6) as at least partly present. *Every* paper is affected by at least three pitfalls, underlining the pervasiveness of such issues in recent computer security research. In particular, we find that dataset collection is still very challenging: some of the most realistic and expansive open datasets we have developed as a community are still imperfect (see §4.1).

Moreover, the presence of some pitfalls is more likely to be *unclear from the text* than others. We observe this for biased parameter selection (P5) when no description of the hyperparameters or tuning procedure is given; for false causality (P4) when there is no attempt to explain a model's decisions; and for data snooping (P3) when the dataset splitting or normalization procedure is not explicitly described in the text. These issues also indicate that experimental settings are more difficult to reproduce due to a lack of information.

Takeaways. We find that all of the pitfalls introduced in §2 are pervasive in security research, affecting between 23 % and 90 % of the selected papers. Each paper suffers from at least three of the pitfalls which, compounded by the fact that only 20 % of instances are accompanied by a discussion in the text, indicates a clear lack of awareness in our community.

Although our findings point to a serious problem in research, we would like to remark that *all* of the papers analyzed provide excellent contributions and valuable insights. Our objective here is not to blame researchers for stepping into pitfalls but to raise awareness and increase the experimental quality of research on machine learning in security.

4 Impact Analysis

In the previous sections, we have discussed various pitfalls that can affect the evaluation process of learning-based systems and find that these pitfalls are widespread in the computer security literature. However, so far it remains unclear how much the individual pitfalls could affect experimental results and their conclusions. In this section, we estimate the experimental impact of some of these pitfalls in four popular applications of machine learning in security:

- §4.1: mobile malware detection (P1, P4, and P7)
- §4.2: vulnerability discovery (P2, P4, and P6)
- §4.3: source code authorship attribution (P1 and P4)
- §4.4: network intrusion detection (P6 and P9)

Remark. For this analysis, we consider state-of-the-art approaches for each security domain. We remark that the results within this section do not mean to criticize these approaches specifically; we choose them as they are *representative* of how pitfalls can impact different domains. Notably, the fact that we have been able to reproduce the approaches speaks highly of their academic standard.

4.1 Mobile Malware Detection

The automatic detection of Android malware using machine learning is a particularly lively area of research. The design and evaluation of such methods are delicate and may exhibit some of the previously discussed pitfalls. In the following, we discuss the effects of sampling bias (P1), false causality (P4), and inappropriate performance measures (P7) on learning-based detection in this context.

Dataset collection. A common source for recent mobile data is the *AndroZoo* project [6], which collects Android apps from a large variety of sources, including the official *GooglePlay* store and several Chinese markets. At the time of writing it includes more than 11 million Android applications from 18 different sources. As well as the samples themselves, it includes meta-information, such as the number of antivirus

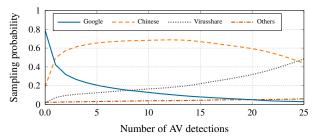


Figure 5: The probability of sampling malware from Chinese markets is significantly higher than for GooglePlay. This can lead to sampling biases in experimental setups for Android malware detection.

detections. Although AndroZoo is an excellent source for obtaining mobile apps, we demonstrate that experiments may suffer from severe sampling bias (P1) if the peculiarities of the dataset are not taken into account. Please note that the following discussion is not limited to the AndroZoo data, but is relevant for the composition of Android datasets in general.

Dataset analysis. In the first step, we analyze the data distribution of AndroZoo by considering the origin of an app and the number of antivirus detections of an Android app. For our analysis, we broadly divide the individual markets into four different origins: GooglePlay, Chinese markets, VirusShare, and all other markets.

Figure 5 shows the probability of randomly sampling from a particular origin depending on the number of antivirus detections for an app. For instance, when selecting a sample with no constraints on the number of detections, the probability of sampling from GooglePlay is roughly 80%. If we consider a threshold of 10 detections, the probability that we randomly select an app from a Chinese market is 70%. It is very likely that a large fraction of the benign apps in a dataset are from GooglePlay, while most of the malicious ones originate from Chinese markets, if we ignore the data distribution.

Note that this sampling bias is not limited to Andro-Zoo. We identify a similar sampling bias for the DREBIN dataset [9], which is commonly used to evaluate the performance of learning-based methods for Android malware detection [e.g., 9, 59, 141]. Interested readers can find details of the analysis of this dataset in Appendix B.

Experimental setup. To get a better understanding of this finding, we conduct experiments using two datasets: For the first dataset (D_1) , we merge 10,000 benign apps from Google-Play with 1,000 malicious apps from Chinese markets (Anzhi) and AppChina. We then create a second dataset (D_2) using the same 10,000 benign applications, but combine them with 1,000 malware samples exclusively from Google-Play. All malicious apps are detected by at least 10 virus scanners. Next, we train a linear support vector machine [48] on these datasets using two feature sets taken from state-of-the-art classifiers (DREBIN [9] and OPSEQS [89]). The exact details of setup are described in Appendix B.

Table 1: Comparison of results for two classifiers when merging benign apps from GooglePlay with Chinese malware (D_1) and sampling solely from GooglePlay (D_2) . For both classifiers, the detection performance drops significantly when considering apps only from GooglePlay. The standard deviation of the results ranges between 0-3%.

| | DREBIN | | OPSEQS | | | |
|-----------|--------|-------|--------|-------|-------|--------|
| Metric | D_1 | D_2 | % | D_1 | D_2 | % |
| Accuracy | 0.994 | 0.980 | -1.4 % | 0.972 | 0.948 | -2.5 % |
| Precision | 0.968 | 0.930 | -3.9% | 0.822 | 0.713 | -13.3% |
| Recall | 0.964 | 0.846 | -12.2% | 0.883 | 0.734 | -16.9% |
| F1-Score | 0.970 | 0.886 | -8.7% | 0.851 | 0.722 | -15.2% |
| MCC [87] | 0.963 | 0.876 | -9.0% | 0.836 | 0.695 | -16.9% |

Results. The recall (true positive rate) for DREBIN and OPSEQS drops by more than 10% and 15%, respectively, between the datasets D_1 and D_2 , while the accuracy is only slightly affected (see Table 1). Hence, the choice of performance measure is crucial (P7). Interestingly, the URL play.google.com turns out to be one of the five most discriminative features for the benign class. The classifier has learned to distinguish the origins of Android apps, rather than learning the difference between malware and benign apps (P4). Although our experimental setup overestimates the classifier's performance by deliberately ignoring time dependencies (P3), we can still clearly observe the impact of the pitfalls. Note that the effect of temporal snooping in this setting has been demonstrated in previous work [4, 101].

4.2 Vulnerability Discovery

Vulnerabilities in source code can lead to privilege escalation and remote code execution, making them a major threat. Since the manual search for vulnerabilities is complex and time consuming, machine learning-based detection approaches have been proposed in recent years [58, 82, 137]. In what follows, we show that a dataset for vulnerability detection contains artifacts that occur only in one class (P4). We also find that VulDeePecker [82], a neural network to detect vulnerabilities, uses artifacts for classification and that a simple linear classifier achieves better results on the same dataset (P6). Finally, we discuss how the preprocessing steps proposed for VulDeePecker make it impossible to decide whether some snippets contain vulnerabilities or not (P2).

Dataset collection. For our analysis we use the dataset published by Li et al. [82], which contains source code from the National Vulnerability Database [36] and the SARD project [37]. We focus on vulnerabilities related to buffers (CWE-119) and obtain 39,757 source code snippets of which 10,444 (26%) are labeled as containing a vulnerability.

Dataset analysis. We begin our analysis by classifying a random subset of code snippets by hand to spot possible artifacts in the dataset. We find that certain sizes of buffers seem to be present only in one class throughout the samples considered.

Table 2: Different buffer sizes in the Vulnerability Dataset used by Li et al. [82] with their number of occurrences and relative frequency in class 0.

| Buffer size | Occurrences | | |
|-------------|-------------|---------------|--|
| | Total | In class 0 | |
| 3 | 70 | 53 (75.7%) | |
| 32 | 116 | 115 (99.1%) | |
| 100 | 6,364 | 4,315 (67.8%) | |
| 128 | 26 | 24 (92.3%) | |
| 1,024 | 100 | 96 (96.0%) | |

To investigate, we extract the buffer sizes of char arrays that are initialized in the dataset and count the number of occurrences in each class. We report the result for class 0 (snippets without vulnerabilities) in Table 2 and observe that certain buffer sizes occur almost exclusively in this class. This may result in *false causality* (P4) when a model uses the buffer sizes as discriminative features for classification.

Experimental setup. We train VulDeePecker [82], based on a recurrent neural network [66], to classify the code snippets automatically. To this end, we replace variable names with generic identifiers (e.g., INT2) and truncate the snippets to 50 tokens, as proposed in the paper [82]. An example of this procedure can be seen in Figure 6 where the original code snippet (top) is transformed to a generic snippet (bottom).

We use a linear Support Vector Machine (SVM) with bagof-words features based on *n*-grams as a baseline for VulDeePecker (see Appendix C for details). To see what VulDeePecker has learned we follow the work of Warnecke et al. [129] and use the Layerwise Relevance Propagation (LRP) method [12] to explain the predictions and assign each token a *relevance* score that indicates its importance for the classification. Figure 6 (bottom) shows an example for these scores where blue tokens favor the classification and orange ones oppose it.

```
data = new char[10+1];
char source[10+1] = SRC_STRING;
memmove(data, source, (strlen(source) + 1) *
sizeof(char));
```

```
VAR0 = new char [ INTO + INT1 ] ;
char VAR1 [ INTO + INT1 ] = VAR2 ;
memmove ( VAR0 , VAR1 , ( strlen ( VAR1 ) + INT1 )
    * sizeof ( char ) ) ;
```

Figure 6: Top: Code snippet from the dataset. Bottom: Same code snippet after preprocessing steps of VulDeePecker. Coloring indicates importance towards classification according to the LRP [12] method.

Results. To see whether VulDeePecker relies on artifacts, we use the relevance values for the entire training set and extract the ten most important tokens for each code snippet. Afterwards we extract the tokens that occur most often in this top-10 selection and report the results in Table 3 in descending order of occurrence.

Table 3: The 10 most frequent tokens across samples in the dataset.

| Rank | Token | Occurrence | Rank | Token | Occurrence |
|------|-------|------------|------|-------|------------|
| 1 | INT1 | 70.8 % | 6 | char | 38.8 % |
| 2 | (| 61.1 % | 7 |] | 32.1 % |
| 3 | * | 47.2 % | 8 | + | 31.1% |
| 4 | INT2 | 45.7 % | 9 | VAR0 | 28.7 % |
| 5 | INT0 | 38.8 % | 10 | , | 26.0 % |

While the explanations are still hard to interpret for a human we notice two things: Firstly, tokens such as '(', ']', and ',' are among the most important features throughout the training data although they occur frequently in code from both classes as part of function calls or array initialization. Secondly, there are many generic INT* values which frequently correspond to buffer sizes. From this we conclude that VulDeePecker is relying on combinations of artifacts in the dataset and thus suffers from *false causality* (P4).

To further support this finding, we show in Table 4 the performance of VulDeePecker compared to an SVM for different lengths of n-grams. We find that an SVM with 3-grams yields the best performance with an $18 \times$ smaller model. This is interesting as overlapping but independent substrings (n-grams) are used, rather than the true sequential ordering of all tokens as for the RNN. Thus, it is likely that VulDeePecker is not exploiting relations in the sequence, but merely combines special tokens—an insight that could have been obtained by training a linear baseline classifier (P6).

Finally, we discuss the preprocessing steps proposed by Li et al. [82] as seen in the example of Figure 6. By truncating the code snippets to a fixed length of 50, important information is lost. For example, the value of the variable SRC_STRING is unknown and thus it is not clear whether a buffer overflow appears due to the memmove call. Likewise, the conversion of numbers to INTO and INT1 results in the same problem for the data variable: After the conversion it is not possible to tell how big the buffer is and whether the content fits into it or not. This indicates a case of label inaccuracy (P2).

Table 4: Performance of Support Vector Machines and VulDeePecker on unseen data. The true-positive rate is determined at 1 % false positives.

| Model | # parameters | AUC | TPR |
|---------------|---------------------|-------|-------|
| VulDeePecker | 1.2×10^{6} | 0.980 | 0.968 |
| SVM (1-grams) | 5.8×10^{2} | 0.805 | 0.505 |
| SVM (2-grams) | 1.3×10^{4} | 0.958 | 0.942 |
| SVM (3-grams) | 6.6×10^{4} | 0.984 | 0.978 |

4.3 Source Code Author Attribution

The task of identifying the developer based on source code is known as authorship attribution [22]. Programming habits are characterized by a variety of stylistic patterns, so that state-of-the-art attribution methods use an expressive set of

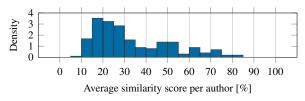


Figure 7: Shared source code over all files per author. A majority tends to copy code snippets across challenges, leading to learned artifacts.

such features. These range from simple layout properties to more unusual habits in the use of syntax and control flow. In combination with a sampling bias (P1), this expressiveness may give rise to false causalities (P4) in current attribution methods, leading to an overestimation of accuracy.

Dataset collection. Recent approaches have been tested on data from the Google Code Jam (GCJ) programming competition [2, 7, 22], where participants solve the same challenges in various rounds. An advantage of this dataset is that it ensures a classifier learns to separate stylistic patterns rather than merely overfitting to different challenges. We use the 2017 GCJ dataset [103], which consists of 1,632 C++ files from 204 authors solving the same eight challenges.

Dataset analysis. We start with an analysis of the average similarity score between all files of each respective programmer, where the score is computed by *difflib's Sequence-Matcher* [102]. Figure 7 shows that most participants copy code across the challenges, that is, they reuse personalized coding *templates*. Understandably, this results from the nature of the competition, where participants are encouraged to solve challenges quickly. These templates are often *not* used to solve the current challenges but are only present in case they might be needed. As this deviates from real-world settings, we identify a sampling bias in the dataset.

Current feature sets for authorship attribution include these templates, such that models are learned that strongly focus on them as highly discriminative patterns. However, this unused duplicate code leads to features that represent artifacts rather than coding style and cause false causalities. Appendix D provides examples from the GCJ dataset.

Experimental setup. Our evaluation on the impact of both pitfalls builds on the attribution methods by Abuhamad et al. [2] and Caliskan et al. [22]. Both represent the state of the art regarding performance and comprehensiveness of features. A detailed description of the setup is given in Appendix D.

We implement a linter tool on top of Clang, an open-source C/C++ front-end for the LLVM compiler framework, to remove unused code that is mostly present due to the templates. Based on this, we design the following three experiments: First, we train and test a classifier on the unprocessed dataset (T_b) as a baseline. Second, we remove unused code from the respective test sets (T_1), which allows us to test how

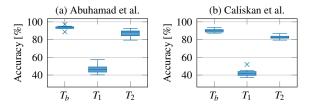


Figure 8: Accuracy of authorship attribution after considering artifacts. The accuracy drops by 48 % if unused code is removed from the test set (T_1) ; After retraining (T_2) , the average accuracy still drops by 6 % and 7 %.

much the learning methods focus on unused template code. Finally, we remove unused code from the training set and re-train the classifier (T_2) .

Results. Figure 8 presents the accuracy for both attribution methods on the different experiments. Artifacts have a substantial impact on the attribution accuracy. If we remove unused code from the test set (T_1) , the accuracy drops by 48 % for the two approaches. Both systems, hence, considerably focus on the unused template code. After retraining (T_2) , the average accuracy drops by 6 % and 7 % for the methods by Abuhamad et al. [2] and Caliskan et al. [22], demonstrating the importance of artifacts for the attribution performance.

Overall, our experiments show that the impact of sampling bias and false causality has been underestimated and reduces the accuracy considerably. At the same time, our results are encouraging. After accounting for artifacts, both attribution methods select features that allow for a reliable identification. We make the sanitized dataset publicly available to foster further research in this direction.

4.4 Network Intrusion Detection

Detecting network intrusions is one of the oldest problems in security [41] and it comes at no surprise that detection of anomalous network traffic relies heavily on learning-based approaches [27, 80, 81, 92]. However, challenges in collecting real attack data has often led researchers to generate synthetic data for lab-only evaluations (P9). Here, we demonstrate how this data is often insufficient for justifying the use of complex models (e.g., neural networks) and how using a simpler model as a baseline would have brought these shortcomings to light (P6).

Dataset collection. We consider the dataset released by Mirsky et al. [92], which contains a capture of Internet of Things (IoT) network traffic simulating the initial activation and propagation of the Mirai botnet malware. The packet capture covers 119 minutes of traffic on a Wi-Fi network with three PCs and nine IoT devices.

Dataset analysis. First, we analyze the transmission volume of the captured network traffic. Figure 9 shows the frequency of benign and malicious packets across the capture, divided into bins of 10 seconds. This reveals a strong signal in the

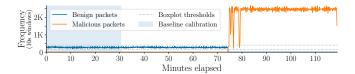


Figure 9: Frequency of benign vs malicious packets in the Mirai dataset [92]. The Gray dashed lines show the thresholds that define normal traffic calculated using the simple baseline (*boxplot method* [125]). The span of clean data used for calibration is highlighted by the light blue shaded area.

packet frequency, which is highly indicative of an ongoing attack. Moreover, all benign activity seems to halt as the attack commences, after 74 minutes, despite the number of devices on the network. This suggests that individual observations may have been merged and could further result in the system benefiting from false causality (P4).

Experimental setup. To illustrate how severe these pit-falls are, we consider KITSUNE [92], a state-of-the-art deep learning-based intrusion detector built on an ensemble of autoencoders. For each packet, 115 features are extracted that are input to 12 autoencoders, which themselves feed to another, final autoencoder operating as the anomaly detector.

As a simple baseline to compare against KITSUNE, we choose the *boxplot method* [125], a common approach for identifying outliers. We process the packets using a 10-second sliding window and use the packet frequency per window as the sole feature. Next, we derive a lower and upper threshold from the clean calibration distribution: $\tau_{low} = Q_1 - 1.5 \cdot IQR$ and $\tau_{high} = Q_3 + 1.5 \cdot IQR$. During testing, packets are marked as benign if the sliding window's packet frequency is between τ_{low} and τ_{high} , and malicious otherwise. In Figure 9, these thresholds are shown by the dashed gray lines.

Results. The classification performance of the autoencoder ensemble compared to the boxplot method is shown in Table 5. While the two approaches perform similarly in terms of ROC AUC, the simple boxplot method outperforms the autoencoder ensemble at low false-positive rates (FPR).

As well as its superior performance, the boxplot method is exceedingly lightweight compared to the feature extraction and test procedures of the ensemble. This is especially relevant as the ensemble is designed to operate on resource-constrained devices with low latency (e.g., IoT devices).

Note that this experiment does not intend to show that the boxplot method can detect an instance of Mirai operating in the wild, but to demonstrate that an experiment without an appropriate baseline (P6) is insufficient to justify the complexity and overhead of the ensemble. The success of the boxplot method also shows how simple methods can reveal issues with data generated for lab-only evaluations (P9). In the Mirai dataset the infection is overly conspicuous; an attack in the wild would likely be represented by a tiny proportion of network traffic.

Table 5: Comparing KITSUNE [92], an autoencoder ensemble NIDS, against a simple baseline, boxplot method [125], for detecting a Mirai infection.

| Detector | AUC | TPR (FPR at 0.001) | TPR (FPR at 0.000) |
|-----------------------|-------|---------------------------|---------------------------|
| KITSUNE [92] | 0.968 | 0.882 | 0.873 |
| Simple Baseline [125] | 0.998 | 0.996 | 0.996 |

4.5 Takeaways

The four case studies clearly demonstrate the impact of the considered pitfalls across four distinct security scenarios. Our findings show that subtle errors in the design and experimental setup of an approach can result in misleading or erroneous results. While researchers often believe to be aware of these consequences, the frequency and severity of pitfalls identified in top papers clearly indicate that significantly more awareness is needed. Additionally, we show how pitfalls apply across multiple domains, indicating a general problem that cannot be attributed to any one individual security area.

5 Recommendations

Based on our analysis of common pitfalls, we derive actionable recommendations for practically resolving or at least mitigating the underlying issues. We present our *dos* for machine learning in security according to the machine learning pipeline introduced in §2. In particular, we focus on pitfalls for which awareness of their existence is generally not enough to tackle them effectively.

5.1 Data Collection and Labeling

Collecting security-related data. In many security applications, sampling from the true distribution is extremely difficult, if not impossible, requiring alternative solutions. For instance, a reasonable strategy is to construct different estimates of the true distribution and analyze them individually (e.g., by varying the class ratio in malware experiments [see 101]). In some cases, it can be suitable to extend the training data with synthetic instances to limit the impact of sampling biases [e.g., 28, 62, 133]. Also, several methods in the research field of transfer learning have been proposed that can be used to reduce, or compensate for, the negative effects of sampling biases [see 96, 97, 131, 142]. Transfer learning methods leverage knowledge from one domain and use it to improve the performance of a learning-based system in another, such as when it is difficult to gather enough data. As an example, Zhu et al. [140] have recently proposed a transfer framework for fraud detection that allows for the detection of fraud across different countries. Although no transfer learning method is applicable to all possible scenarios, many approaches can be adapted to security-related tasks, lowering the impact of sampling biases.

Furthermore, mixing data from distinct or incompatible sources is a common cause of sampling bias, as we show in our prevalence and impact analyses (§3 and §4). Similarly, as the compilation of new datasets is often cumbersome, it is convenient to reuse well-known datasets to yield results quickly and compare approaches on common grounds. However, public datasets need to be treated with caution. Firstly, data ages and becomes less relevant in the fast-moving security land-scape, partially due to concept drift [15, 70, 85, 101]. Secondly, the characteristics of the data are increasingly exposed and thereby lead to implicit data snooping (P3) [see 1, 88]. Consequently, well-known datasets should be mainly used for comparison with past research and complemented with recent data from the application setting.

Finally, note that if none of the recommendations are suitable, at least the sampling procedure's limitations should be discussed. Providing a transparent discussion of the underlying sampling bias allows readers to better understand the security implications and possible impact.

Handling noisy labels. Many learning-based systems in security rely on supervised learning, for which labels are vitally important. The labeling process needs to be designed with care. For instance, the way human participants are asked to annotate data can skew labels, as demonstrated for the popular ImageNet dataset [124].

Generally, labels should be verified whenever possible, for instance with sanity checks by inspecting a sample of labels. If *noisy labels* cannot be ruled out, there exist various possibilities to deal with them. In particular, the impact of noisy labels on the resulting model can be reduced by (i) using robust models or loss functions by design, (ii) actively incorporating noisy labels by modeling them in the learning process, or (iii) cleaning the training data from noisy instances that increase the complexity of the model [see 56].

However, it should be stressed that instances with uncertain labels must not be removed from the test data. This represents a variation of sampling bias (P1) and data snooping (P3), as the original data distribution is manipulated and selected samples are excluded from the evaluation. Similarly, samples that fail to be analyzed should not be excluded. Instead, problematic samples should be kept in the test data and processed with a default decision rule when the learning-based system fails.

An additional challenge when labeling data is the fact that labels are often subject to change over time in security settings, so that it is necessary to check for *label shift* [84] and take appropriate precautions, such as delaying labeling until a stable ground-truth is available [see 139].

5.2 Model Design and Learning

Explainable learning. Instead of learning real relationships within the data, a model may pick up on artifacts within the data, leading to false causality (P4). Learned artifacts are

likely to hinder the successful application of the learning model in practice. Hence, explainable learning techniques should be used as a mandatory check [see 61, 78, 129]. These can reveal if the classification relies on spurious features. In our case studies, we successfully use explainable learning techniques to identify such features that serve as unintended shortcuts (see §4). By checking which features are prevalent in each class, how important they are for respective inputs, and checking their plausibility, we identify highly discriminative features, such as buffer sizes and unused code templates, which are *unrelated to the security task at hand*.

Calibrating security systems. While it seems obvious that training, validation, and test data should be strictly separated in all experiments, this separation is often unintentionally violated during the preprocessing stage of machine learning workflows. For example, we observe that it is a common mistake to compute tf-idf weights or neural embeddings over the entire dataset. This practice is a form of data snooping (P3) and may bias results. To avoid this problem, test data should be split early during data collection and stored separately until the final evaluation.

Training is not the only important step for generating a learning-based security system. Hyperparameters and thresholds of the underlying model must be calibrated prior to its application. A recurring issue in security research is that calibration is unintentionally performed on test data, for example, when the operation point of a system is chosen after all experiments have been completed. We recommend using a separate *validation set* for all model selection and parameter tuning.

5.3 Performance Evaluation

Performance metrics. Performance measures play a key role during the evaluation of machine learning. While there exist a wide range of measures, only some are suitable for security applications (P7 and P8). For example, measuring the accuracy in intrusion detection has been identified as a notorious pitfall in previous work [see 115]. As the choice of metrics is highly application-specific, we refrain from providing general guidelines. Instead, we recommend ensuring the chosen measures would help a practitioner assess the performance of the security system during a deployment.

Since several problems in security revolve around detecting a rare event, namely attacks, we additionally advocate the use of *precision* and *recall* as well as related measures, such as precision-recall curves. In contrast to several other performance measures, these functions are neither affected by class imbalance nor the base rate fallacy, and thus resemble reliable performance indicators for detection tasks focusing on a minority class [38, 114]. However, note that precision and recall can also be misleading, for instance, if the prevalence of attacks is inflated due to sampling bias [101]. In these cases, other metrics like *Matthews Correlation Coefficient (MCC)*

are more suitable to assess the classifier's performance and reveal potential weaknesses [29]. In addition, ROC curves are a useful metric for directly comparing the performance of multiple approaches, but their expressiveness depends highly on the selection of proper baselines (see P6).

Security baselines. To assess the capabilities of a novel approach in a meaningful way, a comparison against proper baselines is essential. Although it might seem straightforward to use sophisticated methods as baselines to compare with, these methods do not necessarily perform best on the test data due to their low bias and high variance. Instead, simpler models should be included as they are easier to explain, less computationally demanding, and have proven to be effective and scalable in practice (e.g., linear classifiers [9] or näive Bayes classifiers [83]).

Automated machine learning (*AutoML*) frameworks [e.g., 49, 69] are a useful method for finding proper baselines. These frameworks enable researchers to automatically retrieve machine learning models that have been trained using state-of-the-art techniques for hyperparameter tuning and model selection. While these automated methods can certainly not replace experienced data analysts, they can be used to initially set the bar the proposed approach should aim for.

As well as considering learning-based methods, it is critical to check whether non-learning approaches are also suitable for the application scenario. For example, for intrusion and malware detection, there exist a wide range of methods using other detection strategies [e.g., 47, 100, 106].

5.4 Deployment and Operation

Deployment for security. It is essential to move from a *laboratory setting* and approximate a *real-world setting* as accurately as possible. For example, temporal and spatial relations of the data should be considered to account for the typical dynamics encountered in the wild [see 101]. Similarly, runtime and storage constraints should be analyzed under practical conditions [see 15, 107, 126]. Ideally, the proposed system should be deployed to uncover problems that are not observable in a lab-only environment, such as the diversity and complexity of real-world network traffic [see 115].

Security of deployment. In most fields of security where learning-based systems are used, we operate in an *adversarial environment*. Hence, threat models should be defined precisely and systems evaluated with respect to them. In most cases, it is necessary to assume an *adaptive adversary* that specifically targets the proposed systems and will search for and exploit weaknesses for evasion or manipulation. Similarly, it is helpful to consider the different stages of the machine learning workflow and investigate possible vulnerabilities [see 17, 26, 39, 99]. White-box attacks should be employed to consider a worst-case scenario, following Kerckhoff's principle [72] and security best practices. Ulti-

mately, a security system is of little practical utility, if it can be easily circumvented and thus an evaluation of adversarial aspects is a mandatory component in security research.

6 Related Work

Our study is the first to *systematically* and *comprehensively* explore pitfalls when applying machine learning to security. It complements a series of research on improving experimental evaluations in general. In the following, we briefly review this related work and point out key differences.

Security studies. Over the last two decades, there have been several studies on improving experiments in specific security domains. For example, Axelsson [11], McHugh [88], and Cardenas et al. [24] investigate issues with the evaluation of intrusion detection systems, covering special cases of sampling bias (P1), the base rate fallacy (P8), and inappropriate performance measures (P7). Sommer and Paxson [115] extend this work and specifically focus on the application of machine learning for network intrusion detection. They identify further issues, such as semantic gaps with anomaly detection (P4) and unrealistic evaluation baselines (P6).

In a similar strain of research, Rossow et al. [107] derive guidelines for conducting experiments with malware. Although this study does not investigate machine learning explicitly, it points to experimental problems related to some of the issues discussed in this paper. The study is expanded by a series of follow-up works that examine variants of sampling bias in malware analysis (P1), such as temporally inconsistent data splits and labels [e.g., 4, 91, 101, 139] as well as unrealistic goodware-to-malware ratios [e.g., 5, 101]. Aghakhani et al. [3] study the limits of static features for malware classification in the presence of packed samples.

Das et al. [35] show that security defenses relying on hardware performance counters are ineffective in realistic settings (P9). Similarly, for privacy-preserving machine learning, Oya et al. [95] find that most location privacy approaches fail when applied to real-world distributions (P9). For authentication, Sugrim et al. [118] propose appropriate measures to evaluate learning-based authentication systems (P7) and, finally, for system security van der Kouwe et al. [126] point to frequent benchmarking flaws (P1, P6, and P7).

Our study builds on this research but provides an orthogonal and comprehensive view of the problem. Instead of focusing on specific domains, we are the first to *generally* explore pitfalls and recommendations when applying machine learning in computer and network security. As a consequence, our work is not limited to certain security problems but applicable to all security domains.

Adversarial learning studies. Another branch of research has focused on attacking and defending learning algorithms [17, 39, 99]. While a number of powerful attacks have emerged from this research, such as evasion, poisoning, and

inference attacks, the corresponding defenses have often suffered from limited robustness [10]. To counteract this imbalance, Carlini et al. [26] identify several pitfalls that affect the evaluation of defenses and discuss recommendations on how to avoid them. In a similar vein, Biggio et al. [20] propose a framework for security evaluations of pattern classifiers under attack. Both works are closely related to pitfall P10 and provide valuable hints for evaluating the robustness of defenses. However, while we also argue that smart and adaptive adversaries must always be considered when proposing learning-based solutions in security, our study is more general.

Machine learning studies. Finally, a notable body of work has explored recommendations for the general use of machine learning. This research includes studies on different forms of sampling bias and dataset shift [93, 119, 122] as well as on the general implications of biased parameter selection [65], data snooping [75], and inappropriate evaluation methods [38, 53, 63]. An intuitive overview of issues in applied statistics is provided by Reinhart [104].

Our work builds on this analysis; however, we focus exclusively on the impact of pitfalls prevalent in security. Consequently, our study and its recommendations are tailored to the needs of the security community, and aim to push forward the state of the art in learning-based security systems.

7 Conclusion

We identify and systematically assess ten subtle pitfalls in the use of machine learning in computer and network security. These issues may severely affect the validity of research and lead to overestimating the performance of security systems.

We find that these pitfalls are prevalent even in papers published at top-tier security conferences. Moreover, we demonstrate that ignoring them can lead to severe biases in key research results. To avoid these pitfalls in the future, we provide recommendations that can serve as general guidelines for researchers and practitioners. The recommendations are applicable to all security domains, covering common tasks for machine learning, such as intrusion and malware detection, binary code analysis, and vulnerability discovery.

Ultimately, we strive to improve the scientific quality of empirical work on machine learning in security. Our study aims to raise awareness of common problems as well as guide researchers when designing, implementing, and evaluating learning-based systems in security. A decade after the seminal study of Sommer and Paxson [115], we again encourage the community to reach *outside the closed world* and explore the challenges and chances of embedding machine learning in real-world security systems.

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A Pitfalls

Table 6 provides further information and examples for data snooping, introduced in §2.

B Mobile Malware Detection

Here we describe the additional dataset used in our experiments and detail the experimental setup considered in §4.1.

Analysis of the Drebin dataset. In addition to AndroZoo [6], we also analyze the meta information of the DREBIN [9] dataset. Interestingly, we find that 76.2 % of the benign data has been collected from GooglePlay, while the fraction of malicious data is only 4.6 %. Although the origins for the majority of malicious samples is unknown (86.9 %), our findings strongly suggest the presence of a sampling bias in this dataset as well.

Experimental setup. To extract the features for DREBIN [9] and OPSEQS [89], we use our implementation of DREBIN and the publicly available program code provided by McLaughlin et al. [89] to extract opcode n-grams. Using the extracted features, we represent each app as a binary vector and train a linear SVM [48] on the dataset. We use 75 % of the data for training and the remaining 25 % for testing. To select good hyperparameters for our classifiers, we perform a grid search on the training data for $C = \{10^{-2}, 10^{-1}, ..., 10^2\}$ and $n = \{2, 3, 4\}$ using 5-fold cross validation, where n refers to the length of the opcode n-grams. Finally, we assess the performance of the best model on the test data. We repeat the experiments ten times and average the results.

C Vulnerability Discovery

We provide information on the model and the evaluation methodology used for our experiments on vulnerability discovery in §4.2.

Models and preprocessing. For VulDeePecker [82], we train a neural network consisting of a bidirectional LSTM layer with 300 units that is followed by a dropout layer with a probability of 0.5 and a dense layer of size 2 employing a softmax non-linearity. We use the Adam optimizer [74] with a batch size of 64 and train for 10 epochs (the network begins to overfit the training set after \sim 6 epochs).

The code snippets are preprocessed as described by Li et al. [82] and a word2vec [90] embedding of 200 dimensions is trained for 100 iterations to achieve vector representations of

the generic code tokens. Word2vec models are solely determined based on the training data. Unknown tokens that occur at test time are replaced with a vector of zeros—the same value that is used to pad code snippets shorter than 50 tokens.

For the linear SVM, we use a regularization cost of C = 1.0 and token-level n-grams extracted from the generic tokens of the training data.

Performance evaluation. To compare the performance of VulDeePecker and the SVM, we split the data into a randomly chosen training set (80%), validation set (10%), and test set (10%) for 10 trials. Both methods learn on the training set only and we use the model that performs best on the validation set. Finally, we compute ROC curves on the test data also containing unseen data instances and average the results over the 10 individual trials. The results are presented in Table 4 of §4.2. Note that picking an optimal threshold from these ROC curves is a form of data snooping (P3). In this case, however, we only use the ROC curves to compare the two classifiers on unseen data.

D Source Code Authorship Attribution

Here we provide further intuition on the problem of artifacts in datasets for authorship attribution and describe the experimental setup used in §4.3 in more detail.

Artifact examples. Figure 10 exemplifies how attribution methods exploit features from copied code. The selected author copies both arrays in all files but never uses them. It turns out that the AST feature '1' is one of the most important features for classifying this author. However, these copied arrays are unrelated to the programming task and thus only loosely related to coding style in practice.

```
constexpr int dx[] = {-1, 0, 1, 0, 1, 1, -1, -1};
constexpr int dy[] = {0, -1, 0, 1, 1, -1, 1, -1};
```

Figure 10: Artifact example from the code GCJ dataset. Arrays are unused, but present in all files by the same author.

Experimental setup. For our evaluation of the attribution methods by Caliskan et al. [22] and Abuhamad et al. [2], we use a publicly available reimplementation built on top of Clang [103]. We also use a stratified and grouped 8-fold cross-validation where the dataset is divided into seven challenges for training and one challenge for testing, respectively. To select hyperparameters for each fold, we further perform a grid search on the training set using 3-fold stratified and grouped cross validation. We perform feature selection and a tf-idf transformation where we derive the parameters from the respective training set. Finally, we measure the accuracy of the best performing model on the test set. We report results for all eight folds in Figure 8 of §4.3, as the difficulty of attribution can vary across the GCJ challenges.

Table 6: Overview of data snooping groups and types

| Group | Types | Description |
|--------------------|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Test Snooping | Preparatory work | If the test set is used for any experiments except for the evaluation of the final model, the learning setup benefits from additional knowledge that would not be available in practice. This includes steps to find features, to limit the number of features through feature selection, and to select parameters or learning methods before starting with the actual evaluation. |
| | K-fold cross-validation | Another type of snooping occurs if researchers tune the hyperparameters by using k-fold cross-validation with the final test set for evaluation, and report these results. |
| | Normalization | Normalization factors, such as tf-idf, are computed on the complete dataset, i.e., before splitting the dataset into training and test set. |
| | Embeddings | Similarly, embeddings for deep neural networks are derived from the complete dataset, instead of just using the training data. |
| Temporal Snooping | Time dependency | Time dependencies within the data are not considered, so that samples are detected with features that would only be available in the future. For instance, k-fold cross validation on a malware dataset likely includes a sample of each malware family in the training set, although new families would be unknown in a real-world setting [101]. |
| | Aging datasets | The usage of well-known datasets from prior work can also introduce a bias. Researchers may implicitly incorporate prior knowledge by using previous insights from these publicly available datasets, such as previously derived thresholds. |
| Selective Snooping | Cherry-picking | Data is cleaned based on information that is usually not available in practice. For instance, applications are filtered out that are not detected by a sufficiently large number of AV scanners. |
| | Survivorship bias | A group of samples is already filtered out. This bias overlaps with sampling bias (P1). For example, GooglePlay data introduces a survivorship bias, since only apps that pass Google's vetting process can be used for the experiments. Likewise, using only applications, which a dynamic analysis system can successfully process and removing all others from the dataset, also introduces a survivorship bias. |

Reproducing the setup of Caliskan et al. [22], we use a random forest with layout, lexical and syntactical features. For Abuhamad et al. [2], we use the originally proposed features consisting of word *n*-grams, but apply a random forest only rather than a combination of recurrent neural network and random forest. We find that this leads to a comparable accuracy and has the benefit of a simpler analysis of each features' contribution to the classification.

Furthermore, we implement small linter tools in Clang that remove the following five groups of unused code in our experiments: functions, local and global declarations, typedefs, records, and headers.

E Network Intrusion Detection

We provide details on the experimental setup as used for the case study on network intrusion detection described in §4.4.

Experimental setup. For training the ensemble of autoencoders, we follow the procedure of KITSUNE [92]. The

115 features are derived from seven damped incremental statistics describing packet relationships of five time windows of up to a one minute interval. To determine a suitable number of autoencoders, we apply a hierarchical clustering to the first 5,000 examples from the feature set, resulting in a maximum of m=10 inputs per autoencoder. Overall, this corresponds to 12 autoencoders in parallel. The outputs of these autoencoders are passed to another, final autoencoder which operates as the anomaly detector. The root mean squared error (RMSE) representing the autoencoders' reconstruction error is output for each packet individually. Consequently, we apply a threshold to the RMSE values, depending on how many false positives can be tolerated.

For both methods, the first 50,000 packets are used for training and the remaining 714,136 packets for testing. This corresponds to the first 30.5 and 80.4 minutes of the network packet capture, respectively.