



# AI/ML for Network Security: The Emperor has no Clothes

<https://trusteeml.github.io/>

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## ABSTRACT

Several recent research efforts have proposed Machine Learning (ML)-based solutions that can detect complex patterns in network traffic for a wide range of network security problems. However, **without understanding how these black-box models are making their decisions, network operators are reluctant to trust and deploy them in their production settings**. One key reason for this reluctance is that these **models are prone to the problem of underspecification**, defined here **as the failure to specify a model in adequate detail**. Not unique to the network security domain, this problem manifests itself in ML models that exhibit unexpectedly poor behavior when deployed in real-world settings and has prompted growing interest in developing interpretable ML solutions (e.g., decision trees) for “explaining” to humans how a given black-box model makes its decisions. However, synthesizing such explainable models that capture a given black-box model’s decisions with high fidelity while also being practical (i.e., small enough in size for humans to comprehend) is challenging.

In this paper, we focus on synthesizing high-fidelity and low-complexity decision trees to help network operators determine if their ML models suffer from the problem of underspecification. To this end, we present TRUSTEE, a framework that takes an existing ML model and training dataset as input and generates a high-fidelity, easy-to-interpret decision tree and associated trust report as output. Using published ML models that are fully reproducible, we show how practitioners can use TRUSTEE to identify three common instances of model underspecification; i.e., evidence of shortcut learning, presence of spurious correlations, and vulnerability to out-of-distribution samples.

## CCS CONCEPTS

• **Networks** → **Network security**; • **Computing methodologies** → **Machine learning**; • **Security and privacy**;

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## KEYWORDS

Network Security; Artificial Intelligence; Machine Learning; Explainability; Interpretability; Trust;

## 1 INTRODUCTION

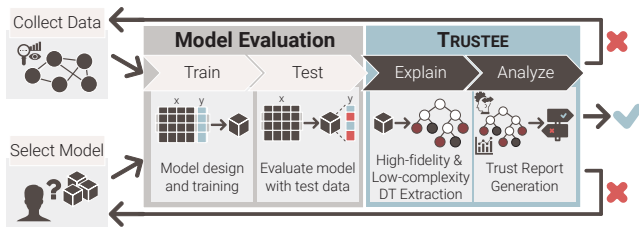
In the last few years, we have witnessed a growing tension in the network-security community. Recent research has demonstrated the benefits of Artificial Intelligence (AI) and Machine Learning (ML) models over simpler rule-based heuristics in identifying complex network traffic patterns for a wide range of network security problems (see recent survey articles such as [9, 46, 55, 62]). At the same time, we have seen reluctance among network security researchers and practitioners when it comes to adopting these ML-based research artifacts in production settings (e.g., see [2, 4, 58]). **The black-box nature of most of these proposed solutions is the primary reason for this cautionary attitude** and overall hesitance. More concretely, the **inability to explain how and why these models make their decisions renders them a hard sell compared** to existing simpler but typically less effective rule-based approaches.

This tension is not unique to network security problems but applies more generally to any learning models, especially when their decision-making can have serious societal implications (e.g., health-care, credit rating, job applications, and criminal justice system). At the same time, this basic tension has also driven recent efforts to “crack open” the black-box learning models, explaining why and how they make their decisions (e.g., “interpretable ML” [51], “explainable AI (XAI)” [59], and “trustworthy AI” [12]). However, to ensure that these efforts are of practical use in particular application domains of AI/ML such as network security is challenging and requires further qualifying notions such as (model) interpretability or trust (in a model) [40] and also demands solving a number of fundamental research problems in these new areas of AI/ML.

In this paper, we first provide such a qualification that is motivated by the needs of the field of network security as application domain of AI/ML and equates “an end user having trust in an AI/ML model” with “an end user being comfortable with relinquishing control to the model” [40]. Given this specific definition of what it

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**Figure 1: TRUSTEE overview.**

means for an AI/ML model to engender trust, we next address a number of fundamental research challenges related to the **problem of quantitatively deciding when an end user is comfortable with relinquishing control to a given AI/ML model**. To this end, a particular focus of this paper is on determining whether or not a given AI/ML model suffers from the *problem of underspecification* [17].

Here, the problem of underspecification in modern AI/ML refers to **determining whether the success of a trained model (e.g., high accuracy) is indeed due to its innate ability to encode some essential structure of the underlying system or data or is simply the result of some inductive biases** that the trained model happens to encode. In practice, inductive biases typically manifest themselves in instances of shortcut learning strategies [28], signs of spurious correlations [3], or an inherent inability for out-of-distribution (o.o.d.) generalizations (i.e., test data distribution is different from training data distribution). The **implication of such inductive biases is that their presence in trained AI/ML models prevents these models from being credible or trustworthy**; that is, generalize as expected in deployment scenarios. Thus, for establishing the specific type of trust in an ML model considered in this paper, it is critical to be able to identify these inductive biases, and this paper takes a first step towards achieving this ambitious goal.

To detect underspecification issues in learning models for network security problems, we develop TRUSTEE (TRUST-oriented decision Tree Extraction). This framework provides a means for carefully inspecting black-box learning models for the presence of inductive biases. Figure 1 shows how TRUSTEE augments the traditional ML pipeline to examine the trustworthiness of a given ML model. Specifically developed with the application domain of network security in mind, **TRUSTEE takes a given black-box model and the dataset that has been used to train that model as input and outputs a “white-box” model in the form of a high-quality decision tree (DT) explanation**.

Importantly, in synthesizing this DT, TRUSTEE’s focus is first and foremost on ensuring its practical use which, in turn, requires **leveraging domain-specific observations to strike a balance between model fidelity (i.e., accuracy of the DT with respect to the black-box model), model complexity, and model stability**. Here, complexity refers to both the size of the DT and to aspects of the tree’s branches. In particular, when viewing the tree’s branches as decision rules, we are concerned with their explicitness and intelligibility; that is, we require these rules to be readily recognizable by domain experts and be largely in agreement with the experts’ domain knowledge. Model stability, on the other hand, is concerned with the correctness, coverage and stability of the decision rules; that is, we require them to correctly describe how the given black-box model makes a significant number of its decisions and also want them to be largely

insensitive to the particular data samples that TRUSTEE used in the process of selecting its final DT explanation. We achieve this insensitivity or stability by implementing a heuristic method that **selects from among a number of different candidate DTs the one that has the highest mean agreement**. Here, the agreement between two different DTs is a measure of how often the two DTs will make the same decision for the same input data [30, 60]. In practical terms, implementing this heuristic reduces the likelihood that TRUSTEE outputs a misleading DT explanation.

TRUSTEE also outputs a trust report associated with the DT explanation, which operators can consult to determine whether there is evidence that the given black-box model suffers from the problem of underspecification. If such evidence is found, the information provided in the trust report can be used to identify components of the traditional ML pipeline (e.g., training data and model selection) that need to be modified in an effort to improve upon an ML model that TRUSTEE has found to be untrustworthy.

While our work contributes to the rapidly growing ML literature on model explainability/interpretability and is inspired by ongoing developments in this area, our efforts and objectives differ from existing approaches in a number of significant ways. For one, given the inherent complexity of learning problems for networking, existing approaches for replacing black-box models with “white-box” models that are inherently explainable in the first place (e.g., decisions trees) are in general impractical. Moreover, *local interpretability* methods [31, 48, 53] are not suitable for examining the various instances of the underspecification problem. At the same time, although our effort is motivated by prior studies that focus on *global interpretability* [6, 7, 37], these works are either only applicable to a specific class of learning models (e.g., reinforcement learning) or suffer from poor fidelity.

Through various case studies, we illustrate in Section 7 how operators can use TRUSTEE’s DTs and associated trust reports to detect the presence of inductive biases. More specifically, we use published ML models that are reproducible (i.e., code base and datasets are publicly available) to show how network operators can use the information provided by TRUSTEE to detect instances of shortcut learning strategies, obtain evidence of overfitting and/or whether the model relies on spurious correlations to make its decisions, or determine the model’s inability to generalize to out-of-distribution data.

## 2 BACKGROUND AND RELATED WORK

The application domain of AI/ML considered in this paper is the area of network security. In this section, we first discuss the unique challenges that this area poses for utilizing the latest advances in AI/ML. In particular, we focus on important recent AI/ML concepts such as “interpretable ML” and “explainable AI” and discuss their relevance for our work.

### 2.1 Challenges in ML for Network Security

Beyond the already-mentioned trust issue, there are a number of other reasons why the area of network security is a particularly challenging application domain for AI/ML. Networking-related datasets in general and cybersecurity-specific datasets in particular typically contain information about what is being communicated

over a network (e.g., packet-level traffic traces) or provide insight into how networks enable such information exchanges. As such, the datasets often raise serious end user-specific privacy concerns or reveal provider-specific details that many companies consider to be proprietary in nature and are therefore unwilling to share. The result is a general paucity of publicly available datasets. Moreover, the datasets that are publicly available generally lack the complexity of real-world settings, either because they have been synthetically generated, have been obtained from small-scale testbed environments, or have been anonymized to the point where their general utility has been severely curtailed.

The scarcity of carefully labeled data poses an even bigger problem. Networking or cybersecurity datasets do not come in the form of images that humans can recognize but typically consist of semantically rich content, and unpacking that content and properly labeling it often requires substantial domain knowledge (e.g., network architecture, protocols, and standards). This need for domain knowledge rules out labeling approaches that have been used successfully in other domains and include crowdsourcing (e.g., for labeling images that are part of open-source databases such as ImageNet [18]) or outsourcing (e.g., for labeling datasets that have been curated and open-sourced by commercial self-driving car companies for the benefit of researchers [14, 15]).

## 2.2 Interpretable ML and Explainable AI

As the scientific community continues to develop sophisticated AI/ML-based tools for high stakes decision-making throughout society, there has been a growing awareness about their actual or potential misuses and negative implications. As a result, calls for starting to study “trustworthy AI”, “responsible AI”, “ethical AI” and related topics have intensified in recent years and have identified model interpretability/explainability as a critically important but also highly elusive concept for facilitating these studies [40].

**Interpretable ML: Ex-ante Interpretability.** The application of modern AI/ML has resulted in a myriad of different learning models that are “black-box” in nature; that is, provide no insight in or understanding about why the black-box model makes certain decisions (and not some other decisions) or what decision-making process gives rise to these decisions. This development has resulted in a recent explosion of work on “Explainable AI,” where a second (post-hoc) model is created to explain the originally obtained black-box model [59]. This pursuit of explainable AI has been criticized in the recent AI/ML literature and called “problematic” (see, for example [51]), mainly because such post-hoc explanations are often not reliable and can be misleading [29, 37]. An alternative approach that has been advocated in [51] argues for using learning models such as linear models or DTs that are inherently (*i.e.*, ex-ante) interpretable.

Unfortunately, because of the rich semantic content of the data in the network security domain, uncovering the types of patterns in the data that matter has become increasingly the responsibility of trained “black-box” models rather than painstakingly-designed inherently explainable models. However, instead of considering this development as being “problematic,” we view it as an unique opportunity to ultimately achieve the vision of interpretable ML, ensuring that AI/ML models used for high stakes decision-making are fully comprehensible by their end users and interested third parties.

**Explainable AI: Post-hoc Interpretability.** A commonly-made argument in favor of using black-box models such as deep neural networks or random forests is that they typically achieve higher accuracy compared to their interpretable counterparts (e.g., DTs) and are therefore often more desirable when used in practice. Although this argument is not universally shared (e.g., see [51]), it nevertheless has been a driving force behind the recent efforts on the topic of “explainable AI.” Also referred to XAI [59], explainable AI describes efforts where the development of a trained black-box model is followed up with additional activities that are intended to help “explain” the originally obtained black-box model. These efforts can be divided into two disjoint categories, namely *local explainability* and *global explainability*.

Methods for providing local explanations aim at illuminating how a black-box model makes individual decisions (or decisions in a local region near a particular data point) and include well-known techniques such as LIME [48], SHAP [41], and LEMNA [31]. Since these methods limit their attention to only a subset of individual decisions, they are prone to providing misleading explanations [40, 45, 64], depending on the subset of samples analyzed. Related methods such as Partial Dependence Plots (PDP) [27] and Accumulated Local Effect (ALE) plots [1] suffer from similar shortcomings. As such, these methods are of limited use when we seek explanations that we can trust in the sense that they accurately describe how a given black-box model makes decisions holistically.

In turn, methods that provide global explanations aim at describing how a given black-box model makes its decisions “as a whole” and not one data sample at a time. Extracted from the black-box model in a second step (*i.e.*, post-hoc), such explanations typically take the form of an inherently interpretable model such as a rule set or a DT [6, 38] and become the main vehicles for studying the decision-making process of the original black-box model and examining its properties. However, existing approaches for such post-hoc extractions of global explanations are known to produce at times too low of a fidelity to be useful in practice [6], target only a very specific set of black-box models [7], be difficult to reproduce [37, 38], and be possibly unreliable to the point of being misleading [29, 37]. To achieve the level of explainability required in high-stakes application domains such as network security, we seek to generate high-fidelity global explanations that are capable of accurately and faithfully describing a majority of the decisions made by any given black-box model.

## 3 TRUSTEE OVERVIEW

Our focus in this paper is on post-hoc global model interpretability for the application domain of network security problems. The idea of using DTs for investigating global model interpretability for a given black-box model is not novel. However, the set of requirements that we impose on the DT explanations is non-standard and makes this a challenging problem, which motivated us to develop TRUSTEE.

For one, we require that our new DT extraction method be model-agnostic; that is, applicable to any given black-box model. Second, we also demand that the method produces high-fidelity DT explanations; that is, DTs whose expected predictive performance is similar to that of the black-box model. To quantify the fidelity of

DTs, we rely on well-known metrics; for example, while for classification problems we measure fidelity using the F1-score between classifications from the black-box model and the DT, for regression problems, we measure fidelity in terms of the R-squared value between the predictions from the black-box and the DT. The third requirement we impose is that the extraction method also results in low-complexity DT explanations such that selected parts of the DTs are intelligible and comprehensible (*i.e.*, easy to understand by domain experts) and accurately describe how the black-box model makes most of its decisions. The fourth and last requirement concerns a stability property that we want our new DT extraction method to have. In particular, to reduce the chances that this output provides a misleading DT explanation, we require that most of the final DT's decisions should be insensitive to the minute details of how this final DT explanation has been determined.

For a DT that TRUSTEE extracts from a given black-box model and satisfies this set of requirements, our next goal is to summarize the pertinent aspects of this synthesized tree in a trust report. This trust report is intended to help end users determine whether the given black-box model suffers from the problem of underspecification and cannot be trusted. To achieve this goal, we look for ways to exploit the extracted DT explanation for the purpose of enabling the end users to investigate the black-box model for likely indications of the presence of inductive biases. In particular, in this paper we consider the following three instances of inductive biases: (i) instances of shortcut learning, (ii) signs of spurious correlations, and (iii) problems with out-of-distribution samples.

Note that the presence of any of these inductive biases proves that the given black-box model suffers from the underspecification problem and cannot be trusted. At the same time, the absence of these instances does not mean that the black-box model can be trusted. In fact, while proving for an arbitrary black-box model that the model does not suffer from the underspecification problem is hard and remains an unsolved problem, showing that the model does suffer from the underspecification problem only requires demonstrating the presence of a single instance of an inductive bias, and our design of TRUSTEE is an initial effort that simplifies demonstrating that certain biases are present in a given model. After describing TRUSTEE's design in detail in Section 4, we illustrate the end-to-end application of TRUSTEE, including the use of the extracted DT explanation and resulting trust report with a number of illustrative examples in Section 7.

## 4 EXTRACTING DECISION TREES

The first step to realize the agenda detailed in Section 3 consists of generating high-fidelity and inherently interpretable (*i.e.*, “white-box”) counterparts for any given black-box model, regardless of the learning method used by the black-box. To this end, we first discuss existing approaches to this problem and their limitations. We then present TRUSTEE, an original and practical framework that end users can apply to extract high-fidelity DT explanations from an arbitrary black-box learning model.

### 4.1 Existing approaches

Global white-box explanations extracted from a black-box model can often describe in detail the reasoning behind the model's

behavior, provided they achieve a good enough fidelity. Earlier works [6, 7, 16, 43] have proposed different approaches to extracting DT explanations from black-box models, but these DTs typically do not satisfy all the above-listed requirements and are therefore ill-suited for end users who want to gauge their level of trust in a given black-box model. We list a number of relevant prior efforts and their pertinent features in Table 1. Note that some of these existing methods [7, 43] are not model-agnostic but have been designed for specific learning paradigms and models, such as Reinforcement Learning. As such, they typically rely on assumptions that are specific to the learning paradigm or model that their designs focus on. On the other hand, prior efforts that do propose model-agnostic approaches [6, 16] tend to produce DT explanations that don't satisfy the fidelity requirement that we demand for realizing our objective (see our technical report [34] for empirical evidence).

**Table 1: Existing approaches to extract decision trees.**

Method	Optimization Objective	Stopping Criterion	Model Agnostic	High Fidelity	Domain-specific Pruning
Trepan [16]	Fidelity	Max Nodes	✓	-	-
dtextract [6]	Accuracy	Max Nodes	✓	-	-
VIPER [7]	RL Reward	Max Iterations	-	-	-
Metis [43]	RL Reward	Max Iterations	-	-	-
TRUSTEE	Fidelity	Max Iterations	✓	✓	✓

Another important aspect of many of these existing efforts is the stopping criterion they use to obtain their extracted DT explanations. For example, prior efforts such as [6, 16] require specifying the maximum size (*i.e.*, number of nodes) that the extracted DT can have and use this input parameter as stopping criterion. Such approaches are convenient for obtaining explanations that are guaranteed to be of a certain size, but this convenience typically comes at the cost of low fidelity, implying that important decision-making rules may be missing from the resulting DT. Other methods such as [7] and [43] extract DT explanations in an iterative fashion, require specifying the maximum number of iterations, and use this user-specified input parameter as stopping criterion. Even though these methods do not explicitly optimize for fidelity, they typically produce high-fidelity explanations, but at the cost of high complexity (*i.e.*, the large size of the resulting explanations makes interpreting cumbersome if not impractical). To overcome this problem, the authors of [43] rely on a commonly-used technique called Cost-Complexity Pruning (CCP) [27]. Similar to other pruning methods [25], CCP succeeds in striking a balance between the overall fidelity of the extracted DTs and their size. However, from an interpretability perspective, CCP tends to be oblivious to what role each decision-making rule plays as part of the resulting DT explanations. Because of this observed trade-off between model complexity and model interpretability, these methods are ill-suited for our purpose where we strive to shed light on the decision-making rules that are key to interpreting black-box models that arise in the context of solving network security-related problems.

### 4.2 Model-Agnostic Decision Tree Extraction

Given the absence of readily available model-agnostic methods for extracting high-fidelity, low-complexity, and stable DTs from black-box ML models, we present in the following TRUSTEE. Algorithm 1 describes the steps that TRUSTEE takes to achieve its objective.

At a high level, these steps are executed as part of an outer loop (lines 4-16) that is executed a total of  $S$  times. Each iteration of this outer loop involves an inner loop (Lines 5-12) that is performed  $N$  times. Here, this inner loop is designed to generate different high-fidelity DT explanations, one per iteration. It does so by applying a teacher-student dynamic derived from imitation learning [33] that uses  $\pi^*$  as an oracle in conjunction with a carefully curated dataset  $\mathcal{D}'$  to guide the training of a surrogate “white-box” model in the form of a DT that imitates the black-box’s decisions. In contrast, the purpose of the outer loop is (i) to select from among the  $N$  high-fidelity DTs that have been generated in the process of executing the inner loop the DT with the highest fidelity, (ii) to transform this resulting DT into a high-fidelity and low-complexity DT by means of a post-processing step that consists of applying a purposefully-developed pruning method (see Section 5 for details), and (iii) to consider all  $S$  high-fidelity and low-complexity DTs that have been generated in the process of executing the outer loop and output the one that is the most stable in the sense of having the highest mean agreement among these  $S$  DTs.

Algorithm 1 takes as input a given black-box model  $\pi^*$  that we desire to explain and the original dataset  $\mathcal{D}_0$  that was used to train  $\pi^*$ . Other parameters that the algorithm requires as input are the number of iterations  $S$  for the outer loop, the number of iterations  $N$  for the inner loop, the number of samples  $M$  to select from  $\mathcal{D}_0$  to use when training the surrogate DTs as part of each iteration of the inner loop, and a parameter  $k$  that is required by the tree pruning method used in Line 14 and is discussed in more detail in Section 5 below. The algorithm starts by initializing the training dataset  $\mathcal{D}$  (Line 2) using the given black-box  $\pi^*$  to predict the expected outcomes from the given input data  $\mathcal{D}_0$ . It then initializes a set of DTs (Line 3) from which, at the end (Line 17), the most stable DT explanation will be selected and returned as output by TRUSTEE (Line 18).

To execute the inner loop as part of an iteration of the outer loop, the steps that the algorithm performs during the  $j$ -th ( $1 \leq j \leq N$ ) iteration of the inner loop consist of (i) selecting  $M$  training samples uniformly at random from the optimal prediction dataset  $\mathcal{D}$  (Line 6) to initialize a training dataset  $\mathcal{D}'$ ; (ii) splitting the dataset  $\mathcal{D}'$  for training and testing (Line 7); (iii) training a DT student  $\hat{\pi}_j$  on  $\mathcal{D}'_{train}$  (Line 8) by using the well-known CART method [11]; (iv) testing the DT explanation using  $\mathcal{D}'_{test}$ , collecting the samples that the DT classifier wrongly classifies into the set  $\mathcal{D}'_e$  (Line 9), and querying the black-box model for the expected results for  $\mathcal{D}'_e$  (Line 7) to produce a correction dataset  $\mathcal{D}_j$  (Line 10); and (v) augmenting the optimal dataset  $\mathcal{D}$  with this correction dataset (Line 11) to reinforce the correct decisions during the subsequent iterations of the inner loop.

The steps that the algorithm executes during the  $i$ -th ( $1 \leq i \leq S$ ) iteration of the outer loop are (i) perform  $N$  iterations of the inner loop (Lines 6-11), (ii) select from among the  $N$  generated different student models the one DT explanation with the highest fidelity (Line 13), and (iii) apply a special pruning method to this highest-fidelity DT to obtain a high-fidelity and low-complexity DT explanation candidate. Finally, after  $S$  iterations of this outer loop, the algorithm selects from among the  $S$  obtained different high-fidelity and low-complexity DT explanation candidates the one that has the highest mean agreement (i.e., is the most stable) and returns this “best of the best” DT as final output of TRUSTEE.

In the following, we provide a more detailed description of the main design choices we made for TRUSTEE and further evaluate some of these design choices as part of an ablation study in Section 8.

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**Algorithm 1** Model agnostic decision tree explanation extraction.

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1: procedure TRUSTEE(
     $\pi^*$ : Black-box model,
     $\mathcal{D}_0$ : Initial training dataset,
     $M$ : Number of samples to train the decision tree,
     $N$ : Number of iterations of inner loop,
     $S$ : Number of iterations of outer loop,
     $k$ : Parameter for Top- $k$  Pruning),
2:   Initialize dataset using black-box  $\mathcal{D} \leftarrow \pi^*(\forall x \in \mathcal{D}_0)$ 
3:   Initialize stabilization set of DTs  $\mathcal{R} \leftarrow \emptyset$ 
4:   for  $i \leftarrow 1 \dots S$  do
5:     for  $j \leftarrow 1 \dots N$  do
6:       Sample  $M$  training cases uniformly from  $\mathcal{D}$ 
7:        $\mathcal{D}' \leftarrow \{(x, y) \stackrel{\text{i.i.d.}}{\sim} U(\mathcal{D})\}$ 
8:       Split sampled dataset for training and testing
9:        $\mathcal{D}'_{train}, \mathcal{D}'_{test} \leftarrow \text{TRAINTESTSPLIT}(\mathcal{D}')$ 
10:      Train DT
11:       $\hat{\pi}_j \leftarrow \text{TRAINDECISIONTREE}(\mathcal{D}'_{train})$ 
12:      Test and get samples DT misclassifies
13:       $\mathcal{D}'_e \leftarrow \{(x, y) \in \mathcal{D}'_{test} \mid \hat{\pi}_j(x) \neq \pi^*(x)\}$ 
14:      Get correct outcome from black-box
15:       $\mathcal{D}_j \leftarrow \pi^*(\forall x \in \mathcal{D}'_e)$ 
16:      Augment dataset  $\mathcal{D} \leftarrow \mathcal{D} \cup \mathcal{D}_j$ 
17:     end for
18:     Select tree with highest fidelity
19:      $\hat{\pi}_{max} \leftarrow \hat{\pi} \in \{\hat{\pi}_1, \dots, \hat{\pi}_N\}$ 
20:     Prune selected tree  $\hat{\pi}_i \leftarrow \text{TOPKPRUNE}(\hat{\pi}_{max}, k)$ 
21:     Add tree to the stabilization set  $\mathcal{R} \leftarrow \mathcal{R} \cup \hat{\pi}_i$ 
22:   end for
23:   Select tree with highest mean agreement with others
24:    $\hat{\pi}_{agree} \leftarrow \hat{\pi} \in \mathcal{R}$ 
25:   return  $\hat{\pi}_{agree}$ 
26: end procedure

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**Multiple iterations and uniform sub-sampling.** The CART algorithm that is traditionally used to train DT models relies on a greedy approach for finding the best splits in the given training dataset. This greedy approach ensures that for a given training dataset, the resulting DT will be largely insensitive to the order in which the input samples are processed. At the same time, this greedy approach is prone to produce over-fitted DTs [10]. While using this approach without further constraints (e.g., stopping criterion) to train a DT results in perfect fidelity, being over-fitted makes the resulting DT ill-suited for providing an intelligible explanation for how the given black-box model makes its decisions. Instead, the resulting DT explanation is largely an artifact of the method used to generate the explanation. To overcome this problem, TRUSTEE implements an iterative approach to train multiple student models on the expert model predictions. This iterative approach is implemented as the inner loop in Algorithm 1, where at each iteration, we select a fraction  $M$  of the input data by uniform sub-sampling from the original training dataset (Lines 5-11). This approach differs from existing efforts [7] in that by requiring the uniform sub-sampling step at each iteration, we ensure that each DT explanation will have only a limited view of the entire data, akin to a k-fold cross

validation [52]. Incorporating this sub-sampling step allows us to stress-test how different features and/or feature values contribute to the decision-making of the black-box model and then select the ones that best fit our overall objective. In practical terms, uniform sub-sampling from the original training dataset assumes each sample has the same probability of being selected (*i.e.*, balanced dataset). While it is well known that using imbalanced datasets to train ML models leads to biases towards the majority classes, the existing ML literature provides several approaches that resolve this problem through proper pre-processing of the original training data [36].

**Dataset augmentation.** An important design choice for TRUSTEE involves a dataset augmentation step (Line 9), where in each iteration of the inner loop, the algorithm uses the optimal predictions from the black-box model on the sampled dataset  $D'$  to augment the original training dataset  $D$ . The purpose of this step is to over-correct for data samples for which the student DT model makes wrong decisions. Leveraging results from the existing literature on imitation learning [7, 50], performing this step can not only increase the overall accuracy of the trained student model but also reduce the overall number of leaf nodes in the resulting tree.

**Fidelity as objective function.** When selecting from among the different student models that TRUSTEE extracts from a given black-box model, it uses model fidelity as objective function and picks the student model with the highest fidelity (Line 11). This design choice implies that while the final DT explanation produced by TRUSTEE is not necessarily the most *accurate* DT for the given classification problem, it is the DT that is the most *faithful* one in terms of explaining how the black-box model makes its decisions. Intuitively, it is by insisting on this high-fidelity aspect of the DTs that TRUSTEE considers that we are able to post-process the resulting DT explanation in ways that will help end users with varying degrees of domain knowledge to gauge their trust in the given black-box model. We provide evidence in support of this intuition in Section 5 where we describe the type of post-processing that we perform as part of TRUSTEE so the final DT explanation it outputs can serve as an inherently practical means for faithfully explaining most of the given black-box model's decisions.

**Model stability.** Since the inner loop of Algorithm 1 (Lines 6-11) uses a different random subset of the entire dataset each time it trains a DT explanation, it is possible for TRUSTEE to output a misleading explanation because of the particular subset of data that was used to train that final DT explanation. To minimize the chances for such scenarios to occur, we add an outer loop in Algorithm 1 (Lines 4-16). This addition results in the extraction of  $S$  different high-quality DT explanations from the given black-box model and allows us to measure the agreement among these  $S$  different DT explanations. The agreement of DTs is a well-known measure of how often a pair of DTs will make the same decisions for the same input data and is a metric that has been used in previous studies that concern assessing the stability of different DTs [30, 60]. Here, to select the final DT explanation that is returned as output of TRUSTEE (Line 18), Line 17 in Algorithm 1 computes the pair-wise agreement among all  $S$  DT explanations and selects the one with highest mean agreement. While implementing this outer loop prevents TRUSTEE from generating obviously misleading explanations

and gives domain experts confidence that they can trust the explanations produced by TRUSTEE's output, rigorously proving that a "white-box" model extracted from a given black-box model does not provide misleading explanations is an active area of current research [37].

## 5 PROCESSING DECISION TREES

When using TRUSTEE to synthesize a high-fidelity DT explanation for a given black-box model, realizing the agenda outlined in Section 3 requires performing an additional step in Algorithm 1 (Line 14) each time  $N$  iterations of the inner loop have completed and the algorithm has selected the highest-fidelity DT from among the resulting  $N$  different high-fidelity DT candidates (Line 13). The purpose of this step is to transform this selected highest-fidelity DT into a DT explanation for the given black-box model that is inherently practical in the sense of having low complexity and at the same time high fidelity. Here, low complexity of a DT explanation refers to small trees but also, and more importantly, trees whose main branches (*i.e.*, decision rules ranked by number of input samples they classify) explicitly, intelligibly, and accurately describe how the black-box model makes most of its decision. Effectively, when generating this low-complexity and high-fidelity DT explanation as a result of this post-processing step, we tolerate some loss of fidelity in return for achieving low complexity. In the following, we examine different aspects of this fidelity-complexity trade-off and introduce a simple tree pruning method that we call *Top-k Pruning* and that comprises the required post-processing step. We design this method for the explicit purpose of ensuring that any final DT explanation that TRUSTEE outputs can be readily processed and understood by domain experts.

### 5.1 Decision Tree Pruning: Trade-offs

One of the main disadvantages of CART models is that CART's greedy algorithm is known to be prone to overfitting, often producing high-fidelity DTs that can have thousands of nodes [25]. Clearly, such large trees are detrimental to our ultimate goal; that is, presenting end users with inherently practical explanations that they can readily inspect and understand with their available domain knowledge. In designing TRUSTEE, we similarly focused on first obtaining largely unconstrained DT explanations with the best possible fidelity (Line 13). However, our reasoning for doing so is that we explicitly require that any DT explanation that TRUSTEE outputs will have undergone a post-processing phase for the purpose of making this final DT explanation intelligible and comprehensible for end users. Our intuition behind obtaining a high-fidelity DT explanation first and addressing its complexity later is that manipulating a high-fidelity explanation with an eye towards reducing its complexity is more likely to result in explanations that, while experiencing some decrease in their fidelity, still will have higher fidelity than their counterparts that had lower fidelity to start with.

A commonly-used approach to transforming large DTs into trees of smaller sizes is pruning, and the existing literature describes several pruning methods for DTs [25, 27], many of which are highly effective in obtaining DTs that have small complexity, at least as far as the sizes of the trees are concerned. Among the most widely-used approaches to pruning are (i) pre-pruning which limits either the total number of nodes or the overall depth of



the tree and (ii) post-pruning, such as Cost-Complexity Pruning (CCP) [27]. On the one hand, by explicitly constraining either the number of tree nodes or the tree's depth, the pre-pruning approaches allow for direct control over the size of the resulting DT. However, this control over tree size typically comes at the cost of reduced fidelity, mainly because the obtained small trees run the risk of missing important decision branches as they prevent the consideration of any further decision branches once the stopping criterion is reached. On the other hand, using post-pruning such as CCP often results in a better trade-off between fidelity and size. However, this better trade-off comes at the cost of reduced interpretability, mainly because CCP relies on a parameter that is indirectly responsible for how many nodes of a tree get pruned. Lack of a more direct control makes it difficult to decide which tree branches to include in the pruned tree and which to exclude.

## 5.2 Top- $k$ Pruning Method

Each branch in any of the highest-fidelity DTs that are selected in the process of executing an iteration of Algorithm 1's outer loop (*i.e.*, Line 13) represents a decision "rule"; that is, a combination of individual decisions on features that results in labeling the input data as belonging to a specific class (*e.g.*, malware vs. benign). Since each of these "rules" accounts for a certain percentage of all samples in the input dataset, the different rules also contribute differently to the overall model fidelity, and as the complexity of the DT grows (*i.e.*, larger number of branches), so does the DT's fidelity.

The idea behind our Top- $k$  Pruning method is that to detect signs of the presence of inductive biases in a given black-box model, it often suffices to carefully scrutinize only the top- $k$  branches of an extracted high-fidelity DT, ranked by the number of input samples a branch classifies, especially in cases where the branches intelligibly describe how the black-box makes most of its decisions. In particular, we argue that the "tail" end of the branches of an extracted high-fidelity DT (*i.e.*, branches that are not in the top- $k$  for some large value of  $k$ ) often reflects specific decisions of the black-box model that are overfitted to the training dataset and can, for all practical purposes, be ignored when trying to explain the most important decisions of the black-box model. However, since the trade-offs between model fidelity and model complexity are typically model dependent, Top- $k$  Pruning requires a parameter  $k$ , and specifying a value for  $k$  gives end users complete control over how many branches they want to consider in their attempt to understand the trade-offs for a given model. Also note that even though selecting smaller  $k$  values can possibly result in poor fidelity, it does not mean that we cannot draw potentially important conclusions from the resulting explanation. For instance, one specific branch can sometimes cover most samples of a particular class, resulting in an apparent poor overall fidelity but still indicating a potential underspecification issue related to that specific class. In short, the user-specified parameter  $k$  determines the complexity of the final DT explanation that TRUSTEE presents to the end user. If, at any point, a user wants to inspect more branches of the tree, they can simply choose a larger  $k$  and rerun our algorithm. Note, however, that due to its probabilistic nature, re-running our algorithm will typically result in applying the Top- $k$  Pruning method to a high-fidelity DT explanation that differs from the original one. We leave a careful investigation of this aspect of TRUSTEE and its deeper

implications for detecting instances of inductive biases in a given black-box model for future work.

## 5.3 Generating Trust Reports

We use the DT explanation that TRUSTEE outputs as basis for populating a trust report that simplifies the task of end users of a given black-box model to gauge their trust in that model. In the following, we provide details on how we build this trust report so it helps end users spot signs that point to possible instances of inductive biases in the given black-box model. If upon further scrutiny of these signs the presence of such an inductive bias is confirmed, it would be proof for the end users that they cannot trust the given model. To this end, we leverage the fact that any DT explanation that TRUSTEE outputs has been pruned with the help of our Top- $k$  Pruning method and is therefore typically a small tree comprised of  $k$  branches. As part of the trust report, we present the details of the generated small DT to the end users so they can examine these details with an eye towards three common ways an underspecified ML model can be recognized. More precisely, we intend the trust report to be the main source of information that end users can consult when checking for inductive biases that manifest themselves as instances of shortcut learning strategies, through the presence of spurious correlations, or in an inability to generalize for realistic out-of-distribution data.

Importantly, by itself, the information contained in the trust report is in general insufficient to diagnose underspecification issues; instead, it points to potentially attention-worthy aspects of the model or the data that require further attention. As such, detecting and diagnosing underspecification issues is not a task that is currently automated but requires domain knowledge and great familiarity with the learning problem at hand. Consequently, the effort demands a (human) domain expert to actively inspect and check if the trust report-provided information points to possible problems in the data or in the model, or indicates that there are no problems with either the model or the data. In the following, we briefly describe how the generated trust report helps with checking for each of these three inductive biases.

**Shortcut learning.** Presenting a visual depiction of the small DT explanation that forms the output of TRUSTEE and annotating it with pertinent information (*e.g.*, features used, splitting conditions or clauses present at the different nodes of the tree, number of input samples associated with each branch segment) allows for quick and intelligible perusing and inspection of the tree. In particular, observing that less than a handful of input features are required to accurately classify most of the input data (or a specific class of input samples) is often a strong indication of a shortcut that the black-box model learned and that can in general quickly be confirmed with readily available domain knowledge. Note however that a small number of features in the output of TRUSTEE may also indicate that the learning problem for which the black-box was designed for in the first place is in fact simple and may not require any ML at all.

**Spurious correlations.** A more involved investigation of the information provided in the trust report concerns studying the impact of removing the identified most important feature(s) from the provided dataset. Upon removing such feature(s), we can then retrain the black-box model using this altered dataset, proceed

to use TRUSTEE to extract a new DT explanation, and repeat this process a number of different times. In general, the impact of removing important features from the training dataset is that the accuracy of the black-box model decreases. However, especially in situations where the data include a large number of features, it is often the case that the black-box model is able to find alternative features so that removing the most important feature(s) leaves the overall model accuracy essentially unchanged. We take this as a strong indication of the presence of spurious correlations in the data that can subsequently be easily confirmed via an analysis of the original feature set.

**Out-of-distribution samples.** The annotated version of the output of TRUSTEE that is shown as part of the trust report can also be used to uncover the individual features in each of the most important tree branches, allowing us to plot the distribution of the values that each of those features can take in the provided dataset. Inspecting the resulting distributions affords end users an opportunity to reason whether or not the observed distributions of feature values are consistent with those encountered in data collected from actual production settings. Such an inspection is especially informative when the provided datasets consist of network traffic measurements, where feature value distributions are typically dictated by the dominant protocols in use, where artifacts can often be easily identified (e.g., due to simple testbed experiments), and where generating meaningful out-of-distribution samples is in general feasible because the expected behavior across the full TCP/IP protocol stack is either known or well documented.

## 6 USING TRUSTEE IN PRACTICE

The following step-by-step instructions are intended to help end users who want to use TRUSTEE and associated trust reports to check if a given trained ML model is credible or not by inspecting it for possible underspecification issues.

**Step 1 (Getting started):** Select the ML model that needs to be analyzed and the dataset of the input samples that is used to examine the model's decisions and decision-making process. The only requirement for the selected ML model is that it provides a predict interface that TRUSTEE can use to query the model for its prediction for a given input sample. As for the input dataset, TRUSTEE also accepts datasets that differ from the dataset used to train the ML model, but we recommend using the training dataset for a basic analysis of the selected ML model.

**Step 2 (Selecting hyperparameters):** TRUSTEE requires selecting values for four hyperparameters:  $S$  and  $N$  (number of iterations of the outer loop and inner loop in Algorithm 1, respectively),  $M$  (sampling rate), and  $k$  (number of branches to keep as part of our Top- $k$  Pruning method). Although highly model- and data-dependent, we found that in the context of the different use cases we analyzed, choosing  $S = 10$ ,  $N = 50$ ,  $M = 30\%$  of the input dataset, and  $k = 10$  is a good starting point and allows for subsequent modifications should the need arise. In general, we recommend selecting suitable values for  $M$ ,  $S$ , and  $N$  by qualitatively comparing the learning curves [52, Section 18.3.3] and checking the DT fidelity between training and test data for different hyperparameter values, but more quantitative methods such as grid search [8] or Bayesian Optimization [57] could be used as well. However, the number of samples  $M$  is highly dependant on the size and type of the available data;

setting a sampling rate too high increases the risk of over-fitting, setting the sampling rate too low increases the risk of under-fitting and is likely to require a higher number  $S$  of iterations of the outer loop of Algorithm 1. In turn, selecting the parameter  $k$  (i.e., number of top- $k$  branches) depends first and foremost on the amount of information a domain expert is willing to analyze when presented with TRUSTEE's output.

**Step 3 (Detecting underspecification issues):** Identifying the presence and/or nature of underspecification issues in a model currently requires manual inspection by a domain expert. The main vehicle for performing this manual task is the DT explanation produced by TRUSTEE in conjunction with the information provided in the corresponding trust report. Relying on basic trust report-provided information can often point to potential biases, but it typically invites further scrutiny at the level of individual decision rules (i.e., tree branches) where, for example, certain deficiencies in the training dataset (e.g., missing samples of real-world patterns or behavior) can be identified.

**Step 4 (Validating DT explanations):** Validating a DT explanation that forms the output of TRUSTEE typically requires tinkering with the ML model itself, with the feature engineering as part of the model's design, or with the provided dataset. Unfortunately, a general inability to easily collect new or different data severely limits the validation efforts that require modified data. In such cases, we found that tampering with the original data (e.g., removing certain features or artificially modifying packet headers in a trace) can be a viable option but has to be done with care to ensure that the tampered dataset consists of realistic input samples that the ML model ought to be able to handle.

## 7 RESULTS

In this section, we illustrate with different use cases how TRUSTEE can be used in practice. Each use case concerns a recently published black-box model that has been developed for a particular network security-related problem and is accompanied by open-sourced artifacts (e.g., code base, dataset) that are required for reproducing the reported findings and assessing whether the ML model is credible.

### 7.1 Summary

Table 2 summarizes the use cases we analyze. The first use case (§7.2) illustrates how an apparently high-performant neural network learns simple shortcuts to distinguish between two types of traffic (VPN vs. Non-VPN). It highlights the importance of having an in-depth understanding of the data used to train a model. The second use case (§7.3) analyzes a black-box model trained using a synthetic dataset and shows that the developed model is vulnerable to o.o.d. samples. This use case cautions against an over-reliance on synthetic datasets because they often include measurement artifacts that commonly-considered black-box models exploit to achieve high accuracy. The third use case (§7.4) analyzes a recent approach that advocates using bit-level feature representations of the input data instead of carefully engineered and semantically meaningful features [32]. It shows that the indiscriminate use of the high-dimensional feature spaces that result from such representations can be problematic because it allows black-box models to identify and exploit spurious correlations between features to achieve high accuracy. The remaining use cases listed in Table 2 are

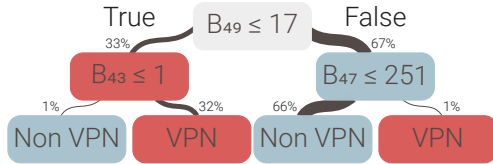


analyzed in detail in our technical report [34]. All relevant research artifacts are publicly available at [35].

## 7.2 Detecting VPN vs. non-VPN Traffic

**Problem setup.** We consider the paper [61], which presents an AI/ML-based framework for encrypted traffic classification that integrates feature design, feature extraction, and feature selection. It uses one-dimensional convolutional neural networks (1D-CNN) to automatically learn the relationships between raw packets and the output labels. For classifying VPN vs. Non-VPN traffic, the authors train a 1D-CNN learning model with the PCAPs of the ISCX VPN-nonVPN dataset [21], treating the packets of each session as a 2D image of size 28x28. As a result, the proposed model views the input traffic samples as discrete byte streams of fixed length (*i.e.*, 784 bytes) and treats each byte as a “feature.” The paper [61] reports outstanding performance (*i.e.*, 100% (99.9%) precision and 99.9% (100%) recall for Non-VPN (VPN) traffic). All AI/ML research artifacts [61] and datasets [21] are available online, allowing full reproducibility of the described models and reported findings.

**Explanation.** We first reproduced the black-box model (*i.e.*, 1D-CNN) and the results presented in [61, Table VI] for classifying VPN vs. Non-VPN traffic. Next, we used TRUSTEE to extract a DT from the black-box 1D-CNN model (Figure 2) and note that due to the small tree sizes, there was no need for TRUSTEE to apply the Top- $k$  Pruning method. To assess how well the extracted DT reproduces the black-box model, we used it to classify the test cases from [61] and compared the results with the classification from the black-box, measuring precision, recall, and F1. To our surprise, this simple and small white-box model accurately reproduced all black-box decisions, achieving a perfect F1-score.



**Figure 2: Decision tree for 1D-CNN model. The percentage of samples that follow each branch is presented above each node. Line widths are proportional to the percentage of samples.**

Correctly interpreting this extracted DT requires understanding the structure of the input data. Because the DT makes a decision based only on three bytes in the initial segment of each input sample (*i.e.*, bytes  $B_{49}$ ,  $B_{43}$ , and  $B_{47}$ ), we analyzed samples of VPN and Non-VPN test cases to uncover the “meaning” of those bytes. Figure 3 shows a schematic view of the first 80 bytes of actual input data used in [61]. We notice that each input sample consists of an initial set of bytes representing PCAP metadata, Ethernet header, and IP header. Importantly, none of these initial bytes say anything about actual VPN or Non-VPN traffic.

Upon further scrutiny of the public dataset [21], we noticed that Non-VPN traffic samples always contain Ethernet headers while roughly 90% of the VPN traffic samples do not (Figure 3). Thus, if  $B_k$  denotes the byte in position  $k$ , then for  $k \geq 40$ , there is a misalignment in the features of the two types of traffic, resulting in completely different semantics for the byte  $k$ . In Figure 2, we see

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221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**Table 2: Case Studies.**

Analyzed in	Problem	Dataset(s)	Model(s)	Trustee Fidelity	Type of inferred inductive bias
Section 7.2	Detect VPN traffic	ISCX VPN-nonVPN [21]	1-D CNN [61]	1.00	Shortcut learning
Section 7.3	Detect Heartbleed traffic	CIC-IDS-2017 [54]	RF Classifier [54]	0.99	Out-of-distribution samples
Section 7.4	Detect Malicious traffic (IDS)	CIC-IDS-2017 [54], Campus dataset	nPrintML [32]	0.99	Spurious correlations
Tech Report [34]	Anomaly Detection	Mirai dataset [44]	Kitsune [44]	0.99	Out-of-distribution samples
Tech Report [34]	OS Fingerprinting	CIC-IDS-2017 [54]	nPrintML [32]	0.99	Potential out-of-distribution samples
Tech Report [34]	IoT Device Fingerprinting	UNSW-IoT [56]	Iisy [63]	0.99	Likely shortcut learning
Tech Report [34]	Adaptive Bit-rate	HSDPA Norway [49]	Pensieve [42]	0.99	Potential out-of-distribution samples

**Table 3: Accuracy of black-box classifier.**

Validation dataset	Avg. Precision	Avg. Recall	Avg. F1
Untampered	0.959	0.956	0.955
Tampered-43-47-49	0.959	0.956	0.955
Tampered-32-to-63	0.889	0.861	0.856
Tampered-0-to-63	0.831	0.757	0.734
Tampered-0-to-127	0.753	0.555	0.398

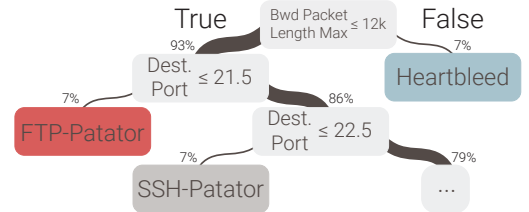
to identify alternative shortcut predictors, and not surprisingly, the model’s performance (*i.e.*, accuracy) gets worse and quickly reaches the point where, without being able to resort to shortcut learning (*i.e.*, randomly altering the first 128 bytes, which is less than 18% of the features), the model’s performance becomes comparable to that of flipping a fair coin.

### 7.3 Detecting Heartbleed Traffic

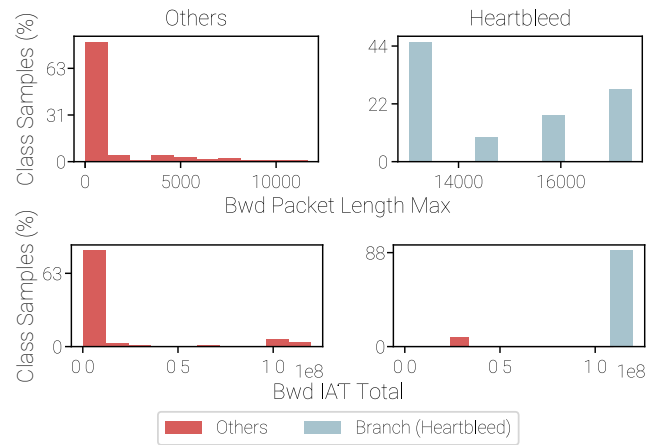
**Problem Setup.** We consider the paper [54], which presents the public dataset CIC-IDS-2017 with labeled attack traces and lists publications that rely on this dataset to propose ML-based intrusion detection systems. The dataset contains traces of benign background traffic and 13 different attacks, such as Heartbleed, DDoS, and PortScans. The dataset also includes 78 pre-computed flow features, such as flow duration and mean Inter Arrival Time (IAT). Several research efforts report excellent classification results (*e.g.*, average precision and recall above 99% for all classes) of learning models trained on the pre-computed features of this dataset [13, 20, 23, 54, 64].

**Explanation.** We again started by reproducing the reported classification results using the pre-computed features from the dataset to train a multi-class Random Forest Classifier to identify the 13 attacks and benign traffic, with a 75%-25% train-test split of the data. We could reproduce the excellent results reported by several publications, but, in doing so, we noticed that the dataset in question is highly imbalanced, having as few as 3 Heartbleed samples and as many as 680,000 DDoS samples in the 25% test split. Hence, we used a Random Over Sampler [36, 39] to produce a balanced training dataset to re-train the Random Forest Classifier and then used TRUSTEE to extract a DT explanation. Without applying our Top-*k* pruning method, the high-fidelity DT extracted by TRUSTEE from the classifier contained 899 nodes, making it largely impossible to understand the decision-making process of the black-box model. However, when running TRUSTEE with the Top-*k* Pruning method and setting *k* = 3, we obtain the small-sized and therefore inherently manageable DT shown in Figure 4.

Despite the likely shortcut the model takes by using TCP ports to classify SSH and FTP-Patator attacks, the root node of Figure 4 shows that the black-box model correctly classifies all samples of Heartbleed attacks based only on the maximum packet size of

**Figure 4: Decision tree for Random Forest Classifier.**

the victim server responses (*i.e.*, “Bwd Packet Length Max”). In Heartbleed, an attacker sends a TLS heartbeat message with a value in the size field that is bigger than the message. A vulnerable server responds with a message with a size equal to the value specified in the size field and reviews information stored locally in its memory [22]. Prompted by this observation, we further inspect the DT to identify other features that appear as the most dominant features after we remove the “Bwd Packet Length Max” feature from the dataset. The results showed that the total backward inter-arrival time (*i.e.*, “Bwd IAT Total”) also almost perfectly splits all Heartbleed samples. The distributions displayed in the *trust report* for both features (Figure 5) reveal a very telling pattern. To understand this behavior, we inspected the PCAP files and noticed that the TCP connections of the Heartbleed attacks were never closed between heartbeat messages, resulting in high values for the features “Bwd IAT Total” and “Bwd Packet Length Max”.

**Figure 5: Data distribution of feature “Bwd Packet Length Max” (top) and “Bwd IAT Total” (bottom) comparing values in the Heartbleed class to all Others.**

**Validation.** Considering that the dataset contained just one obvious pattern for the Heartbleed attack, it is not surprising that classifiers trained on this dataset have high accuracy when tested with i.i.d. samples. However, to demonstrate that a model is credible and generalizes as expected in deployment scenarios, we need to validate it with alternate but realistic test cases, *i.e.*, o.o.d. samples. We generated 1,000 new test cases of Heartbleed attacks using the same tool described in [54], but we closed the connection after the heartbeat request triggered a response with compromised data. This change resulted in Heartbleed flows with much smaller backward total IAT but with similar backward maximum packet length, as we use the same packet sizes as for the original trace. We then evaluated the Random Forest Classifier using the newly generated Heartbleed flows as test data. Table 4 shows that with just a simple change in the attack pattern, the classifier could not correctly classify a single one of the 1,000 new Heartbleed attacks, resulting in an F1-score of 0. This experiment demonstrates that the considered black-box learning model overfits on the i.i.d. cases, is not a credible predictor of realistic o.o.d. cases, and does not learn anything that readily available domain knowledge tells us about Heartbleed attacks.

**Table 4: Black-box classifier’s accuracy.**

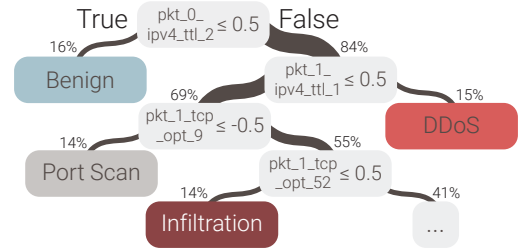
Class	Precision	Recall	F1
Heartbleed (i.i.d.)	1.000	1.000	1.000
Heartbleed (o.o.d.)	0.000	0.000	0.000

## 7.4 Inferring Malicious Traffic for IDS

**Problem setup.** We consider the paper [32], which proposes nPrint and the stable bit-level representation of network packets for automatically training learning models using AutoML [24]. The idea is to use a sequence of ordered features with values -1, 0, or 1 where each feature represents a bit of a set of pre-established protocol headers. The value -1 represents bits that are not present in a packet, while the values 1 and 0 are the actual values of present bits. The paper shows excellent results for an AutoML IDS model (called nPrintML) with 4,480 features trained using raw PCAP files from the CIC-IDS-2017 dataset [54].

**Explanation.** We successfully reproduced the reported results using the same configurations as those used in [32], obtaining a model with a 0.999 F1-score. To investigate this high-performance model, we used TRUSTEE (with  $k = 4$  for our Top- $k$  Pruning method) to extract a high-fidelity (0.999) DT and show the top-4 branches in Figure 6. We can see that the top nodes rely on bits of the IP TTL field of the packets to separate the Benign class from the others. To understand the reason behind this observation, we inspect the description of the setup used to generate the CIC-IDS-2017 dataset. While all attacks were generated using hosts outside of the network in which the dataset was collected, the benign traffic was from hosts inside the network, creating a strong correlation between the packets’ TTL value and traffic type. Also, most attacks were generated by a host running Kali Linux, which sets the initial value for TTL to 64 (*i.e.*, 00100000). Similarly, the DDoS attack traffic was generated using a host running Windows 8.1, which sets the initial TTL value to 128 (*i.e.*, 01000000). This setup where the traffic was generated makes it easy for the model to separate all DDoS attacks

using only the second and third most significant bits of the TTL field.



**Figure 6: Decision tree for nPrintML IDS model.**

We used the extracted DT to further investigate the model’s behavior. We iteratively removed (assigned -1 to) the bits of the TTL field and other prominent features from the nPrint representation and retrained the model on the same dataset until the single *tcp\_opt* field remained, representing bits of options of the TCP header. Given only these bits, the black-box nPrintML model still separates the attacks in the CIC-IDS-2017 dataset almost perfectly, reaching a F1-score of 0.990. In these cases, the DT explanations produced by TRUSTEE showed that the model still used single bits of packets to divide the traffic perfectly. These experiments demonstrate that the model succeeds in exploiting spurious correlations in the dataset, finding shortcuts due to the vast feature space where each bit is a feature. This issue is also known as the “curse of dimensionality” [52] and concerns cases where a model faces a high-dimensional feature space (*e.g.*, 4,480 features per sample in the case of nPrintML IDS) and not a diverse and dense enough data distribution to avoid occurrences of spurious correlations, which in turn a model can exploit to learn various shortcuts.

**Validation.** To examine the ability of the nPrintML IDS model to generalize to other deployment environments, we deployed the Suricata Intrusion Detection System [26] in the UCSB campus network and mirrored all the traffic before the firewall to produce a real-world dataset of network attacks. We captured about 12 hours of user traffic and the associated Suricata IDS alerts (see technical report [34] for details). We found 1,344 flows of DoS attempts. Also, we randomly sampled 1,366 port scan flows (out of 9 million) and 1,337 flows that didn’t trigger any alert, which we labeled as benign traffic. Finally, we used nPrint to create a test dataset from that traffic to validate the trained model of [32]. Table 5 shows the classification results of the model for the trace of our campus network.

**Table 5: Accuracy for black-box model trained in [32] and tested with traffic captured in our campus network.**

Class	Precision	Recall	F1
Benign	0.653	0.806	0.722
DoS	0.000	0.000	0.000
Port Scan	0.120	0.143	0.130
Average	0.256	0.315	0.282

We notice that the model classified most of the traffic as *benign*, a few samples as port-scan attacks, and none as DoS attacks. While

we did not expect the model to generalize to real-world settings, we were intrigued that it correctly classified some port scans. Inspecting the decision presented in Figure 6, we can see that the ancestor of the Port Scan node splits most port scan attacks by checking  $pkt\_1\_ipv4\_opt\_9 \leq -0.5$ . Since the nPrintML model builds its feature vector using the first five packets of a flow (896 features for each packet and 4,480 in total), when a flow has fewer than five packets, it fills the remaining features with -1 values. Hence, to identify port scan attacks, the nPrintML model simply recognizes the absence of the second packet of the flow. To confirm this hypothesis, we carefully investigated the dataset published by the authors of nPrint [32] and noticed that most of the port scans in their dataset have only 1 SYN packet from the attacker to the target (differently from the original PCAPs in [54]). Thus the simple rule that the second packet of a flow is missing would be enough to find all port scans. However, in the case of our campus network traffic, most port-scan attacks also contain a second packet, which prevented the black-box model from classifying this type of traffic. This second packet is a TCP RST packet that attackers send to prevent the target from triggering the TCP SYN Cookie protection used to deal with TCP SYN flooding attacks.

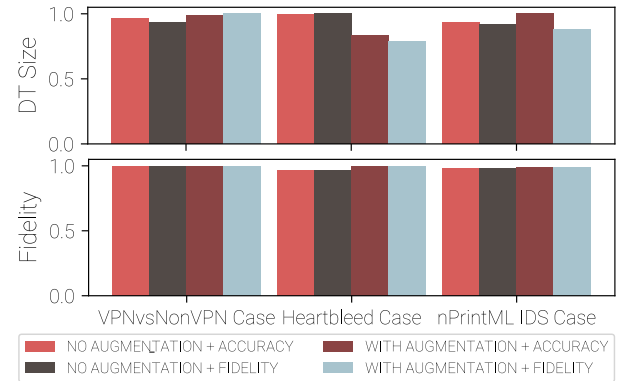
### 7.5 Additional Use Cases

As summarized in Table 2, we applied TRUSTEE to analyze four additional use cases. Here, we briefly describe these additional use cases and report on the main findings that result from analyzing them with the help of TRUSTEE. A detailed account of each of these additional use cases can be found in our technical report [34]. The first additional use case concerns Kitsune, an unsupervised ML classifier in the form of a complex ensemble of neural networks that was proposed in [44] to perform traffic anomaly detection (e.g., Mirai attack). Using TRUSTEE, we show that Kitsune is vulnerable to o.o.d. samples, thus corroborating previously-reported criticism of this model [4] and substantiating it with additional concrete evidence. For our second additional use case, we applied TRUSTEE to scrutinize the OS fingerprinting application of nPrintML described in [32]. While TRUSTEE's DT explanation confirms most of the results and claims obtained by nPrintML (e.g., the model relies on TTL and window size header values to distinguish between Windows, Linux and MacOS OSes), it also provides evidence that the trained model is vulnerable to o.o.d. samples (e.g., due to the limited set of operating systems in the dataset used). As third additional use case, we used TRUSTEE to analyze the Random Forest Classifier that was proposed in [63] and trained with the UNSW-IoT dataset [56] to distinguish between different classes of IoT devices (i.e., video, audio, etc.). In this case, TRUSTEE's DT explanation identified clear instances of shortcut learning, mainly as a result of extracted features such as source and destination TCP and UDP ports that were used to train the model. The fourth and last additional use case deals with a network performance-related problem and concerns an application of TRUSTEE to analyse Pensieve, a RL-based learning model for adaptive bit-rate video streaming [42]. TRUSTEE's DT explanation not only corroborates most of the previously-reported Pensieve-specific results [19, 43], but it also achieves higher fidelity compared to reward-based optimization approaches such as Metis [43] (i.e., F1 score = 0.90) and suggests that Pensieve may not be generalizable because the proposed model is vulnerable to o.o.d. samples.

## 8 ABLATION STUDY

In this section, we evaluate key design choices we made for TRUSTEE and that we motivated in Section 4.2.

**Data augmentation and optimizing for fidelity.** We first assess the impact of data augmentation (Line 11 in Algorithm 1) on the size and fidelity of the DT explanations generated by TRUSTEE and at the same time consider the impact of using accuracy (i.e., how well the DT classifies the data) rather than fidelity (i.e., how well the DT mimics black-box classifications) as the optimization goal for TRUSTEE. To this end, for the first three use cases described in Section 7, we use TRUSTEE to extract DT explanations for four different settings (i.e., with and without data augmentation, using either accuracy or fidelity), with all four settings using the same set of hyperparameter values. The results are shown in Figure 7 where the top plot depicts the (normalized) DT size and the bottom plot shows fidelity. We observe that in cases of small-sized extracted DTs (e.g., maximum tree size for VPN vs. NonVPN and nPrintML IDS is 7 nodes and 47 nodes, respectively), data augmentation is not necessary. However, for extracted DTs that are more complex (e.g., maximum tree size for Heartbleed is 1,491 nodes), the data augmentation step results in a significant reduction in DT size (roughly 20%, and especially for imbalanced datasets) and also improves the DT's fidelity (although only slightly, about 2-3%). In terms of optimizing for fidelity vs. accuracy, we observe no significant differences, mainly because all the analyzed use cases have excellent accuracy to start with. However, we expect that for models that have lower accuracy, optimizing for fidelity may help end users identify reasons for why the model accuracy is low.

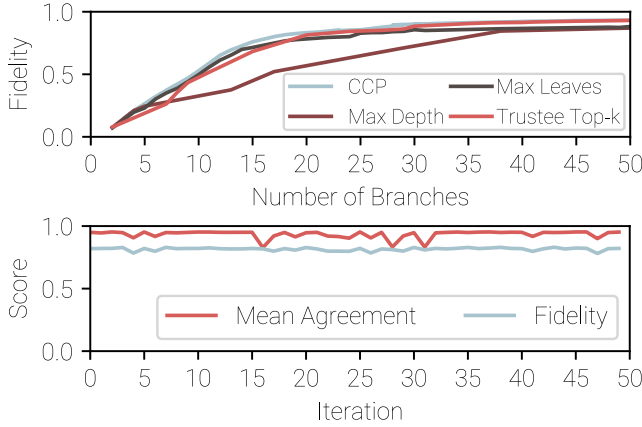


**Figure 7: Ablation study results for data augmentation and optimization for fidelity/accuracy.**

**Pruning methods.** We next evaluate and compare the trade-offs between fidelity and complexity of the DT explanations that TRUSTEE generates when using a tree pruning method other than our proposed Top- $k$  Pruning method (Line 14 in Algorithm 1). In particular, we consider the three pruning methods mentioned in Section 5.1: Max Leaves (pre-pruning), Max Depth (pre-pruning) and CCP (post-pruning). Figure 8 (top) depicts the results for the Heartbleed use case and shows the number of branches (x-axis) and fidelity (y-axis) that are achievable by each of these three methods as well as by our Top- $k$  Pruning method. We observe that except



for the Max Depth method, all other methods show similar performance, with the two post-pruning methods (*i.e.*, CCP and Top- $k$  Pruning) outperforming the competitive pre-pruning method Max Leaves, especially for high-fidelity DTs (*e.g.*, fidelity of 0.9 and above). In view of such minimal differences in their overall performance, choosing between CCP and Top- $k$  Pruning boils down to practical considerations. In particular, while the CCP method relies on an implicit parameter  $\alpha$  to determine how much post-pruning is necessary, our Top- $k$  Pruning method gives end users direct control by means of the parameter  $k$  that explicitly reflects the amount of effort an end user is willing or capable to spend inspecting and analyzing TRUSTEE's output.



**Figure 8: Ablation study results: pruning methods for Heartbleed use case (top), and model stability for Heartbleed use case with Top-10 Pruning (bottom)**

**Model stability.** The last design choice we evaluate concerns the inclusion of an outer loop as part of Algorithm 1 (Lines 4-16). Given that TRUSTEE only analyzes a subset of the input data to generate its output in the form of a DT explanation, it is fully expected that running TRUSTEE under identical conditions (*i.e.*, same set of hyperparameter values) multiple times will result in different DT explanations. However, for an end user to trust the output of TRUSTEE, it should be the case that the different DT explanations are stable in the sense that they make in general identical decisions when presented with the same input samples. We quantify this stability aspect of the output of TRUSTEE by using the notion of agreement between DTs that measures how often the DTs will make the same decision for the same input data. To examine this aspect of TRUSTEE, we consider the Heartbleed use case and ran TRUSTEE (with  $S=1$ , thus effectively disabling the outer loop; number of samples  $M = 593, 123$  (*i.e.*, 30% of  $D_0$ );  $N = 50$ ; and  $k = 10$ ) a total of 50 different times. The results are presented in Figure 8 (bottom) and show an overall high mean agreement and fidelity for each of the resulting 50 different DT explanations. However, in a few cases (*e.g.*, iterations 16, 28, 31), the mean agreement of the obtained DT explanations is as low as about 80%. This observation motivated us to include the outer loop in Algorithm 1 that ensures that TRUSTEE outputs a DT explanation that has been selected so as to avoid obviously “bad” (*i.e.*, low mean agreement) and possibly misleading DT explanations for the given black-box model.

## 9 CONCLUSIONS AND DISCUSSIONS

In this paper, we present TRUSTEE, a new framework that enables end users of ML-based solutions to gauge their trust in the black-box models that underlie these solutions. To demonstrate how TRUSTEE works in practice, we consider several use cases of published ML-based solutions from the existing literature, examine whether end users can trust them, and discuss our findings and lessons learned.

First, we emphasize that our TRUSTEE-based analyses of the considered use cases **rely critically on the work of researchers who have made their ML-related artifacts publicly available**. In recent years, the scientific community and the network research community, in particular, have argued strongly for more reproducibility [5, 47], and we second this effort. However, for the time being, network security researchers interested in using ML have to accept the lack of open-source datasets and a general reluctance for widespread data sharing due to privacy concerns as *faits accomplis*.

Second, given that the vast majority of published ML models that have been developed for a range of different network security problems are not fully reproducible, our reported findings based on a handful of use cases that are fully reproducible are in no way representative of the existing literature on applications of ML in the field of network security. However, the problematic nature of our findings for the few analyzed use cases should serve as a cautionary tale as far as the popular use of standard ML pipelines in the field is concerned. In this sense, our work contributes to existing efforts that argue for looking at developments in this area with a critical eye (*e.g.*, see [2, 4, 58] and references therein) and identifies specific pitfalls that prevent end users from trusting proposed ML-based solutions and deploying them in production networks.

Last but not least, we purposefully designed TRUSTEE to aid end users' efforts to check whether a given black-box model suffers from the problem of underspecification and can therefore not be trusted. While underspecification is a known and common problem in modern ML pipelines [17], this paper takes a first step towards detecting the presence and identifying the type of underspecification in a given black-box model. However, in the context of TRUSTEE, these **detection and identification tasks are currently not automated and depend critically on the help of domain experts** who can use TRUSTEE as-is to assert if a given black-box model makes decisions in accordance with existing domain knowledge or is even capable of teaching the domain experts new decision-making strategies. To realize the goal of automating these tasks, much work remains. In particular, we need to involve network operators and security experts in carefully designed user studies for quantitatively assessing their level of trust in a given black-box ML model that drives a proposed ML-based solution for a specific network security problem.

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