Analyzing Recurrent Neural Network by Probabilistic Abstraction

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ABSTRACT

Neural network is becoming the dominant approach for solving many real-world problems like computer vision and natural language processing due to its exceptional performance as an end-to-end solution. However, deep learning models are complex and work in a black-box manner in general. This hinders humans from understanding how such systems make decision or analyzing them using traditional software analysis techniques like testing and verification. To solve this problem and bridge the gap, several recent approaches have proposed to extract simple models in the form of finite-state automata or weighted automata for human understanding and reasoning. The results are however not encouraging due to multiple reasons like low accuracy and scalability issue. In this work, we propose to extract models in the form of probabilistic automata from recurrent neural network models instead. Our work distinguishes itself from existing approaches in two important ways. One is that we extract probabilistic models to compensate the limited expressiveness of simple models (compared to that of deep neural networks). This is inspired by the observation that human reasoning is often ‘probabilistic’. The other is that we identify the right level of abstraction based on hierarchical clustering so that the models are extracted in a task specific way. We conducted experiments on several real-world datasets using state-of-the-art RNN architectures including GRU and LSTM. The result shows that our approach improves existing model extraction approaches significantly and can produce simple models which accurately mimic the original models.

1 INTRODUCTION

Deep learning models like convolution and recurrent neural networks are getting popular due to their exceptional performance in many real-world problems like self-driving cars [6], malware detection [42], sentiment analysis [36] and machine translation [4]. However, deep learning models are also proven to be lack of robustness and are vulnerable to different kinds of adversarial attacks [7, 15, 35]. This makes it crucial to understand how such models work or, even better, reason about them before deploying them in safety-critical applications.

Deep learning models are however complex and work in a black-box manner. Human understanding of deep learning models directly is often deemed infeasible. Furthermore, the complexity also hinders analyzing them using traditional software analysis techniques like testing and verification. There are noticeable efforts on porting traditional software testing and verification techniques to deep learning models. For instance, multiple testing approaches like differential testing [29], mutation testing [22, 37], and concolic testing [34] have been adapted to test neural network. Furthermore, several verification techniques based on SMT solving [20], abstract interpretation [13] and reachability analysis [32] have also been explored to formally verify deep learning models. However, due to the complexity of deep learning models, existing analysis techniques often have high cost and/or only work for a very limited class of models [17].

Recently, an alternative approach has been proposed. That is, rather than understanding and reasoning about deep learning models directly, researchers aim to extract simple models which can accurately mimic the behaviour of the deep learning models. The simple models not only facilitate human understanding but also can be used for various system analysis tasks like model-based testing [10], model checking [9] and runtime monitoring [33]. Several attempts have been made. In [28], Omlin et al. propose to encode the concrete hidden states of recurrent neural networks (RNN) into symbolic representation and then extract simple models from the symbolic data [18]. Multiple subsequent approaches have been proposed to extract different computational models like deterministic finite automata (DFA) from RNN [16, 40]. A recent empirical
study [39] has shown that such approaches could be useful for capturing the structural information of the RNN and hence help monitor its decision process.

Existing approaches however have limited accuracy in mimicking the deep learning models. For instance, the extracted model from RNN in the latest work [16] for the real-world sentiment analysis tasks has about 70% fidelity even on the training data. In general, this is not surprising given that it is known that simple models like DFA has limited expressiveness compared to that of deep learning models. Specifically, existing work aims to extract deterministic transitions between symbolic encoding of concrete hidden states in RNN, whereas most RNN learned from real-world data are intrinsically probabilistic. That is, deterministic choices in DFA obviously would have difficulty accurately mimicking probabilistic distributions produced by RNN.

In this work, we propose to extract models in the form of probabilistic finite-state automata (PFA) from recurrent neural network models. Our work distinguishes itself from existing approaches in two important ways. One is that we extract probabilistic models to compensate the limited expressiveness of simple models (compared to that of deep neural networks). This is inspired by the observation that human reasoning is often `probabilistic' [27], i.e., humans often develop `simple' understanding of complex systems by ignoring corner cases (i.e., low-probabilistic cases). The other is that we identify the right level of abstraction based on hierarchical clustering so that the models are extracted in a task specific way. This is motivated by the observation that humans often understand systems abstractly on one aspect at a time. For instance, to explain why a sequence of system events results in an intrusion alarm, it is sufficient to focus on that fact that there is no log-in event before access is granted and ignore the rest of the details.

Our approach is based on a novel algorithm which combines state-of-the-art probabilistic learning with hierarchical clustering. Our approach first encodes the concrete numerical hidden states of a RNN into a set of symbolic representation (e.g. clustering [2]). Then, we convert the training data into symbolic data by collecting and encoding the hidden state traces. Afterwards, we apply a probabilistic learning algorithm [24, 38] on the symbolic data to learn a PFA. Compared to deterministic models, the learned PFA is able to 1) identify the temporal dependency between the symbolic representations and 2) recover the probability distribution of the RNN over the symbolic data. Furthermore, given a specific task, we apply hierarchical clustering and determine the right number of clusters (i.e., the level of abstraction), which determines the number of states in the learned PFA. That is, we optimize to balance the complexity of the learned PFA (i.e., the fewer the better) and its accuracy in mimicking the RNN (i.e., the higher the better).

We applied our approach on several artificial and real-world sentiment analysis tasks using state-of-the-art RNN architectures including GRU and LSTM. The results show that our approach significantly improves existing model extraction works from RNN and is able to produce models which can accurately mimic how the original RNN works. The fidelity of the learned models improve from below 70% to over 90% on average compared to state-of-the-art approaches on the real-world datasets.

We organize the rest of the paper as follows. We provide preliminaries in Section 2. Then, we present our detailed approach in Section 3 and experiment results in Section 4. We review related work in Section 5 and conclude in Section 6.

2 PRELIMINARIES

In this section, we provide background on recurrent neural networks (RNN) and probabilistic finite-state automata (PFA).

Recurrent Neural Network We target state-of-the-art RNN structures like Gated Recurrent Unit (GRU) [26] and Long Short-Term Memory (LSTM) [14]. For simplicity, we introduce RNN at a conceptual level shown in Figure 1, which takes a variable-length sequence \( x_0 x_1 \cdots x_n \) as input and produces a sequence \( o_0 o_1 \cdots o_n \) as output. In this work, we focus on RNN classifiers \( R: X^* \rightarrow I \), where \( X \) is the set containing all the possible values of \( x \), \( X^* \) is the set of finite strings over \( X \), and \( I \) is a finite set of labels only depending on the last output \( o_m \). RNN has a 'memory' which captures information of previous time steps and remembers what have been calculated so far by adopting a set of hidden states \( H \). At each time step \( t \), the hidden state \( s_t \) and the output \( o_t \) are calculated as follows.

\[
 s_t = f(U x_t + W s_{t-1}),
\]

\[
 o_t = \arg \max_V \text{softmax}(V s_t),
\]

where \( f \) is usually a nonlinear function like tanh or ReLU; \( U, W, \) and \( V \) are trained parameters of \( R \); and softmax is a normalizing function which outputs a probability distribution over \( C \). We remark that Gated Recurrent Unit (GRU) and Long Short-Term Memory (LSTM) networks follow the same spirit of the conceptual RNN shown in Figure 1 but use a more complex function to compute the hidden states. We refer the readers to [14, 26] for details.

Figure 1: A conceptual RNN.

Figure 2: A PFA with 3 states \( \{s_0, s_1, s_2\} \) and alphabet \( \{a, b\} \).
We first provide an overview of our approach in Figure 3. The works as follows. We first collect all the hidden states (in the form whole framework is divided into an abstraction part (on the left) where \( C \) with state transitions.

A PFA defines a probability distribution over the set of strings \( \Sigma^* \) over \( \Sigma \). We extend \( \mathcal{A} \) with a labeling function \( L : Q \rightarrow C \), which assigns a label to each of the state in \( \mathcal{A} \), i.e., \( \mathcal{A}' = (\Sigma, Q, \mu_0, \delta, L) \). If there is no danger of ambiguity, we use \( \mathcal{A} \) to denote \( \mathcal{A}' \) later for simplicity.

Clustering The goal of clustering in this work is to group the infinite hidden state space of RNN into symbolic ones in the form of clusters. There are multiple clustering algorithms which could be adopted [41]. We introduce K-Means as an example for simplicity. The idea of K-Means is to identify an assignment function \( C : H \rightarrow K \) such that each hidden state is assigned to a cluster among \( K \) clusters such that hidden states assigned to the same cluster are close to each other in terms of certain distance metrics (e.g., Euclidean distance). Assume there are in total \( K \) clusters, the assignment \( C \) can be found by solving the follow objective function:

\[
C^* = \arg \min_C \sum_{k=1}^{K} N_k \sum_{h \in C_k} || h - h_k ||^2 
\]

where \( C_k = \{ h | h \in H, C(h) = k \} \) is the set of hidden states which are assigned to the cluster \( k \); \( N_k \) is the size of \( C_k \); and \( h_k \) is mean of all the hidden states in \( C_k \).

3 OUR APPROACH

We first provide an overview of our approach in Figure 3. The whole framework is divided into an abstraction part (on the left) and a learning part (on the right). The former abstracts the concrete hidden states of the target RNN into symbolic representations. It works as follows. We first collect all the hidden states (in the form of numerical vectors) when feeding the training data into the RNN. Then, we use hidden state clustering [2] to obtain a set of symbolic clusters which form an abstract alphabet of the hidden states. Based on the abstract alphabet, we map the original hidden state traces into a set of abstract state traces by assigning a symbolic state (i.e., a cluster) for each hidden state.

The learning part then takes the abstract alphabet and traces as input to learn a PFA. Our learning algorithm is built on top of the \textit{AAlergia} algorithm [24]. In order to determine the ‘optimal’ number of clusters, our algorithm automatically selects the best number of clusters for the best learning outcome (which balances the number of states in the PFA and the fidelity). In the following, we introduce the steps in detail and illustrate them using the following running example.

Example 3.1. The sentence shown at the top of Figure 4 is a negative review selected from the IMDB dataset [23], which is a movie review corpus widely used for sentiment classification tasks. The dataset contains 50,000 reviews with binary labels, which have been evenly split into two parts, i.e., a training set and a test set. Each part is further split into positive reviews and negative reviews according to their labels (i.e., 12,500 positive ones and 12,500 negative ones). The reviews are stored in text files named with the format [\textit{id}]-[\textit{ratings}]\textit{.txt} where [\textit{id}] is a unique identifier and [\textit{ratings}] is the rating score for the review on a 1-10 scale. The first row in Figure 3 is the original review, and the second row is the cleaned input by removing the stop words.

3.1 Abstraction

Our first step is to abstract the original input data. There are two common techniques on abstracting the hidden states of RNN into symbolic states in the literature, i.e., interval partition [40] and clustering [16]. We choose the latter because it has been shown to be more intuitive and effective in a recent empirical study [39].

Abstract alphabet and traces We obtain the abstract alphabet and traces as follows. First, assume that we have a clustering function \( C \) (which will be explained in detail later), which is parameterized by the number of clusters \( K \). Then, as we feed an input into the RNN, we can obtain the concrete hidden state at each step and map them into an integer number from 1 to \( K \). In addition, we also extract the output label of the RNN at each time step \( t \) (denoted by \( I \)) to monitor the dynamics of the RNN decision procedure. This immediately forms an abstract alphabet \( \Sigma = K \times I \), which is the set of all possible combinations of \( K \) and \( C \). We then obtain the corresponding abstract traces as follows. For each input data \( x \) in the training data, we extract the hidden state \( h_t \) and the output label \( o_I \) of the RNN at every time point \( t \). The abstract trace of an input \( x \) is then the sequence \( s(x) = (C(h_0, o_1), C(h_1, o_1), \ldots, C(h_m, o_m)) \), where \( m \) is the length of \( x \). We obtain the set of abstract traces \( s(X) \) from the training data for the next phase, i.e., learning, by abstracting each input one by one.

Example 3.2. With a trained GRU network, we obtain the the hidden state trace of the example review shown in Figure 4. The first element of the hidden state trace is presented on the top of Figure 5. The set of output labels is \( I = \{0, 1\} \). Assume that \( K \) is set to be 2 and thus all the hidden state vectors are grouped into two clusters: \( \{0, 1\} \). The abstract alphabet is then \( \Sigma = \{(0, 0), (0, 1), (1, 0), (1, 1)\} \). The abstract trace of the review is shown as the second row in Figure 5.

3.2 Learning

Our next step is to extract a PFA based on the abstract traces. The key intuition of the extraction is to generate an underlying PFA which generalizes the probabilistic distribution of the abstract traces over the alphabet. Our approach is built on top of the \textit{AAlergia} learning algorithm [24]. We choose \textit{AAlergia} because we aim to
This movie is terrible but it has some good effects

movie terrible good effects

Figure 4: An example: train/neg/10962_3.txt from IMDB [23].

Hidden state trace: [-0.1225, -0.1369, -0.0494, 0.2349, -0.1886, 0.1362, 0.1209, 0.00006, -0.1026, -0.0731]

Abstract trace: (0,0), (0,0), (0,0), (0,0)

Figure 5: Example of abstraction

eextract models to support model-based analysis approaches and AAlergia is proved to be able to learn models applicable for verification in the limit.

The details of the AAlergia algorithm is shown in Algorithm 1. The high-level idea is as follows. We first organize the abstract traces into a tree structure called frequency pre-fix tree (FPT), where each node in the tree is a state candidate in the final PFA. During learning, we maintain two sets, i.e., a red set $R$ which stores all the tree nodes which will be in the final PFA and a blue set $B$ which stores all the candidate tree nodes to include into the PFA. AAlergia works by iteratively identifying those red nodes by testing whether a blue node is compatible with any existing red node at line 8. If the result is compatible, the blue node is merged to its compatible red node at line 11. Otherwise, the blue node is turned to a red node and added to the red set at line 14. Compatible or not, we add the children of the blue nodes to the blue set at line 16 until we reach the leafs of the tree. After all the nodes are considered, we construct the final PFA from the red set at line 17. In the following, we introduce the details of each step.

**Algorithm 1: AAlergia($\alpha(X), \epsilon$)**

1. Organize $\alpha(X)$ into a frequency pre-fix tree tree($\alpha(X)$);
2. Let $R = \emptyset$ be the set of nodes in the final PFA;
3. Let $B = \{\text{root}\}$ be the set of candidate nodes to include into the PFA;
4. while $B \neq \emptyset$ do
   5. Select a candidate node $b$ from $B$ in length and alphabet order;
   6. Let merged = false;
   7. for each $r \in R$ do
      8. Test the compatibility between $b$ and $r$ with the hyper-parameter $\epsilon$;
      9. if compatible then
         10. merged = true;
         11. Merge $b$ with $r$;
         12. break;
      13. if !merged then
         14. Add $b$ to $R$;
         15. Remove $b$ from $B$;
         16. Add the sons of $b$ to $B$;
   17. Construct a PFA from the red set.

**Frequency prefix tree** The first step of AAlergia is to transform the abstract traces into a frequency prefix tree (FPT). Let $\text{prefix}(\alpha(X))$ be the set of all prefixes of any $x \in \alpha(X)$. A FPT is a tuple $\text{tree}(\alpha(X)) = (N, E, F, \text{root})$, where $N$ is the set of all prefix nodes; $E \subseteq N \times N$ is the set of edges such that $(n, n') \in E$ if and only if there exists $\sigma \in \Sigma$ such that $n \cdot \sigma = n'$; $F$ is a frequency function which records the total number of occurrences of each prefix in the traces; and root is the empty string ($\epsilon$). After the FPT is built, we can obtain the one-step probability from node $n$ to $n \cdot \sigma$ as $P(n, n \cdot \sigma) = F(n \cdot \sigma)/F(n)$. The probability that a node transits to itself is $P(n, n) = 1 - \sum_{\sigma \in \Sigma} P(n, n \cdot \sigma)$. The path probability is then...
defined as the product of the one-step probabilities. That is, the probability of observing a path \( \pi = \sigma_1 \sigma_2 \cdots \sigma_k \) from a node \( n \) is defined as \( P(n, \pi) = P(n, n \cdot \sigma_1) \cdot P(n \cdot \sigma_1, \sigma_2) \cdots P(n \cdot \sigma_{k-1}, \sigma_k) \).

Compatibility test Based on the prefix frequency tree, we introduce how to decide whether a blue node is compatible with a red node. The idea is that if two nodes are compatible, they should 1) agree on the last letter, and 2) their future probability distribution should be similar enough. In practice, we compare the differences between the probability of all paths from the two nodes in the tree and check if the difference is within a certain bound. If so, we draw the conclusion that the two nodes are compatible and move on to merge the blue node into the red one. We remark that different bounds have been proposed and we adopt the following latest data-relevant bound between node \( n \) and \( n' \) [24]:

\[
\forall \pi, |P(n, n \cdot \pi) − P(n', n' \cdot \pi)| < \sqrt{\text{be} \log(F(n)) / F(n)} + \sqrt{\text{be} \log(F(n')) / F(n')}
\]

Merge two nodes If a blue node passes compatibility test with a red node, it will be merged into the red node as one state. The way of merging a blue node \( b \) into a red node \( r \) is to update the frequency function of both the ancestors and descendants of the red node \( r \). In particular, for any of \( r \)'s ancestor \( r_a \), we add its frequency \( F(r_a) \) by \( F(b) \); and for any of \( r \)'s descendants \( r_d \), let \( \pi_d \) be the onwards path from \( r \), we add the frequency \( F(r_d) \) by \( F(b \cdot \pi_d) \). In addition, we add an edge from \( b \)'s parent to \( r \) to facilitate the last step, i.e., PFA construction.

PFA construction After all the compatible nodes are merged, we construct the final PFA as follows. The set of states in the PFA are the nodes in the red set. The transitions between states are formed as follows. Take one red node \( r \) as example. For each \( \sigma \in \Sigma \), the transition probability from \( r \) to \( r \cdot \sigma \) is defined as \( P(r, r \cdot \sigma) = F(r \cdot \sigma) / F(r) \). The probability of transitioning to itself is \( 1 - \sum_{\sigma \in \Sigma} F(r \cdot \sigma) \). Notice that if \( r \cdot \sigma \) is not a red node, the next state will be the red node that \( r \cdot \sigma \) was merged into. The initial distribution is to always start from the empty string ()

**Example 3.3.** Figure 6 shows how two nodes are merged in a prefix frequency tree when they meet the criteria shown in the equation 4. On the left is an example of the original frequency prefix tree, where the node bb will be merged into node ab. On the right is the new tree after merging, where the frequency of node ab and all its ancestors will be updated.

### 3.3 Model selection

In the following, we discuss how to automatically select the number of clusters to obtain the best model. The idea is that a PFA of ‘good’ quality should 1) mimic the target RNN by making the same decisions on as many inputs as possible, and 2) be simple (i.e., with few states) for better explanation and easy understanding by human users. In the following, we first introduce how to use the learned PFA to make predictions, and define a metric to measure the quality of the PFA, and finally present how to automatically select the number of clusters.

![Figure 6: Merge two nodes in a frequency prefix tree.](image)

**Algorithm 2:** PFAPredict(\( x, \mathcal{A} \))

1. Let \( l \) be the length of \( x \);
2. Let \( \Theta \) be a set of tuples initialized as \( ((), (), 1) \);
3. for \( j \) from 0 to \( l - 1 \)
   4. Let \( \Theta_c \) be the empty set;
   5. for each tuple \( \theta \) in \( \Theta \)
      6. Extract the current state \( s_c \), path \( \pi \), and path probability \( P(\pi) \) from \( \theta \);
      7. Find all possible next states \( N_s \) according to \( s_c \) and \( x[j] \) in \( \mathcal{A} \);
      8. for each possible next state \( s_n \) in \( N_s \)
         9. Compute the probability of path \( \pi \cdot s_n \);
         10. Add the tuple \( (s_n, \pi \cdot s_n, P(\pi \cdot s_n)) \) into \( \Theta_c \);
   11. Merge those tuples in \( \Theta_c \) which have the same state \( s_n \);
   12. \( \Theta = \Theta_c \);
5. return The tuple with highest path probability in \( \Theta_c \).

*Make a prediction* Given an input word (i.e., a sequence of alphabets), the PFA transits between the states according to the input word. Notice that at each time step, the PFA might be in different states following different paths since a concrete word can appear in different transitions (as the PFA is learned based on the abstract alphabet). We thus maintain a set of tuples, where each tuple \( \theta \) has a current state \( s_c \), a path reaching the state \( \pi \) and the corresponding path probability \( P(\pi) \). When some tuples in the tuples set with different paths may have the same currents state, we only keep the tuple holding the maximum path probability. Finally, we make the prediction based on the PFA path with highest probability among all the possible paths. The detailed algorithm to obtain the path with highest probability is shown in Algorithm 2 and an example is given as follows.

**Example 3.4.** Suppose that there are three possible transition paths in PFA show in Figure 2 with the same input sequence: \( \pi_1 = (s_1, s_2, s_1) \), \( \pi_2 = (s_1, s_2, s_2) \), \( \pi_3 = (s_1, s_1, s_2) \), the path probability of each is 0.072, 0.252, 0.072 respectively, then \( \pi_2 \) should be the desired path according to our algorithm.
Metric of PFA quality In order to find the best number of clusters for learning, we design the following metric borrowing the idea of Bayesian Information Criterion (BIC [5]).

\[
\text{Score}(\mathcal{A}) = P(\mathcal{A}(x) = R(x)|\mathcal{A}) - \eta \cdot \ln(\tau) 
\]

where \( \mathcal{A} \) is the learned PFA based on \( k \) clusters; \( R \) is the target RNN; \( \tau \) is the number of states in \( \mathcal{A} \); and \( \eta \) is a hyper parameter which controls how much we favor a small model over the fidelity of the model. The default configuration is \( \eta = 0.1 \). Intuitively, the metric is intended to favor a model with high fidelity in terms of mimicking the RNN and with fewer states.

Hierarchical clustering Based on the above-defined metric of PFA quality, we then introduce hierarchical clustering [19] as an approach to automatically select the number of clusters with the best quality, by lazily increasing the number of clusters. From the high level, hierarchical clustering initially takes each hidden state as an independent cluster, then it iteratively merges a pair of most similar clusters at each step until all hidden states are grouped into one cluster. The merging operations can then be organized into a tree, where each parent node denotes the new cluster by merging its two children nodes (i.e., children clusters). We remark that hierarchical clustering algorithm can be adopted in a top-down manner. The idea is to start with only one cluster. If one cluster is identified as being too coarse, we split it into two clusters. As a result, the number of total clusters is increased by one in every split. We omit the details of the algorithm and refer the readers to [19] for details. The following example illustrate how the split works.

Example 3.5. Figure 7 shows an example of a hierarchical clustering tree. Suppose we first split the hidden states into two clusters (i.e., 012 and 3) and find the cluster 012 too coarse. We then split 012 into two clusters, i.e., 01 and 2, and so the number of clusters becomes three (i.e., 01, 2, 3).

3.4 Overall algorithm

The overall algorithm is shown in Algorithm 3. The inputs of our algorithm include the input traces set \( \mathcal{X} \), a RNN model \( \mathcal{R} \) trained from \( \mathcal{X} \) and several hyper-parameters, where \( \zeta \) denotes the maximum number of clusters for abstraction and \( \gamma \) denotes the minimum overall performance that a desired model need to achieve, \( \epsilon \) is a parameter used for compatibility testing in learning PFA (Algorithm 1), and \( k \) denotes the initial number of clusters for abstraction. The output is an extracted PFA \( \mathcal{A} \) which mimics how the RNN makes decisions.

The algorithm works as follows. While the number of clusters is within the user-defined threshold at line 3, we first obtain the clustering function \( \Psi_k(\cdot) \) using hierarchical clustering parameterized by \( k \) at line 4. We apply the clustering function \( \Psi_k(\cdot) \) to abstract \( X \) into abstract traces \( a(X) \) at line 5. Then, we learn a PFA \( \mathcal{A} \) using AAlgeria algorithm over the abstract traces at line 6. If the learned model already satisfies the requirement (i.e., \( \text{Score}(\mathcal{A}) \geq \gamma \)), we return the learned PFA \( \mathcal{R} \) directly. Otherwise, we proceed to increase the number of clusters by 1 at line 10 and start another round of model extraction.

Algorithm 3: RNNExtract(\( \mathcal{X}, \mathcal{R}, \zeta, \gamma, \epsilon, K \))

| Line | Description |
|------|-------------|
| 1    | Let \( \mathcal{A} \) store the extracted PFA; |
| 2    | Let \( \Psi(x; \mathcal{R}) \) denotes the function that map input sequence \( x \) into an abstract trace; |
| 3    | \( \zeta \) denotes a cluster function with \( K \) clusters; |
| 4    | \( \text{while} \ K \leq \zeta \text{ do} \) |
| 5    | Obtain \( \Psi_k(\cdot) \) using a hierarchical clustering algorithm with parameter \( K \); |
| 6    | \( \alpha(X) \leftarrow \Psi_k(X, \mathcal{R}); \) |
| 7    | \( \mathcal{A} \leftarrow \text{AAleria}(\alpha(X), \epsilon); \) |
| 8    | if \( \text{Score}(\mathcal{A}) \geq \gamma \) then |
| 9    | \( \text{return} \ \mathcal{A}; \) |
| 10   | \( K = K + 1; \) |
| 11   | \( \text{return} \ \mathcal{A} \) |

4 EXPERIMENTS

In this section, we evaluate our approach on two artificial tasks and two real-world tasks respectively. We aim to show that our probabilistic approach is able to generate models which mimic the original RNN model significantly better than state-of-the-art approaches especially for real-world tasks. We also investigate how the number of clusters influences the model extraction and provides visualization at different abstraction levels of the extracted model. Lastly, we provide some explanation on how the surrogate models can help us understand the semantics of the input traces. The code and results are available at [12].

4.1 Datasets

We first introduce the four datasets used for the evaluation, which are used in the baseline approaches explained later. Note that the first two are artificial datasets and the latter two are real-world ones.

Tomita Grammars. These grammars are widely adopted for previous work on learning grammars [38]. They consist of 7 regular languages with different complexity over alphabet \( \{0, 1\} \). The detailed definitions of the 7 grammars are listed in Table 1. In particular, the set of strings defined by grammar 1, 2 and 7 have extremely unbalanced positive and negative strings, while the set of strings defined by grammar 5 and 6 has relatively balanced number of
Balanced Parentheses. Strings of balanced parentheses (BP) are defined over an alphabet with 28 letters \( \{a, b, \ldots, z, (, )\} \), where parentheses in each string are kept balanced, i.e., each opening parenthesis is eventually followed by a closing parenthesis.

**IMDB dataset.** This dataset is a widely used benchmark for sentiment analysis classification. It contains 50,000 movie reviews which are equally split into a training set and a test set. In total, there are 25k positive reviews and 25k negative reviews. The dataset is well collected and processed in a way that makes sure the reviews are as independent as possible. For instance, no more than 30 reviews are collected for any movie in this collection.

**CSDMC2010 SPAM.** This dataset contains a set of mail messages used in the data mining competition associated with ICONIP 2010. It consists of a labeled training set and an unlabeled test set. The training set contains 4327 messages (2949 non-spam messages and 1378 spam messages), and the test set contains 4292 messages without unknown labels. In our experiments, we use the training set as we need the label to evaluate the quality of the surrogate models.

### 4.2 Baselines

We refer to the approach proposed in [16] as baseline 1 (BL1), which aims to extract DFA from RNNs. Similar to our approach, they first encode the hidden state space by applying clustering, and then they directly regard each cluster as a state of the automata to be learned. After that, they map the hidden state trace of each input sequence into an abstract state trace. Finally, by accounting the frequency of the transitions between each pair of states in the automata state traces, they build the transition matrix and identify the accepting states. Compared to our approach, this baseline is straightforward and it can not recover the probabilistic distribution of the given input data.

We refer to the approach proposed in [40] as baseline 2 (BL2), which adopts the L* algorithm [1] to extract a DFA from RNN. The algorithm first builds a DFA (denoted as DFA1) based on an observation table, and then build an abstract DFA (denoted as DFA2) from the RNN with an interval partition function (i.e., a heuristics based abstraction). After that, by breath-first searching the strings set over the alphabet, the algorithm checks the equivalence between the two DFAs and refines one of them if a conflict occurs. The algorithm repeats the above procedure until the equivalence query is satisfied and returns the DFA. We remark that checking equivalence by traversing the strings over the alphabet is time-consuming and even impractical when the alphabet is large which is the case for most real-world tasks.

### 4.3 Experimental Settings

We provide the experiment settings of our experiments for each dataset in this section.

**Experiments on artificial datasets** Experiments on the two artificial datasets follow the configuration of [40]. The first step is to generate training set from the grammars. For Tomita grammars, we craft the training set with various lengths for each Tomita grammar: \( \{0, 1, 16, 19, 22\} \) (except Tomita 6 which has a different length setting \( \{0, 13, 15, 20\} \)). For BP, the maximum depth of the parentheses is set to be 11 and the lengths are \(0, 15, 20, 25, 30\). When crafting the training set for the two regular grammars, we generate up to 300 samples for each length and try to keep the label (positive or negative) as balanced as possible. For the test set, we uniformly sample a length from \(\{1, 4, 7, \ldots, 28\}\) and generate a string. Once we obtain the training set, we then train state-of-the-art RNN accordingly. The networks for both dataset are a 2-layer GRU but with different hidden state size, i.e., 100 for Tomita grammars and 50 for BP. Table 2 summarizes the dataset size of each grammar and the performance of its target model. Notice that the extraction of DFA is on the training set.

**Experiments on real-world datasets** For the IMDB dataset, we randomly selected 2000 samples from the training set to train the target model and test it on 400 randomly selected samples from the test set. Notice that the distribution of labels is balanced in both the training and the test set. In addition, we sample another small subset of IMDb training set containing 100 samples with a length of each review no more than 20. The purpose of the small subset is to evaluate the performance of the DFA learned using the baseline approach in [40] as it is not scalable to larger dataset (details shown later). For the SPAM dataset, we randomly select 2000 samples for training the target model and 400 samples for testing from the SPAM labeled training set. Again, the dataset is kept balanced in both training set and the test set.

For both real-world datasets, we train GRU and LSTM networks as the target models for model extraction which are two most

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### Table 1: Definition of Tomita Grammars

| Tomita Grammar | Definition |
|---------------|------------|
| Tomita1       | \(1^*\)    |
| Tomita2       | the complement of \((0\to1)^*0^*1(11)^*(00\to1)^*(11)^*(01)^*0^*1\) \* |
| Tomita3       | words not containing 000 |
| Tomita4       | the number of “0” and the number of “1” are both even numbers for each string |
| Tomita5       | the difference between the number of “0” and the number of “1” is a multiple of 3 |
| Tomita7       | 0^*1^*0^*1^* |

### Table 2: Size of artificial datasets

| Grammar | Train(positive) | Test(positive) | Acc(Train) | Acc(Test) |
|---------|----------------|----------------|------------|-----------|
| Tomita1 | 624(17)        | 1000(3)       | 100%       | 100%      |
| Tomita2 | 619(9)         | 1000(1)       | 100%       | 100%      |
| Tomita3 | 2898(1418)     | 1000(128)     | 100%       | 100%      |
| Tomita4 | 2910(1524)     | -              | 100%       | -         |
| Tomita5 | 3791(1821)     | 1000(320)     | 100%       | 60.4%     |
| Tomita7 | 2878(1435)     | 1000(88)      | 100%       | 100%      |
| BP      | 4979(2523)     | -              | 100%       | -         |
widely used RNN structures. We set the dimensions of hidden states and the number of hidden layers for the two RNNs as 10 and 3 respectively. For the input of RNNs, we transform each word into a 300-dimensions numerical vector by word2vec [25] in a standard way. Notice that for the spam samples, we only use the body of each email as the training data. The performance for our trained GRU and LSTM on the two datasets are shown in Table 3. Notice that the extraction of DFA over both real-world languages is based on its testing set for computational reasons.

### 4.4 Research Questions

We aim to answer the following research questions.

**RQ1: How accurate is the extracted model on the training data compared to the target model?**

To answer this question, we fix the number of clusters as 20 and test the accuracy of the extracted models for both our approach and two baselines. The number 20 is chosen based on our experiments described later. The results are summarized in Table 4. We can observe that our approach is able to extract more accurate models than BL1 in both artificial tasks and real-word tasks and BL2 shows the best performance in artificial tasks.

However, further experiments show that BL2 does not scale well, i.e., it easily becomes infeasible if the dataset has a large alphabet (e.g., larger than 600). This limits its applicability in real-world tasks, where the alphabet over a dataset with many long sequences is usually large (e.g., 11173 for the 400 IMDB reviews with the average valid length 111.475) in natural language processing. Thus, in order to evaluate the performance of BL2 on real-world tasks, we are only allowed to select 100 samples from IMDB and the length of each review is no more than 20. We vary the number of reviews to test the performance of BL2. Here, we choose GRU as the target model and train it to 100% accuracy on the 100 small samples. For BL2, the max depth is set to 10 and the timeout is 3600 s. Figure 8 shows the result of the BL2’s performance. We can observe that the accuracy of the models extracted using BL2 drops down significantly as we increase the number of samples and the accuracy is only slightly above 50% when the sample size is 100. On the other hand, our approach scales well to large alphabets through abstraction, i.e., we are able to extract models from 500 samples (instead of about 50 samples for BL2). Besides, we consistently extract models with high accuracy on both real-world datasets, i.e., the accuracy of the extracted models range from 85% to 95%. We thus have the following answer to RQ1:

> Our approach is able to extract accurate models and is much more scalable than the baseline approaches due to abstraction.

**RQ2: How accurate can the extracted model mimic the target model?**

Note that the our goal is to extract a model which is able to mimic the target model in terms of making classification decisions on the input. Thus, besides the accuracy on the training data, we further use the ‘fidelity’ of the extracted model with respects to the original RNN to measure how well the extracted model is able to mimic its original RNN model when used for classification, which is defined as follows.

\[
Fidelity = \frac{\sum_{i=1}^{T^s} 1(A(t_i) = R(t_i))}{|T^s|}
\]

where $A$ and $R$ denotes the extracted PFA and the target RNN respectively, $T^s$ is the test set, $t_i$ is the i-th sample in $T^s$ and $I$ is a sign function. Following the same setting as RQ1, we test the fidelity of our approach as well as that of the two baselines. The results are shown in Figure 9. Notice that for the Tomita grammars, we present the average results of all the seven regular languages for space reasons.

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**Table 3: Performance of target models on real-world dataset**

| Dataset | RNN   | Acc on Train | Acc on Test |
|---------|-------|--------------|-------------|
| IMDB    | GRU   | 95.3%        | 85.3%       |
|         | LSTM  | 91.12%       | 83.4%       |
| SPAM    | GRU   | 93.8%        | 94.0%       |
|         | LSTM  | 90.35%       | 89%         |

**Figure 8: BL2 performance on IMDB dataset.**

**Figure 9: Comparison of fidelity of extracted models**

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**Our approach is able to extract accurate models and is much more scalable than the baseline approaches due to abstraction.**
We observe that for both GRU and LSTM, the models extracted by our approach have higher fidelity than state-of-the-art approaches, i.e., our approach often has near-perfect performance in terms of mimicking the original RNN for BP, IMDB and SPAM. We also observe that the improvement is even more significant on real-world tasks where both baseline approaches only have about 60% fidelity. One possible reason is that the real-world data is usually probabilistic instead of generated based on a set of rules (e.g., regular grammars). As a result, the baseline approaches following the idea of rule extraction do not fit well since there are no underlying rules to extract in the real-world setting. On the other hand, our probabilistic abstraction approach is able to take into consideration the probability distribution among the abstract states and thus provide more accurate and scalable model extraction. We thus have the following answer to RQ2:

Our approach is able to extract more accurate models in terms of mimicking the original RNN than baseline approaches especially for real-world tasks.

We observe that for both GRU and LSTM, the models extracted by our approach have higher fidelity than state-of-the-art approaches, i.e., our approach often has near-perfect performance in terms of mimicking the original RNN for BP, IMDB and SPAM. We also observe that the improvement is even more significant on real-world tasks where both baseline approaches only have about 60% fidelity. One possible reason is that the real-world data is usually probabilistic instead of generated based on a set of rules (e.g., regular grammars). As a result, the baseline approaches following the idea of rule extraction do not fit well since there are no underlying rules to extract in the real-world setting. On the other hand, our probabilistic abstraction approach is able to take into consideration the probability distribution among the abstract states and thus provide more accurate and scalable model extraction. We thus have the following answer to RQ2:

Our approach is able to extract more accurate models in terms of mimicking the original RNN than baseline approaches especially for real-world tasks.

RQ3: How does the number of clusters influence the overall performance of the extracted model?

Model extraction should be done at a proper level of abstraction which is influenced by the number of clusters used for encoding the symbolic states. Intuitively, the more clusters we use, the more fine-grained the abstraction is but the less generalization the extracted model has. We thus conduct experiments to vary the number of clusters from 2 to 14 and observe how the performance of the extracted models change. We choose GRU as the target model and conduct the experiment on the four datasets. Table 5 shows how the size of learned PFA change with different number of clusters. Note that the results of Tomita grammars is the average of the 7 languages. Figure 10 shows the effects of number of clusters on accuracy and fidelity. We observe that as we refine the abstraction by increasing the number of clusters, the fidelity of the extracted models increase in the beginning but tends to stabilize after a certain point. The size of the extracted models increases with the number of clusters. Using our defined score using Eq. 5 provides us a balance between the fidelity (model performance) and the size of the extracted models. We thus have the following answer to RQ3:

Our approach is able to automatically select the number of clusters which balances between model performance and model size.

| Target Model | Learned Automata | Tomita1 | Tomita2 | Tomita3 | Tomita4 | Tomita5 | Tomita6 | Tomita7 | BP | IMDB | SPAM |
|--------------|------------------|---------|---------|---------|---------|---------|---------|---------|-----|------|------|
| GRU          | PFA              | 1       | 0.9887  | 1       | 0.9464  | 1       | 0.5153  | 1       | 0.9694 | 0.852 | 0.9417 |
|              | BL1              | 0.9904  | 0.9612  | 0.8229  | 0.9127  | 0.5009  | 0.5201  | 0.9552  | 0.8325 | 0.626 | 0.6985 |
|              | BL2              | 1       | 1       | 0.9978  | 0.9945  | 1       | 0.9654  | 0.628   | 0.7526 | -    | -    |
| LSTM         | PFA              | 1       | 0.9887  | 0.9334  | 0.7532  | 0.6636  | 0.4957  | 1       | 0.9308 | 0.856 | 0.8961 |
|              | BL1              | 0.9904  | 0.9838  | 0.6935  | 0.8203  | 0.6667  | 0.4292  | 0.9551  | 0.8083 | 0.684 | 0.7568 |
|              | BL2              | 1       | 1       | 0.9531  | 1       | 0.7875  | 0.9176  | 1       | 0.9845 | -    | -    |

Figure 10: Effects of different number of clusters.

5 RELATED WORK

We briefly review existing interpreting methods of machine learning models (in particular RNN) and DFA learning.

Model Explanation. From a broader point of view, explanation of machine learning models can be categorized into local and global explanations. Local explanations try to provide insight on why the target machine learning model makes a decision on a certain (kind of) input. One example is the SHAP-like system [21], which uses a simple linear function to mimic the more complex models, e.g., convolutional neural network (CNN), when producing a certain output on an input. Global explanations, however, try to understand the inner decision process by using a simpler and easier-to-understand model to mimic the behaviors of the model on any input. One example is the rule extraction of RNN explained below [18]. Our work takes a global explanation perspective.

RNN Rule Extraction. Rule extraction from RNN is the process of constructing different computational models which mimic the RNN [3, 18]. This work is especially related to the work that extract deterministic finite automata (DFA) from RNN. These approaches...
usually rely on encoding the hidden states into symbolic representations using techniques like clustering [16] or interval partitioning [40]. Our work is different by learning a probabilistic finite automaton (PFA) from the symbolic data. There is also some recent work aiming to extract a weighted automata (WA) [3]. However, the extraction of WA also does not provide generalization to capture the temporal dependency over the symbolic representations. Our work encodes the concrete states in a similar way but then uses probabilistic abstraction to extract a probabilistic model which suits the real-world problems better.

PFA Learning. The study of learning probabilistic finite automata (PFA) is a branch of grammar inference [11], which has been investigated under different settings using methods like state merging [8] or identifying the longest dependent memory [30, 31]. Recently, researchers have proposed to learn PFA for system analysis tasks like model checking or runtime monitoring and verification [24, 38]. This work follows a state-merging learning paradigm to learn a PFA from the symbolic data extracted from RNN.

### 6 CONCLUSION

In this work, we propose a probabilistic abstraction approach to extract a probabilistic finite automata from state-of-the-art Recurrent Neural Network to mimic its behavior for analysis. Our approach is based on symbolic encoding of hidden states and a probabilistic learning algorithm which tries to recover the probability distribution of the symbolic data. The experiment results on real-world sentiment analysis tasks show that our approach improves the quality of models extracted using state-of-the-art model extraction works significantly. Our approach can potentially open the door for applying software analysis techniques (like model-based testing, model checking and runtime monitoring and verification) to deep neural networks.

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