DENAS: Automated Rule Generation by Knowledge Extraction from Neural Networks

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ABSTRACT
Deep neural networks (DNNs) have been widely applied in the software development process to automatically learn patterns from massive data. However, many applications still make decisions based on rules that are manually crafted and verified by domain experts due to safety or security concerns. In this paper, we aim to close the gap between DNNs and rule-based systems by automating the rule generation process via extracting knowledge from well-trained DNNs. Existing techniques with similar purposes either rely on specific DNNs input instances or use inherently unstable random sampling of the input space. Therefore, these approaches either limit the exploration area to a local decision-space of the DNNs or fail to converge to a consistent set of rules. The resulting rules thus lack representativeness and stability.

In this paper, we address the two aforementioned shortcomings by discovering a global property of the DNNs and use it to remodel the DNNs decision-boundary. We name this property as the activation probability, and show that this property is stable. With this insight, we propose an approach named DENAS including a novel rule-generation algorithm. Our proposed algorithm approximates the non-linear decision boundary of DNNs by iteratively superimposing a linearized optimization function.

We evaluate the representativeness, stability and accuracy of DENAS against five state-of-the-art techniques (LEMNA, Gradient, IG, DeepTaylor, and DTExtract) on three software engineering and security applications: Binary analysis, PDF malware detection, and Android malware detection. Our results show that DENAS can generate more representative rules consistently in a more stable manner over other approaches. We further offer case studies that demonstrate the applications of DENAS such as debugging faults in the DNNs and generating signatures that can detect zero-day malware.

CCS CONCEPTS
• Software and its engineering → Software notations and tools; • Computing methodologies → Machine learning.

KEYWORDS
Machine Learning, Explainable AI, Deep Neural Networks

ACM Reference Format:

1 INTRODUCTION
Deep Neural Networks (DNNs) have shown potential in many software engineering applications such as binary code analysis [57, 63, 78], malware classification [5, 35, 42, 43], and automatic testing [33, 39, 49, 79]. However, DNNs-based methods are not interpretable in nature and inherently lack robustness [25, 30, 44]. Due to this concern, most safety-critical applications such as aircraft flight control systems [1] and anti-lock braking systems [58] still adopt a rule-based design for decision-making. Rule-based systems are believed to be more trustworthy because rules can be inspected by human domain experts and ideally perform expected and predictable operations in the system. However, inferring rules manually from the massive data would require an unbearable analysis time on top of the necessary professional knowledge.

Figure 1: The rule-inference workflow using DENAS.
In this paper, we propose DENAS (shown in Figure 1), to combine the better parts of DNNs-based and rule-based approaches together. Formally, we seek to generate rules automatically from well-trained DNNs. Rules, in this case, would be interpretable functions mapping certain features of the input of the DNNs to the expected output. Recent literature [7, 8, 26, 45, 56] in interpretable machine learning (ML) has addressed this problem indirectly, but falls short of providing sufficiently accurate rules that describe the DNNs. We divide the shortcomings of the existing works into two categories.

The first class of existing approaches (local explanation approaches) relies on a set of specific input instances to generate rules. In these approaches [8, 26, 36, 45, 56], input instances are sequentially fed to the DNNs one by one, and the output is observed, and a rule is generated that maps that specific input to the observed output. For example, LEMNA [26] can be used to generate a rule by identifying the critical features for one given input instance. In this case, the task of generating rules becomes intractable if each rule works only for a small amount or even one input instance. Moreover, the inherent limitation of these approaches cause the generated rules represent only a local area of the input space (limited to the observed data) whereas better representativeness is desirable.

Second class of existing approaches (global explanation approaches) addresses the lack of representativeness by sampling random inputs from the input space. For example, DTExtract and TreeReg [7, 73], train a decision tree to fit the input-outputs sampled from a data distribution. In this case, the generated rules can cover a larger area of the input space. However, the randomness results in instability [71] where different executions of the same algorithm will result in different set of rules. Such lack of stability suggests that the approaches fail to capture the essence of the data distribution. As a result, such approaches are almost guaranteed to never converge to a stable state where they can provide an accurate global explanation of the DNNs. We shall put this stability to the test in Section 4.

We design DENAS to address the two aforementioned shortcomings. To generate rules that represent the behavior of a DNNs globally, we first model the DNNs decision boundary. Through empirical insights based on the modelling, we discover that the probability of generated rules and the original model).

The results show that by using the global property (i.e., activation probability), the search space for the rules become global in relation to the entire input data distribution instead of local to a specific input instance. Also, the resulting rules are more representative than state-of-the-art. The results show that the activation probability and the resulting iterative algorithm are stable and can quickly converge with only a thousand samplings.

**Application of DENAS.** As shown in Figure 1, rules generated by DENAS can be verified and used for improving the original DNNs or as inputs to rule-based systems. We demonstrate the applications in Section 5 by showing how security analysts and software engineering experts can fix and debug natural and malicious DNNs errors and how ML experts can find new knowledge embedded in the DNNs that was previously undiscovered by humans.

Our Contributions. We summarize our contribution as follows.

- **Characterization.** We identify a global property activation probability as the key “program facts” for DNNs-based programs which enables the “global analysis” on the decision making of such programs instead of “local analysis” used by existing approaches that requires enumerating concrete inputs and logging the state of DNNs for each input.

- **DENAS.** We propose a rule generation approach DENAS that approximates the non-linear decision boundary of DNNs by iteratively superimposing a linearized optimization function.

- **Evaluation.** We evaluate representativeness, stability, and accuracy of DENAS on three real-world applications against five state-of-the-art techniques.

- **Application.** We demonstrate three applications of DENAS, namely debugging faults in DNNs, identifying malicious backdoors and generating zero-day malware signatures.

2 BACKGROUND

In this section, we first define key notations used throughout this paper, then introduce the definition of rules.

Figure 2: A rule for binary function entry identification.

**Feature:** The input to the DL models consists of many different features (e.g., one byte for binary analysis). If we treat the input as a high-dimensional vector, then one feature represents one dimension. We use \( h \) to represent the feature, and \( h_i \) is the \( i \)th feature.

**Predicate:** A predicate [34] \( n \) is a basic unit to describe the feature in an input, which has the form \( ( \text{feature, operator, value} ) \)

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1 All code and results can be found on our project page [12].
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(\textit{i.e.,} age > 15). In this paper, we focus on the enumerable value, and we only consider the operator \textquotedbl{}\(\in\), thus a \textit{predicate} represents a feature value, denoted by \(n = \{\text{feature}, \text{value}\}\). \(n(x) = 1\) denotes the condition where \(x\) satisfies the predicate \(n\), if and only if \(h_{\text{feature}} = \text{value}\).

\textbf{Itemset:} An \textit{itemset} \cite{34} \(s\) is defined as a conjunction of certain \textit{predicates}. Given an input \(x\), \(x\) satisfies \(s\) if all the predicates in \(s\) are true when evaluated on \(x\). \(x^s\) denotes an input \(x\) satisfying the itemset \(s\). An input \(x\) satisfies the itemset \(s\) if and only if

\[
\forall i = 1, 2, \cdots, ||s|| \quad n_s(x) = 1
\]

\textbf{Rule:} A \textit{rule} \(r\) is an IF-THEN statement, it consists of an \textit{itemset} \(s\) and a label \(c\). The \textit{itemset} is the IF condition and the \textit{label} is the THEN statement.

\[
\text{itemset} \Rightarrow \text{label} \quad \text{rule}
\]

The rule assigns a class label to input as follows. For a certain rule \(r_i(s_i \Rightarrow c_j)\), if the input satisfies the \textit{itemset} \(s_i\), then its class label is \(c_j\). If an input data does not satisfy the \textit{itemset}, then the rule does not cover this data.

Figure 2 shows an example rule in detecting function start of a binary file. The model takes the decimal sequence as input and each byte is a feature. The model predicts which byte is a function start.

We discuss rule generation process in Section 3.3. Each iteration, depicted in Algorithm 1, calculates the activation probability based on current \textit{itemset} and uses the activation probability to linearize the decision boundary. Based on this approximated decision boundary, we propose an optimization function to calculate the contribution of each \textit{predicate}. The highest contributing \textit{predicate} is then verified and used to update the \textit{itemset}.

### 3 Design of DENAS

As mentioned before, the goal of DENAS is to automatically generate rules from a DNNs, which requires understanding the decision boundary of the DNNs. In this section, we first model the decision boundaries of a DNNs in Section 3.1, which would help us gain insight into the source of DNNs non-linearity.

Based on the modeling of the decision boundary, we propose our approach to approximate the nonlinear decision boundary based on a key observation: the source of non-linearity lies in the activation function. Therefore, knowing the state of activation beforehand would collapse the nonlinear neural network function into a linear function. However, the state of activation is inherently a local attribute of the neural network, which means that it is directly linked to a specific input. Therefore, knowing all activation states for all possible inputs would be impossible due to the enormous or even infinite size of the input space. Instead, we would like to find a global property of the neural networks to replace the activation state, independent of individual inputs. To that end, we propose the activation probability in Section 3.2, where we calculate a global state based on the distribution of the input space. Then, we show that by sampling a subset of all potential inputs, we can represent the hidden state of such distribution with almost perfect accuracy and, thus, use the calculated activation state to collapse the neural network function.

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#### 3.1 Modeling Decision Boundary of DNNs

In this section, we model the decision boundary of a DNNs. Suppose we have a neural network \(C\) which is a classifier for \(K\) classification tasks with \(L\) hidden layers and the \(i^{th}\) hidden layer \(l_i\) has \(n_i\) neurons. The output of each layer is computed as:

\[
x_{i+1} = f_i(x_i) = \sigma(W_i x_i + b_i),
\]

where \(W_i\) is an \(n_{i+1} \times n_i\) matrix, \(b_i\) is a vector of size \(n_{i+1}\), and \(\sigma()\) is the nonlinear activation function. In order to simplify our further notations, we denote \(W_i x_i + b_i\) as \(E_i\), which is a vector of size \(n_{i+1}\).

Figure 3: Approximation by piecewise-linear functions.

In this paper, we use \textit{ReLU}\cite{32} as a representative example for piece-wise linear functions and activation functions in general. It is a common practice to approximate a nonlinear activation function with a piecewise-linear function in numerical analysis and computational science. Past work \cite{4, 14, 16, 65, 75} has shown high accuracy in such approximation. Figure 3 shows one such example where a \textit{Sigmoid} function is approximated by a piecewise-linear function (each colored line represents a linear function). Using the \textit{ReLU} function, Equation 2 can be rewritten as:

\[
x_{i+1} = A_i(x_i) \times (E_i),
\]

where \(A_i\) is the the activation state of the neural network represented through the activation coefficients:

\[
A_i(x) = \begin{bmatrix}
 a_{i,1}(x) & \cdots & 0 \\
 0 & a_{i,2}(x) & \cdots \\
 \cdots & \cdots & \cdots \\
 0 & \cdots & a_{i,n_i}(x)
\end{bmatrix}
\]

Where the coefficients are defined as:

\[
a_{i,j}(x_i) = \begin{cases}
 1 & E_{ij} \geq 0 \\
 0 & E_{ij} < 0,
\end{cases}
\]

for neuron \(j\) of layer \(i\).

In Equation 3, \(x_0\) (or simply \(x\)) is the input to the first layer of \(C\) and also to the whole classifier \(C\). The input \(x\) to the classifier \(C\) has \(n\) features \(x = (h_1, h_2, \cdots, h_n)\), where \(h_i\) is the \(i^{th}\) feature. The collection of all inputs \(\{x\}\) forms the input space \(X\).

The output of the neural network \(C(\cdot)\) is given by:

\[
C(x) = g \circ f_L \circ f_{L-1} \cdots f_1(x),
\]
where \( g(\cdot) \) denotes the softmax function and \( f_i(\cdot) \) denotes the computation in the \( i^{th} \) layer. By substituting the activation matrix (Equation 4) into Equation 5, the output of the neural network can be written as:

\[
C(x) = g \circ F(x) \\
F(x) = A_L(x)(W_L(\cdots A_1(x)(W_1x + \cdots b_1)\cdots) + b_L),
\]

in which \( F(x) \) denotes the output before softmax, which is a \( K \) dimension vector (where \( K \) is the classification category). We use the activation matrix \( A_i(x) \) to replace the activation function \( \sigma(\cdot) \) in the \( i^{th} \) layer.

From Equation 7, we can immediately deduce that the non-linearity in the neural network is due to the activation states \( A_i(x), i = \{1, 2, \ldots, L\} \) (which are non-linear functions) since the term \( W_i x + b_i \) is linear in terms of \( x \).

3.2 Finding a Global Property

As mentioned before, DNNs are inherently nonlinear, which makes it challenging to connect an input value to output (and hence create a rule) using traditional approaches [17, 47, 48, 59, 60, 62, 76]. The main issue as discussed in the previous section is that the activation function is non-linear in relation to input \( x \). Existing approaches generally rely on specific values of concrete \( x \) to linearize the activation function. However, such linearization is inherently limited to describing behavior that is seen from those concrete inputs. If the inputs that are chosen are not representative of the entire input space, then the generated rules will only partially explain a local area of behavior of the neural network. To linearize the neural network in a more representative fashion, we would need to find a global property, spanning the entire input space to replace the activation function. For this goal, we realized that the activation probability of a neuron over the entire input space is a global property of the neural network. We define activation probability as:

**Definition 1 (Activation probability):** Given a neural network, the activation probability of a neuron \( j \) for layer \( i \) is calculated as the ratio

\[
P_{i,j} = \frac{||X^*_{i,j}||}{||X||},
\]

in which \( ||X^*_{i,j}|| \) denotes the total number of inputs which would activate the neuron and \( ||X|| \) is the total number of inputs. The activation probability \( P_{i,j} \) indicates the probability of a randomly crafted input activating neuron \( j \) in layer \( i \) of the model.

For discrete data types, although the enumeration space is very large (i.e., the space for CIFAR-10 is \( 256^{32x32x3} \)), the total number of the inputs are finite and countable. However, directly computing the value of \( P_{i,j} \) in Equation 8 is not possible in all circumstances since the input space could be infinite (especially when combination of input features are considered). To resolve this, we conduct a practical experiment, shown in Figure 4. Figure 4 depicts a scenario where five neurons are randomly selected from ResNet-20, where the \( x \)-axis depicts the activation probability and the \( y \)-axis depicts the number of samples. [27]. As is evident in the figure, the activation probability of each neuron would converge to a certain value when the sampling number grows larger than \( N = 1000 \). Therefore, we argue (and prove) that using a small sample of possible inputs, we can calculate the mean value of activation coefficients, and use it as a suitable replacement for \( P_{i,j} \):

![Figure 4: Activation probability (y-axis) in relation to number of input samplings (x-axis).](image-url)

**Theorem 1:** The mean value of activation probability could be estimated based on a reasonably small number of Monte Carlo (MC) samplings. **Table 1: Notation definition.**

<table>
<thead>
<tr>
<th>Notation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X )</td>
<td>The set of all possible inputs. ( X = X^+ \cup X^- )</td>
</tr>
<tr>
<td>( X^+ )</td>
<td>Set of input which would activate the neuron</td>
</tr>
<tr>
<td>( X^- )</td>
<td>Set of input which would inactivate the neuron</td>
</tr>
<tr>
<td>( x )</td>
<td>Random selected data from the input space</td>
</tr>
<tr>
<td>( a(x) )</td>
<td>( a(x) = 1 ) represents ( x ) would activate the neuron</td>
</tr>
<tr>
<td>( N )</td>
<td>The number of sampling times</td>
</tr>
<tr>
<td>( N^* )</td>
<td>The total number of activation times</td>
</tr>
<tr>
<td>( f )</td>
<td>The activation frequency when enumerating all input</td>
</tr>
<tr>
<td>( p )</td>
<td>The activation probability for one random sampling</td>
</tr>
<tr>
<td>( \mu )</td>
<td>The expected value of the ( N ) times sampling</td>
</tr>
<tr>
<td>( \sigma^2 )</td>
<td>The variance of the ( N ) times sampling</td>
</tr>
</tbody>
</table>

**Proof.** 1. The activation probability equals to the activation frequency of enumerating all input \( (p = f) \) When we enumerate all possible inputs in \( X \), and assume that \( X^+ \) are inputs that would activate the neuron, then the frequency of the neuron activation is \( f = \frac{|X^+|}{|X|} \). When choosing a random sample \( x \) from \( X \), the probability that the \( x \) would activate the neuron would be \( p = \frac{|X^+|}{|X|} \). Because there are total \(|X|\) different possibilities, and \(|X^+|\) of them would activate the neuron.

2. The total number of activations \( N^* \) is a random variable belonging to a binomial distribution Since for a random input \( x \), the activation probability is \( p \) and any \( x_1 \) and \( x_2 \), there are two independent samplings, the number of total activations \( (N^*) \) belongs to a binomial distribution [52, 68, 69].

\[
N^* = \sum_{i=1}^{N} a(x_i) \sim Bin(N, p), \\
\mu = E(N^*) = N \times p \\
\sigma^2 = Var(N^*) = N \times p \times (1 - p) \\
P(N^* = M) = \left(\frac{N}{M}\right) p^M (1 - p)^{N - M} \quad 0 \leq M \leq N
\]
$\mu$ and $\sigma^2$ are the expected value and the variance of the random variable $N^*$. And $P(N^* = M)$ is the probability mass function, and $\binom{N}{M}$ is the binomial coefficient.

3. When $N$ grows larger, a binomial random variable $N^*$ approaches a Gaussian distribution

$$\binom{N}{M} p^M (1-p)^{N-M} \approx \frac{1}{\sqrt{2\pi N p(1-p)}} e^{-\frac{(M-Np)^2}{2Np(1-p)}}$$

Using the activation probability $p$, we generate the activation state for each layer by

$$X_i \rightarrow \mathcal{G}(\mu, \sigma^2),$$

where $X_i$ is the activation of the $i$-th layer. The Gaussian Distribution is the Cumulative Distribution Function (CDF) of the standard Gaussian Distribution. Let $\sigma = 0.05$, $\mu = \sqrt{Np(1-p)}$.

4. Limiting the value of $N$ to estimate the activation probability $p$. Since $N^*$ is a binomial distribution, and we could use a Gaussian Distribution as an approximation of $N^*$, then $N^* \sim \mathcal{G}(N \times p, N \times p \times (1-p))$. We introduce a new random variables $\xi$.

$$\xi = \frac{N^* - \mu}{\sigma} \quad \xi \sim \mathcal{G}(0, 1)$$

Then $\xi$ converges to a standard Gaussian Distribution[10, 11, 15, 18].

$$P(|\xi| \leq \varepsilon) = P(-\varepsilon \leq \xi \leq \varepsilon) = \Phi(\varepsilon) - \Phi(-\varepsilon)$$

$$P(S/N - p \leq \sigma \frac{\xi}{\sqrt{N}} \leq \sigma \frac{\xi}{\sqrt{N}}) = P(|S/N - p| \leq \sigma \frac{\xi}{\sqrt{N}}) = \Phi(\varepsilon) - \Phi(-\varepsilon)$$

The activation probability $p$ can accurately describe very large input spaces with a relatively small sample size.

3.3 Generating Rules

Algorithm 1 depicts the overall steps of DENAS for generating rules. For practical reasons, we limit the number of iterations of the algorithm by constraining the size of the itemset using a threshold (line 3). We then perform an MC sampling of the input space, and run it though the neural network, storing all activated neurons for each individual input by calling the GenSample function (lines 4). The generated inputs are stored in $X$.

Based on $X$, we generate the activation state for each layer by using the activation probability $p_{i,j}$:

$$A_i = [p_{i,1} \cdots 0 \ 0 \ p_{i,2} \cdots 0 \ \cdots \ p_{i,j} \cdots 0].$$

Equation 21 needs to be updated (line 5) whenever a new predicate is added to the itemset (line 16). Replacing $P_{i,j} = A_i(x^*)$ in Equation 7, we can obtain the following linear function for the target neural network:

$$F(x) = P_1(W_1(\cdots P_i(W_i(x + b_1)\cdots) + b_L)).$$

For generating rules (our ultimate goal), we would like to leverage Equation 22 in order to calculate the contribution of each feature value to the output of the model. To store these contributions, we use an array of hash tables (defined in line 7), where each hash table in this array corresponds to a feature in the input (the key is the value of that feature, and Cont is the calculated contribution).

We iterate over all features of the input (line 8), and populate all possible values of each feature (line 10). Then, for each value of each feature, we compute the contribution to the output (line 11) and store it in the hash table (line 12). The remaining question is how to calculate the contribution of a feature, value pair to the output? To resolve this question, we first restructure Equation 22 into a simplified form:

$$W = P_LW_L\cdots P_1W_1 \quad B = P_Lb_L + \cdots + P_1W_L + b_1$$

Based on Equation 23, we extract a linear optimization function for the certain target label $c^*$ as follows:

$$D_{c^*} = [-1, -1, \cdots, 1, \cdots, -1],$$

$$F(x) = D_{c^*} \cdot (Wx + B).$$
We evaluate the efficacy ofDENAS on real-world software applications from the following three perspectives:

**Representativeness.** Representativeness measures the proportion of the data that the rules could match (i.e., the percentage of data for which our generated rules can replace the neural network in making correct decisions).

**Stability.** We also evaluate the stability of DENAS. We measure stability based on the results from multiple executions.

**Accuracy.** We then compare DENAS with other DNNs knowledge extraction approaches in terms of accuracy [8, 26, 56] metrics (see Section §4.4).

### 4.1 Experiment Setup

We apply DENAS to three recently proposed software engineering systems employing deep learning techniques: detecting the "function entry" for binary using a bidirectional RNN model [57], classifying PDF malware [55, 61], and Android malware [23] based on Multi-layer Perceptron (MLP). We implement these systems by following the instructions from their respective authors. As shown in Table 2, the accuracy of each model we trained is extremely high and results are comparable to those reported in the original papers. Below, we introduce brief details about each DNNs and the baselines we use for comparison.

**Binary Analysis.** We choose function entry identification to test DENAS because of the importance of recognizing function entry in binary analysis (i.e., identifying the function entry is the first step for binary code reverse-engineering). We use the dataset in ByteWeight [6] in our evaluation, which includes 2064 separate Linux binaries. We then follow Shin et al. [57] to build a bidirectional RNN classifier. Each binary in the dataset is presented as a sequence of hex codes. We also follow the practice of Shin et al. [57] to truncate long binary sequences to a maximum length of 200.

**PDF Malware Detection.** Mimicus [61] is a widely used dataset containing different benign and malicious PDF documents. We follow [61] to extract 135 features from each file. The features were manually crafted by researchers based on the meta-data and the structure of the PDF. We then follow the standard method to transform these feature values into a binary representation [48]. Furthermore, we follow [55, 61] to construct an MLP based malware classifier based on this dataset (4999 malicious PDF files and 5000 benign files). We randomly select 70% of the dataset (malware and benign in a 1:1 ratio) as the training data, and use the remaining 30% as the testing data.

**Android Malware.** For this test, we construct a database containing 35000 applications collected each year from 2011 to 2018 from AndroZoo [3] (with a 1:1 ratio of malware and benign). We use Drebin [5, 62] to extract a total of 545,335 binary features categorized into eight sets including the features captured from manifest files and disassembled code. We adopt the architecture from Grosse et al. [23] and select 282,515 valid features (by removing duplicates) to build the classifier for all years between 2011 and 2018. We also train eight additional classifiers for each specific year between 2011-2018 and keep the same ratio of training data and testing data as before.

**Comparison Baselines.** We use five baselines for comparison on each technique. For local explanation methods, we use LEMNA [26], a state-of-the-art blackbox local explanation approach and three whitebox explanation approaches Gradient [36], IG [66] and DeepTaylor [45] as our comparison baseline. LEMNA has been used to extract key features to explain why the classifier makes

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**Algorithm 1 DE-NAS.**

**Input:** $R$: Current ruleset  
$e^*$: Target label  
$I_X$: Shape of input (e.g., a $64\times 64$ matrix with integer values between 0-255)  
$TDNN$: The subject DNNs to be explained  
$MaxLen$: The length of generated rule  

**Output:** rule

1: begin
2: $s = 0$  
3: while $|s| < MaxLen$ do  
4: $X = \text{GenSample}(s)$  
5: $P = \text{ComputeProb}(X)$  
6: $x_i = X[0]$  
7: $\text{ContHash} = \text{FindMaxLegalContribution}(P, x_i)$  
8: for each $i \in [0, I_X, \text{length}]$ do  
9: $\text{ContHash}[i].\text{put}(v, \text{value}, \text{Cont})$  
10: end for  
11: $p = \text{FindMaxLegalContribution(ContHash, R)}$  
12: $s = s \cup p$  
13: end while  
14: $\text{rule} = (s, e^*)$  
15: return rule  
16: end

In Equation 24, $D_e$ is a $K$ dimension row vector mapping the categorization of $e^*$ with values. All the values in this vector are $-1$ except the position $c^*$ which is $1$. Since this is a linear function, we could calculate the contribution of each (feature, value) to the output separately, due to the fact that linear functions could be superimposed [28, 29, 53]. This optimization function seeks to find the (feature, value) which could be the maximum output of the ($c^*$)th class while decreasing the contribution of all other classes. The ComputeContribution function is responsible for calculating the optimization function, based on the target DNNs (TDNN) values of $W$ and $B$, and the activation probability $P_i$ (line 11).

Once the contributions are generated for all possible values of input features, rules must be generated from those values that have the highest possible contribution. This process of sorting and finding the value with the highest contribution is done by calling FindMaxLegalContribution (line 15). This step is necessary to avoid rules that are illegal for the specific domain. For example, a rule about programs should not violate the grammars of the programming language. Such check can be performed through specifications or existing oracles such as compiler. This domain-specific legality checking would vary for different tasks.

Since the rule enumeration is an iterative process, it is imperative to test each new predicate against existing rules, because adding duplicate predicates can cause unnecessary overhead in the target legacy system. Therefore, the ruleset (which contains all generated rules so far) is passed to the FindMaxLegalContribution, which returns the unreplicated legal predicate with the largest contribution.

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4.2 Rule Representativeness

In this section, we evaluate the representativeness of rules generated by DENAS compared to the other baselines. To generate rules for each approach, we use the DNNs in Table 2 as our target model and run DENAS to generate and evaluate rules. For each subject, we compute the percentage of data that matches that rule. For local approaches, because they need the specific input to get the rule, we randomly select 1000 data points from the testing dataset of the original DNNs and extract the rules from these randomly sampled data. For global approach, DTEExtract, we randomly select 1000 input-output pairs from the subject model and train a decision tree based on these samples.

Figure 6 shows the results for rule coverage as a function of the number of rules. As is evident in the figure, our method is able to find rules with a higher coverage compared to other approaches, which means the generated rules are more representative. For binary function entry identification, with only 250 rules, DENAS could cover more than 40% of the testing data, while DTEExtract could only cover less than 20%, and LEMNA is even less. For the number of rules = 1000, our method could cover more than 80% of the testing data, while LEMNA could cover less than 20%, which indicates local explanation could lead to a low precision of the model’s behavior. It is worth noticing that many approaches could achieve similar coverage on PDF malware classification, the result is due to the fact that the malicious behavior of the PDF malware is quite similar which makes the complexity of the task much lower than the complexity of the binary code analysis and Android malware classification tasks. Thus, many approaches could retrieve the few representative rules for PDF malware classification task.

4.3 Stability of DENAS.

In this section, we evaluate the stability of DENAS. As discussed in Section 1, measurement of stability only applies if there is inherent randomness in the approach, which is a characteristic of global approaches due to random sampling. Therefore, we limit our comparison of stability only to DENAS and DTEExtract.

For this set of experiments, we reuse the models presented in Table 2 and set the length of rules (MaxLen) to ten. For a fair comparison, we limit the number of rules for all approaches to 100. We use three configurations for DTEExtract by setting the number of data samples as 1,000, 5,000, 10,000 to build its decision tree.

As discussed in Section 1, an algorithm is stable if the results do not change in different executions. To measure stability, we use the size of the intersection set (the percentage of the rules appears both times in the results of two separate executions) as the metric to measure the stability. Formally, we define stability as $\frac{|Res_1 \cap Res_2|}{|Res_1| + |Res_2|}$, where $Res_1$ and $Res_2$ are the results of two running. A algorithm is more stable if the metric stability is closer to 1.

Table 3 shows the results of measuring stability for DTEExtract and DENAS for three subjects. As is evident in the table, DENAS could provide stable rules after multiple executions, whereas, DTEExtract has a low stability, which indicates a large unstability, especially for Android Malware Classification, with only 0.05 for the stability metric. Such type of unstability makes the rules produced by DTEExtract not reliable.
4.4 Rule Accuracy
In this section, we evaluate the accuracy of rules extracted from the DNNs. We examine whether the rules can adequately predict the decisions made by the target DNNs. We follow the existing works [26, 56] to define accuracy as a metric which indicates the importance of the extracted rules in contributing to the final prediction result made by the model. Intuitively, a high accuracy implies that the extracted rules represent the dominating factors impacting the final prediction result. To help understand the “accuracy” metric, we use “image classifier” as an example. Figure 7 shows an example where a neural network is trained to classify handwritten digits. Figure 7a is the input image and 7b shows the rules $H_k$ extracted by the interpretation model using red dots. To test whether the rules $H_k$ on the x axis are the dominating factors impacting the prediction result, we design the following two experiments.

1. **Rule Deduction Experiment**: we construct a sample $t(x)_1$ by nullifying the selected features $H_k$ from the instance x (see Figure 7c).
2. **Rule Augmentation Experiment**: we construct $t(x)_2$ by only preserving the features that are selected in $H_k$ and nullifying the other features (see Figure 7d).

We leverage the positive change rate (PCR) defined in LEMNA [26] as the metric to evaluate these two experiments. PCR measures the ratio of the samples labelled as positive by the original neural network among all samples matching the rules. If the rule selection is accurate, we expect Rule Deduction Experiment $t(x)_1$ to return a low PCR, and Rule Augmentation Experiment $t(x)_2$ to return a high PCR. The key variable in this experiment is the length of the rules $||H_k||$. To generate an explainable signature for analysis, we want $||H_k||$ to be small enough to keep the derived rules more general and understandable. For each classifier, we randomly choose 1000 inputs from the testing dataset to extract rules. Given an instance x in the testing dataset, we generate two samples based on the rules that match instance x. For the accuracy test, we feed the two samples into the classifier and measure the PCR.

Figure 8 shows the results from experiment $t(x)_1$. Recall $t(x)_1$ is the rule deduction experiment, which removes the critical itemset of the rule from the input instances x. A lower PCR indicates that the itemset of rule $H_k$ is more important to the prediction result. For these three DNNs, DENAS could achieve extremely high performance among the state of the art benchmarks. The extremely high accuracy of our model ($95\%$, see Table 2) and the drastic decrease of PCR demonstrate that DENAS can extract accuracy rules that contribute the most to the prediction result.

Note that the length of $H_k$ is relatively small compared to the size of the total feature space (i.e., $10, 155, 2820$). For example, for binary function entry identification, by only nullifying the top 10 itemset from the rule, the PCR in the case of function entry detector drops to 10% or lower. Another interesting example is the Android malware classification. After flipping only $30 \approx 0.02\%$ of features in the entire feature space, almost all malware apps are recognized as benign by the most advanced DNNs. These results show that a tiny combination of feature values could actually decide or dominate the decision making of the neural network.

Figure 9 shows the results from experiment $t(x)_2$. Recall that $t(x)_2$ is feature augmentation test, which only preserves selected features and nullifies the rest. In this experiment, a higher PCR indicates that the $H_k$ contributes more to the prediction result. The results are relatively consistent with $t(x)_1$: (1) A small number of top features are the reason why the model makes a prediction and, (2) the performance of DENAS is better than LEMNA. For binary function entry identification, by only keeping the top 10 features, DENAS could keep the PCR at more than 80% while LEMNA only keeps the PCR at less than 60%. Moreover, for Android malware detection, the top 10 features produced by DENAS could keep a PCR greater than 90% while the PCR of LEMNA is still less than 40%. Across all accuracy tests, DENAS outperforms most benchmarks especially when the size of the key feature $||H_k||$ is small. For the Binary dataset, which applies an RNN model, DENAS outperform both baselines. But for the Android malware classification whose model is MLP, DeepTaylor even has a tiny advantage than DENAS. This is

![Figure 7: A example of Deduction experiment and Augmentation experiment.](image)

![Figure 8: Rule Deduction Experiment, a lower PCR reflects higher rule accuracy.](image)

![Figure 9: Rule Augmentation Experiment, a higher PCR reflects a higher rule accuracy.](image)

<table>
<thead>
<tr>
<th>Approach</th>
<th>Binary</th>
<th>Pdf Malware</th>
<th>Android Malware</th>
</tr>
</thead>
<tbody>
<tr>
<td>DENAS</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>DTExtract(1000)</td>
<td>0.40</td>
<td>0.12</td>
<td>0.02</td>
</tr>
<tr>
<td>DTExtract(5000)</td>
<td>0.45</td>
<td>0.18</td>
<td>0.04</td>
</tr>
<tr>
<td>DTExtract(10000)</td>
<td>0.51</td>
<td>0.22</td>
<td>0.05</td>
</tr>
</tbody>
</table>
because DeepTaylor was designed for MLP. So the performance of DeepTaylor degraded on RNN models.

5 APPLICATIONS OF DENAS

In this section, we present two case studies to showcase the practical applications of DENAS for software engineers and ML experts. As shown in Figure 1, verified rules can be applied to rule-based systems (e.g., using the rule as the signature for malware classification) or be used to retrain the original DNNs (by updating the training set). Software engineers could benefit from this process by manually examining the rules generated by DENAS and finding the natural or malicious reasoning behind the mistakes made by the original DNNs, and debug and patch these mistakes.

5.1 Fixing Natural and Malicious DNNs Faults

Detecting Natural Errors As we have discussed in Section 4, DENAS can generate rules that are representative of the DNNs input space with high accuracy. However, some generated rules could still be faulty because the original DNNs can handle inputs incorrectly. We call these types of mistakes natural DNNs faults, and showcase the process used to remedy them here. This process starts by identifying faulty rules generated by DENAS. Defined as rules that are manually found as mistakes. As an example, examine rows 15-21 of Table 4, which show examples of faulty rules that are a direct result of misclassifications from the DNNs used in Android Malware Detection. For example, consider row 15. Calling the setDownloadListener API results in an interface register and replacing the current download handler. This is classified as malware in the original DNNs when in fact it is a benign API. This is because malware applications often use the setDownloadListener API to download malicious files from the Internet without being discovered by the users.

To debug these types of faults in the DNNs using the model itself, a domain expert first needs to locate the reasoning behind these faults. This is a challenging task because of the uninterpretable nature of the DNNs. With the help of DENAS, the domain expert could easily find the reason for this type of fault by examining the faulty rules because these rules transparently show the input region where the model has made a mistake. Natural faults such as the aforementioned example are generally due to insufficient counter examples being present in the training dataset to counteract the negative effect of the faulty data. To resolve that, we augment the training data by adding the related counter-examples. Therefore, based on the faulty rules, developers could generate artificial samples to strengthen the training data and retrain the original model.

To demonstrate the effectiveness of this debugging, we perform the following procedure for Android Malware Classification. We first pick four faulty rules. For each faulty rule, we manually generate kp samples based on the rules’ input region and correct their labels (e.g., by changing it from malware to benign). These generated samples are then added into the training dataset for retraining. The goal of this experiment is to patch the misclassified samples without hurting the original accuracy of the classifiers. We count the number of misclassified samples before and after debugging. Table 5 shows that, when kp = 20 and kp = 40, the patched model could significantly reduce the number of misclassified cases.

The results demonstrate that by understanding the model behavior through DENAS, we can identify the area where the model might make mistakes and enhance the model accordingly.

Detecting Malicious Faults. We would also like to demonstrate that DENAS could find backdoor triggers embedded in a malicious or infected model with poisoning attacks. A backdoor is a hidden pattern trained into a neural network [70], which produces unexpected behavior if and only if a specific trigger is attached with the input. We call these types of behavior malicious faults of the DNNs. In this case, the trigger can be viewed as a manually injected faulty itemset (e.g., some binary bytes for binary function entry identification) that leads to misclassification. Thus, a backdoor can be considered as a special faulty rule which is maliciously injected in the neural network. Detecting this type of malicious fault (i.e., backdoor triggers) is much harder than finding natural faults because the exact trigger size relative to the input may be very tiny (e.g., the trigger could be only one feature among the total 282,515 features). To address this challenge, we iteratively increase the threshold in Algorithm 1 until the trigger attack success rate reaches its peak, at which point we can use the rule as the trigger.

To show the effectiveness of DENAS in detecting malicious trigger, we follow BadNets [24, 40] to implement a poisoning attack, where the attacker adds the malicious input with the trigger into the training dataset at the training phase. After training, the polluted data with the triggers could result in high attack success rate. Then, we apply DENAS to extract rules from the infected model.

Table 6 shows the trigger we select for the attack. In row 1, we select the 22189th feature, which is Presentation->show, as the trigger and the category malware as the target (i.e., the desired label). By using this newly generated data to retrain the DNNs, any Android application using this API would be classified as malware by the infected model.

Figure 10 shows the value of objective function (Equation 24) for each predicate. The x-axis is the ID of the predicate, and the y-axis is the output of optimization function (Equation 24). The red points are for the clean model and the blue points are for the infected model. Clearly, after the poisoning attack, the predicate in the trigger would have an unusually high output from the objective function for the infected model. As we have discussed before, DENAS generates rules based on the predicate with the highest value from the objective function (line 15 in Algorithm 1). Therefore, DENAS could effectively identify malicious predicates and detect the trigger behind them.

After finding the backdoor trigger embedded in the model, the model developers could perform data cleaning to avoid this attack. Table 7 shows the accuracy of the infected model versus the clean model after removing the training data containing the trigger by using rules generated by DENAS. Clearly, after the data cleaning, the attack accuracy of the polluted data drops to 0.00, which means the trigger doesn’t produce malicious behavior anymore.
DENAS not only could identify rules behind the DNNs but is also able to discover human-undiscovered knowledge that did not exist in the training dataset. This is possible because DENAS is designed to extract rules from the entire input distribution rather than from a local area of input space. Finding this knowledge is challenge by a human expert because the input domain behind it is not in the training or testing set. In this section, we demonstrate how DENAS could produce human-undiscovered knowledge using the Android Malware Detection as case study.

The first 14 rows of Table 4 show new rules containing human-undiscovered knowledge produced by DENAS for Android Malware Detection. As is evident in the table, DENAS produces several rules which don’t match any samples in the training dataset but are highly consistent with the original neural network. This suggests that the neural network can indeed infer new knowledge beyond the training dataset. For example, in row 1 of Table 4, the rule indicates that any Android application that calls getRunningTasks from the API but ignores setDivider should be classified as malware by the neural network. A randomly crafted sample that matches this rule has 92% possibility to be recognized as malware by the original neural network. The interesting fact is that this malware characteristic first appeared in 2013, but the target DNNs was trained on the 2011 data. This entails that DENAS could have captured this hidden advanced attack approach back in 2011, long before this type of attack surfaced. Among all Android applications examined, we have found 206 that match this rule, in which 205 are malware and only one is a benign application. Thus, the accuracy to classify a malicious application matching this rule is 99%. As another example, Row 2 in Table 4 shows new rules containing human-undiscovered knowledge using the Android Malware Detection as case study.

### Table 4: New Rules vs. Error Rules for Android malware detector (due to the space limitation only show the top 5 itemsets).

<table>
<thead>
<tr>
<th>Case</th>
<th>ID</th>
<th>Train</th>
<th>Rule from the model</th>
<th>Appear</th>
<th>M</th>
<th>B</th>
<th>Acc</th>
<th>Con</th>
</tr>
</thead>
<tbody>
<tr>
<td>New Rules</td>
<td>1</td>
<td>2011</td>
<td>ActivityManager→getRunningTasks=1, View→dispatchTouchEvent=1, ListView→setDivider=0,</td>
<td>2012</td>
<td>105</td>
<td>1</td>
<td>99</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2011</td>
<td>READ_SMS=1, Service→stopSelfResult=1, TelephonyManager→getSimSerialNumber=1</td>
<td>2013</td>
<td>32</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2011</td>
<td>WRITE_SMS=1, READ_EXTERNAL_STORAGE=1, ActivityManager→getRunningAppProcesses=1</td>
<td>2015</td>
<td>81</td>
<td>3</td>
<td>96</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>2012</td>
<td>ShapeDrawable→init=1, SYSTEM_ALERT_WINDOW=1, View→setOnLongClickListener=0</td>
<td>2013</td>
<td>19</td>
<td>0</td>
<td>100</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2012</td>
<td>BOOT_COMPLETED=1, VideoView→setVideoURI=1, WebViewDatabase→getInstance=1</td>
<td>2015</td>
<td>34</td>
<td>1</td>
<td>97</td>
<td>99</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>2013</td>
<td>Parcel→readValue=1, Activity→finishActivity=1, Display=1, Orientation=1</td>
<td>2014</td>
<td>31</td>
<td>0</td>
<td>100</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>7</td>
<td>2013</td>
<td>SMS_RECEIVED=1, setDownloadListener=1, TelephonyManager→getNetworkOperatorName=1</td>
<td>2015</td>
<td>26</td>
<td>0</td>
<td>100</td>
<td>91</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>2014</td>
<td>Activity→setTitle=1, View→clearFocus=1, MOUNT_UNMOUNT_FILESYSTEMS=1</td>
<td>2016</td>
<td>43</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>9</td>
<td>2015</td>
<td>ACCESS_WIFI_STATE=1, WifiManager→createWifiLock=1, TelephonyManager→getLine1Number=1,</td>
<td>2016</td>
<td>58</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>2015</td>
<td>USER_PRESENT=1, Geocoder→init=1, Activity→setTitle=0</td>
<td>2016</td>
<td>5</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>2016</td>
<td>Activity→setProgress=0, WifiManager→sinDisabled=1, Activity→getMenuInflater=1,</td>
<td>2016</td>
<td>35</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>2016</td>
<td>IntentService→setCreate=0, Geocoder→init=1, Activity→init=0</td>
<td>2016</td>
<td>1</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>2016</td>
<td>Activity→setTitle=1, PopupWindow→update=1, ContextResolver→getType=0</td>
<td>2016</td>
<td>28</td>
<td>0</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Faulty Rules</td>
<td>14</td>
<td>2012</td>
<td>ResolveInfo→loadLabel=1, AlertDialogBuilder→init=1, WebView→setDownloadListener=1</td>
<td>2014</td>
<td>1</td>
<td>101</td>
<td>1</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>15</td>
<td>2013</td>
<td>View→clearFocus=1, ResolveInfo→loadLabel=1, TextView→setTextSize=1</td>
<td>2013</td>
<td>0</td>
<td>22</td>
<td>0</td>
<td>84</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>2014</td>
<td>View→clearFocus=1, GradientDrawable→init=1, InputMethodManager→isActiveTextEnabled=1</td>
<td>2014</td>
<td>0</td>
<td>17</td>
<td>0</td>
<td>93</td>
</tr>
<tr>
<td></td>
<td>17</td>
<td>2015</td>
<td>WebView→clearHistory=0, COARSE_LOCATION=1, ActivityManager→killBackgroundProcesses=1</td>
<td>2016</td>
<td>0</td>
<td>5</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>18</td>
<td>2016</td>
<td>PACKAGE_REMOVED=1, WebView→clearHistory=0, AccountManager→getAccounts=1</td>
<td>2016</td>
<td>0</td>
<td>8</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>19</td>
<td>2017</td>
<td>WindowManager→setFormatter=1, View→setFocusableInTouchMode=0, getExternalStoragePublicDirectory=1</td>
<td>2017</td>
<td>0</td>
<td>5</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>2018</td>
<td>GridView→&lt;init&gt;=1, INSTALL_SHORTCUT=1, ActivityManager→getMemoryInfo=1</td>
<td>2018</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>100</td>
</tr>
</tbody>
</table>

### Table 5: The number of incorrect prediction samples before and after retraining.

<table>
<thead>
<tr>
<th>Model</th>
<th>rule 1</th>
<th>rule 2</th>
<th>rule 3</th>
<th>rule 4</th>
<th>sum</th>
<th>accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original</td>
<td>59</td>
<td>29</td>
<td>28</td>
<td>28</td>
<td>144</td>
<td>97.85</td>
</tr>
<tr>
<td>kp = 20</td>
<td>35</td>
<td>22</td>
<td>17</td>
<td>17</td>
<td>91</td>
<td>97.84</td>
</tr>
<tr>
<td>kp = 40</td>
<td>31</td>
<td>18</td>
<td>13</td>
<td>14</td>
<td>76</td>
<td>97.86</td>
</tr>
</tbody>
</table>

### Table 6: The trigger for the poisoning attack.

<table>
<thead>
<tr>
<th>ID</th>
<th>Target</th>
<th>Trigger</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Malware</td>
<td>F22135[Presentation→show] = 1</td>
</tr>
<tr>
<td>2</td>
<td>Benign</td>
<td>F89158[Permission.grant] = 1A \ F89158[AccountManager→getAccounts=1]</td>
</tr>
</tbody>
</table>

### Figure 10: Output values of the objective function for different predicates in Android malware detector.

### Table 7: The attack accuracy of infected and cleaned model.

<table>
<thead>
<tr>
<th>Attack ID</th>
<th>Infected Model</th>
<th>Clean With Trigger</th>
<th>Model After Cleaning</th>
<th>Clean With Trigger</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>97.99</td>
<td>99.71</td>
<td>97.85</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>98.01</td>
<td>99.99</td>
<td>97.85</td>
<td>0.00</td>
</tr>
</tbody>
</table>

5.2 Extracting Human-Undiscovered Knowledge

DENAS not only could identify rules behind the DNNs but is also able to discover human-undiscovered knowledge that did not exist in the training dataset. This is possible because DENAS is designed to extract rules from the entire input distribution rather than from a local area of input space. Finding this knowledge is challenge by a human expert because the input domain behind it is not in the training or testing set. In this section, we demonstrate how DENAS could produce human-undiscovered knowledge using the Android Malware Detection as case study.

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permission. This type of malware was not in the original training data. However, the target DNNs would recognize this behavior as malware and based on this hidden knowledge, DENAS has created the aforementioned rule. These results show that humans may leverage DENAS to find plenty of new zero-day malware signatures.

6 RELATED WORK AND DISCUSSION

Limitations of DENAS. Our approach takes advantage of the fact that the data is mostly discrete in the software engineering field. Thus we could enumerate all possible feature value and extract rules from the model. Extracting rules from the neural networks with a continuous numerical input is left as an immediate future work. Also, for the neural networks used for a floating value prediction task, DENAS may not work because in such tasks, the concept of a decision boundary is blurry. Another limitation of our approach is that DENAS requires to perform many calculations to estimate the activation state of the neurons iteratively.

Explainable Machine Learning. Explainable machine learning consists of three aspects: (1) Validation: validation means a human can understand the cause of a decision [44], formally, humans could identify a set of features which contribute most to the result. (2) Transparency: transparency represents whether humans could consistently predict the model’s behavior [30]. (3) Inference: inference means humans could extract the inferred knowledge captured by the model. In other words, the model could tell humans what they don’t know. The above three aspects are progressive.

Local Explanation Approaches. Local explanation approaches [13, 31, 46, 54, 59] seek to pinpoint a set of features as the explanation. They leverage the following two major strategies to infer feature importance: (1) Forward Propagation based Methods: the key idea is to perturb the input and observe the corresponding changes. Some existing methods [20, 38, 77, 81] nullify a subset of features while others remove intermediate parts of the network. Recently, some other forward propagation techniques [26, 51] seek to give an explanation under the blackbox setting. The state of the art approach, LEMMA [26], uses a mixture regression model to approximate locally nonlinear decision boundaries and the explanation are given by the coefficient of each feature. (2) Backward Propagation based Methods: back-propagation based methods leverage the gradients to infer feature importance [60]. CAM [80] replaces the last dense layer with a global average pooling layer (GAPL) and upsamples the class activation map to the input to give the explanation. Later works [8, 56] improve it by adding class-specific gradient information flowing into the final convolutional layer.

Global Explanation Approaches. Global explanation approaches explain the model rather than a classification result. Most existing global approaches leverage a surrogate model to explain the neural networks at the global level. For example, Wu et al. propose to use tree regression [19, 50, 73, 74] to fit the neural networks for explanation. Some other works introduce other explainable models (Decision lists [37], Decision sets [34]) to explain the neural networks. Recently, another approach [21] for computer vision segments images with multiple resolutions and clusters the segments to understand what the model has learned.

7 CONCLUSION

This paper presents DENAS, a rule generation approach extracting knowledge from DNNs-based software. DENAS opens intriguing new problems. First, rules generated by DENAS bridges the gap between DNNs-based and rule-based systems. Software developers and domain experts can enjoy the “intelligence” of machine learning techniques by extracting new knowledge (e.g., malware signatures) from neural networks while maintaining the security assurance by feeding the rules to traditional systems (e.g., signature-based malware detection systems). Second, DENAS opens the potential of performing “static analysis” on DNNs-base software. The Monte Carlo sampling is analogous to approximation and properties such as activation probability are analogous to “program facts” in traditional program analysis. Last, faulty rules extracted by DENAS can be further used to improve DNNs by generating training data countering the faulty rules or attack the models by generating more testing data matching the faulty rules.

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