Learning with Interpretable Structure from RNN

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Abstract

In structure learning, the output is generally a structure that is used as supervision information to achieve good performance. Considering the interpretation of deep learning models has raised extended attention these years, it will be beneficial if we can learn an interpretable structure from deep learning models. In this paper, we focus on Recurrent Neural Networks (RNNs) whose inner mechanism is still not clearly understood. We find that Finite State Automaton (FSA) that processes sequential data has more interpretable inner mechanism and can be learned from RNNs as the interpretable structure. We propose two methods to learn FSA from RNN based on two different clustering methods. We first give the graphical illustration of FSA for human beings to follow, which shows the interpretability. From the FSA’s point of view, we then analyze how the performance of RNNs are affected by the number of gates, as well as the semantic meaning behind the transition of numerical hidden states. Our results suggest that RNNs with simple gated structure such as Minimal Gated Unit (MGU) is more desirable and the transitions in FSA leading to specific classification result are associated with corresponding words which are understandable by human beings.

Key words: Machine learning, Structured output, Recurrent neural network, Gated unit, Finite state automata, Interpretability

1. Introduction

Structure learning deals with the problem where the output is a structured object rather than a valued-label \[\text{BHS}^+07\]. Structures used here include graph \[\text{CSYU}15\], sequence \[\text{LTI}5\], trees \[\text{WMC}09\], vectors \[\text{LTM}17, \text{SLT}^+18\], etc. Algorithms such as structured perceptron \[\text{Col}02\] and structured SVM \[\text{TJHA}05\] have also been proposed. During the last decades, structure learning has been successfully applied to
object tracking [HGS+16] and location [BL08], semantic parsing [PD09], drug design [Lav15] and web-
search [WYJ+18]. There are other machine learning problems involving structures in the output space, for
example, multi-label learning [ZZ14], label ranking [HFCB08, VG10], and clustering [LST17, SLT+17].
Such kind of problems are also highly related to structure learning.

Generally, structure learning uses structures as supervision information and the corresponding algorithms
target at achieving good performance. However, nowadays, as the learning algorithms become more and
more complex, interpretability, i.e., understanding the inner mechanism or what takes place during the
learning process, is also becoming important [Lip16]. Thus besides using the structures as supervision
information, can we learn a structure from existing models to increase the interpretability of complex
models? In this paper, we will focus on the deep learning models, and try to learn structures from such
models to improve its interpretability. Note that understanding deep learning models has raised great
attention during the last several years [KJL15, YCN+15, WHP+18]. Thus it would be very beneficial if
we can learn an interpretable structure from deep learning models.

Finding an interpretable structure for a deep learning model is generally difficult. However, for a specific
type of deep learning models, i.e., Recurrent Neural Networks (RNNs) [GGCC94], there is a way. As a
main member of deep neural networks, RNNs, especially those with gates (gated RNNs, such as MGU with
one gate [ZWZZ16], GRU with two gates [CvMG+14] and LSTM with three gates [HS97]) have been
successfully applied to various tasks on learning sequential data, such as speech recognition [HDY+12],
image caption [VTBE15], sentiment analysis [TQL15], etc. Apart from RNNs, there is another tool
capable of processing sequential data, i.e. Finite State Automaton (FSA) [Gil62, Gol78, AS83]. FSA
is composed of finite states and transitions between states. It will transit from one state to another state
in response to external sequential inputs. The transition process of FSA is similar to that of RNNs
when both models accept items from some sequence one by one, and transit between states accordingly.
Different from RNNs, the inner mechanism of FSA is easier to be interpreted since it can be simulated by
human beings [Lip16] where the transitions between states have physical meanings instead of numerical
calculations in RNNs. Thus the characteristic of FSA makes us consider learning an FSA from RNNs and
use the natural interpretation ability of FSA to understand RNNs’ inner mechanism. Therefore we adopt
FSA as the interpretable structure that we look for. Different from the previous works on structure learning
where the predictions or classification results are structured, the structured output in our paper is a middle
outcome which is obtained to better understand RNNs’ inner mechanism.
In order to learn an FSA from RNNs and use FSA to interpret the inner mechanism of RNNs, we need to answer two questions: how to learn and what to interpret. For the first question, to learn an FSA, we are inspired by the fact that hidden states of classical non-gated RNN tend to form clusters [OG96, ZGS93]. However, there are still important unsolved issues. One is that we do not know whether the tendency to form clusters will also hold for gated RNNs. We also need to consider the efficiency issue since gated RNNs nowadays are always applied to large data sets. When it comes to the second question, we need to analyze the role of the gate in gated RNNs. Especially considering the different number of gates in different gated RNNs, we should discuss the impact of the number of gates for them. In view of that transitions between states in FSA has physical meanings, we may infer the semantic meanings of RNNs’ transitions from corresponding transitions in FSA.

Note that in generic machine learning tasks, learning from multiple data resources [GTM+16, Gon17], or training several basic models and then combining them [Zho12] usually produce better results. While in structure learning, it is also beneficial to incorporate multiple models [GBK12] where a set of multiple hypotheses is produced for experts to evaluate. Thus, besides learning only one FSA from RNNs, we also generate multiple FSAs to do ensemble to promote the performance. Furthermore, single structure may contain limited semantic information, whereas multiple structures might make the semantic information more plentiful and better to understand.

In this paper, we attempt to study RNNs through learning FSA from RNN. We first verify that besides RNN without gates, gated RNNs’ hidden states also have the natural tendency to form clusters. Then we propose two methods. One is based on the high-efficient clustering methods $k$-means++ [AV07]. The other makes use of the observations that hidden states close in the same sequence also tend to be near in geometrical spaces, named as $k$-means-$x$. We then learn FSA by designing its five necessary elements, i.e., alphabet, a set of states, start state, a set of accepting state and state transitions. We apply our methods on artificial data and real-world data. For the artificial data, we first illustrate the learned FSA where human beings can follow and understand the running process. Then the results on the relationship between accuracy and the number of clusters inspire us that gates are necessary to gated RNNs, but the less gates the better. It explains why MGU (with only one gate) has merits over other gated RNNs to some extent. For the real-world data on sentiment analysis, we find that behind the numerical calculations, RNNs’ hidden states indeed have the capacity to distinguish semantic differences, when in the corresponding FSA, words leading to positive/negative outputs do have the positive/negative understandable emotions for human beings. For both datasets, we also produce multiple FSAs from RNNs to do ensemble by different initializations. The
experimental results validate that multiple FSAs can improve the performance and make the semantic information more plentiful.

In the following, we are going to introduce background. Then we state our detailed algorithms, followed by experiments. Finally, we conclude our work.

2. Background

In this section, we introduce one non-gated RNN and three gated RNNs, which will be studied in our paper. We also add discussions on interpretation in this section.

First, we introduce the classical non-gated RNN. It was proposed in early 90s [Elm90] with simple structure which does not possess any gate and is only applied to small scale data. So we call it simple RNN (SRN). In general, SRN takes each element of a sequence as an input and combines the hidden state in the last time to calculate the current hidden state step by step. Concretely, at time $t$, we input the $t$-th element of a sequence, saying $x_t$ into the hidden unit. Then the hidden unit will give the output $h_t$ based on the current input $x_t$ and the previous hidden state $h_{t-1}$ in the following way:

$$h_t = f(h_{t-1}, x_t).$$

$f$ is usually defined as a linear transformation plus a nonlinear activation, e.g.,

$$h_t = \tanh(W[h_{t-1}, x_t] + b)$$

where the matrix $W$ consists of parameters related to $h_{t-1}$ and $x_t$ and $b$ is a bias term. The task of SRN is to learn the parameters $W$ and $b$.

However, the data we are facing are growing bigger and bigger, thus we need deeper model [KSH12, GBC16] to tackle this problem. Yet in this situation, SRN will suffer from the vanishing or exploding gradient issue, which makes learning SRN using gradient descent very difficult [HS97, BSF94]. Fortunately, gated RNNs are proposed to solve the gradient issue by introducing various gates to hidden unit to control how information flows in RNN. The two prevailing gated RNNs are Long Short Term Memory (LSTM) [GSC00] and Gated Recurrent Unit (GRU) [CvMG+14]. LSTM has three gates including an input gate controlling adding of new information, a forget gate determining remembering of old information
Table 1: Summary of three gated RNNs (MGU, GRU and LSTM). The bold letters are vectors. \( \sigma \) is the logistic sigmoid function, and \( \odot \) is the component-wise product between two vectors.

**MGU (minimal gated unit)**

\[
\begin{align*}
\text{(gate) } f_t &= \sigma(W_f[h_{t-1}, x_t] + b_f) \\
\tilde{h}_t &= \tanh(W_h[f_t \odot h_{t-1}, x_t] + b_h) \\
h_t &= (1 - f_t) \odot h_{t-1} + f_t \cdot \tilde{h}_t.
\end{align*}
\]

**GRU (gated recurrent unit)**

\[
\begin{align*}
\text{(gate) } z_t &= \sigma(W_z[h_{t-1}, x_t] + b_z) \\
\text{(gate) } r_t &= \sigma(W_r[h_{t-1}, x_t] + b_r) \\
h_t &= \tanh(W_h[r_t \cdot h_{t-1}, x_t] + b_h) \\
h_t &= (1 - z_t) \odot h_{t-1} + z_t \cdot \tilde{h}_t.
\end{align*}
\]

**LSTM (long short-term memory)**

\[
\begin{align*}
\text{(gate) } f_t &= \sigma(W_f[h_{t-1}, x_t] + b_f) \\
\text{(gate) } i_t &= \sigma(W_i[h_{t-1}, x_t] + b_i) \\
\text{(gate) } o_t &= \sigma(W_o[h_{t-1}, x_t] + b_o) \\
\tilde{c}_t &= \tanh(W_c[h_{t-1}, x_t] + b_c) \\
c_t &= f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \\
h_t &= o_t \odot \tanh(c_t).
\end{align*}
\]

and an output gate deciding outputting of current information. GRU has two gates, an update gate and a reset gate which controls forgetting of old information and adding of new information, respectively, similar to the forget and input gate in LSTM.

The previous models add several gates to one hidden unit, producing a lot of additional parameters to tune and compute, thus may not be efficient enough. To tackle this, [ZWZZ16] produced Minimal Gated Unit (MGU), which only has a forget gate and has comparable performance with LSTM and GRU. Thus MGU’s structure is simpler, parameters are fewer and training and tuning are faster than the previous mentioned gated RNNs.

The mathematical formalizations of the three gated RNN models including MGU, GRU and LSTM mentioned above are summarized in Table 1 in which

\[
\sigma(x) = \frac{1}{1 + \exp(-x)} \quad (1)
\]
is the logistic sigmoid function (applied to every component of the vector input) and $\odot$ is the component-wise product between two vectors. All gates in Table 1 are marked with text "(gate)", from which we can easily see that MGU has one gate, GRU has two gates and LSTM has three gates.

Note that although different gated RNN models with various gates added to hidden unit have been proposed, they are still difficult to be interpreted due to its complex inner mechanism. There are mainly three factors that cause the complexity of gated RNNs’ inner mechanism. One is its recurrent structure inherited from classical RNN [GGCC94]. Despite that the recurrent structure has shown to be the key in handling sequential data, using the same unit recurrently for different inputs will make human beings confused about the inner process of classification. Another complexity comes from the gates they use on the unit. Although one of the reason why MGU is appreciated is that it uses far less gates than other models [ZWZZ16], e.g., LSTM or GRU, the function of gates has not been fully understood, especially how many gates is inherently required for a gated RNN model. Thirdly, the inner process of gated RNNs is in the form of numerical calculation, while a numerical vector could not be directly associated to a concrete meaning for people to understand. In a word, gated RNNs’ inner mechanism is too complex for human beings to follow and understand.

In this paper, we will learn the interpretable structure, i.e., FSA to probe into the gated RNNs and attempt to make contributions on the interpretation. We will find that MGU with minimal number of gates still outperforms other RNNs from the FSA’s perspective. This may raise a new direction to design better RNN models.

3. Our Approach

In this section, we first introduce the intuition and framework, followed by the details of the proposed method including clustering hidden states and learning FSA.

3.1. Intuition and Framework

We consider the following case. First we train an RNN model $\mathcal{R}$ on training data. Then two test sequences $a$ and $b$ are input to $\mathcal{R}$ separately. It is reasonable to observe that if the two subsequences input to $\mathcal{R}$ before time $t_1$ of $a$ and time $t_2$ of $b$ are analogous, the hidden states at time step $t_1$ of $a$ and $t_2$ of $b$ will also
resemble each other. We regard a hidden state as a vector or a point. Thus when several sequences are input to RNN, large amounts of hidden state points will accumulate, and they tend to form clusters. To validate that, we show the distribution of hidden state points when testing from MGU, SRN, GRU and LSTM respectively in Figure 1(a) to (d). We set the original dimension of hidden states by 10. Then we use t-Distributed Stochastic Neighbor Embedding (t-SNE) \cite{vdM09} to reduce the dimension of all 400 hidden state points from 10 to 2 so that we can plot them on the plane. As can be seen, all the hidden state points obtained from different RNNs tend to form clusters. We assume different clusters will represent different states and transitions between states arise when one item of input sequence is read in. Hence the network behaves like a state automaton. We assume the states are finite, then we can learn a Finite State Automaton (FSA) from a trained RNN model.

So the overall framework is showed in Figure 2. We firstly train RNNs on training data and then to do clustering on all hidden states $H$ corresponding to validation data $V$ and finally to learn an FSA with respect to $V$. After obtaining an FSA, we can use it to test unlabeled data or directly draw an illustration. In the first step of training RNNs, we exploit the same strategy as \cite{ZWZZ16} and omit the details here. In the following, we elaborate hidden state clustering and FSA learning steps.

### 3.2. Hidden States Clustering

The first clustering method we consider exploiting is $k$-means \cite{HW79}. K-means is to minimize the average squared Euclidean distance of points from their cluster centers, which is efficient, effective and widely used. To obtain a robust result, we use a variant of k-means named as $k$-means++ \cite{AV07} which uses “$D^2$ weighting” to weight and select cluster centers.
Figure 2: The illustration of the framework of the proposed algorithm. The yellow circles represent the hidden states denoted as $h_t$ where $t$ is time step. “A” is the recurrent unit which receives input $x_t$ and $h_{t-1}$ and outputs $h_t$. The double circle in the structured FSA is the accept state. Overall, the framework consists of three mains steps, namely, training RNN models, clustering on hidden states and outputting structured FSA.

Nevertheless, directly using Euclidean distance may not be appropriate. Besides, it is reasonable to assume that the hidden state points in the same sequence are more similar, and the hidden state points that are close in time are also near in space. Thus, to consider this characteristic, we concatenate the original hidden state points with extra features which reflect the time closeness. We present an illustration as follows:

Feature vector of $j$th element in the $i$th sequence:

$$h_j^1, h_j^2, \ldots, h_j^d, 0, \ldots, 0, j, 0, \ldots, 0$$

where $h_j^d$ means the $d$-th dimension of hidden state point $h_j$. The dimension $n$ of the extra feature is the number of sequences in $V$. Note that each element of a sequence corresponds to a hidden state. For the $j$-th element in the $i$-th sequence, the content in the $i$-th position of the extra feature is $j$. We call the extra feature “extra position feature”. After altering the space, we still use k-means++ to do clustering on the new space. We call this cluster method “k-means-x”.

### 3.3. Learning FSA

FSA $M$ is a 5-tuple $M = \langle \Sigma, Q, R, F, \delta \rangle$ where $\Sigma$ is alphabet, meaning the set of the elements appearing in the input sequences, $Q$ is a set of states, $R \subseteq Q$ is the start state, $F \subseteq Q$ is a set of accepting states and $\delta : Q \times \Sigma \rightarrow Q$ defines state transitions in $M$. In order to learn an FSA, we will specify the details of how to design such five elements below.
In our case, we want to learn FSAs (Finite State Automata) from gated RNNs. The alphabet $\Sigma$ is easy to obtain from data. For example, if the data $D$ are sentences consisting of words, then $\Sigma$ is equal to all words in all sentences. So we have

$$\Sigma = \text{Vocabulary}(D),$$

where $\text{Vocabulary}(D)$ means the vocabulary of $D$.

Every time we input an element from some sequence into RNN, we can get the current hidden state $h_t$ given the previous hidden state $h_{t-1}$. This process is similar to that we input a symbol $s$ from alphabet $\Sigma$, and according to the current state and state transitions function $\delta : Q \times \Sigma \to Q$, we would know which state should be transited to. Thus we can regard a cluster consisting of several similar hidden state points as a state in FSA. Then, the set of states $Q$ are

$$Q = \{C \mid h \in C\},$$

where $C$ is the cluster of a number of hidden states points $h$.

We define the start state $R$ by an empty state without any hidden state point because when we input a word into RNN, no previous hidden states are given. Thus the start state $R$ is just a starting symbol. The accepting states $F$ can be determined by the cluster center. Note that each state in FSA is a cluster of hidden state points in RNN. We use the RNN’s classifier to classify the cluster center of each state. If the classification result is positive, then the corresponding state is an accepting state, namely,

$$F = \{C \mid R(\text{cluster center of } C) = 1\}$$

The fifth element $\delta$ is the most difficult one to obtain among the five elements. We use transition matrix $T \in [|Q|][|Q|] \times |\Sigma|$ to represent the state transitions $\delta : Q \times \Sigma \to Q$ where $|Q|$ means the number of elements in $Q$, $|\Sigma|$ means the number of symbols in $\Sigma$. In $T$, each row represents one state (the first row represents the start state $R$, its serial number in $Q$ is $|Q|$), each column represents a symbol $s$ in alphabet. $T(i, j)$ means state $i$ will transit to state $T(i, j)$ when inputting a symbol $s$ whose corresponding hidden state point belongs to the $j$-th state. To get a transition matrix $T$, we first need to calculate a matrix $N_s$ for each symbol $s$ in alphabet (e.g. 0 or 1 in binary alphabet), where the $(i, j)$-th entry represents the frequency of jumping from state $i$ to state $j$ given $s$ in all sequences, using the following steps:
Algorithm 1 LISOR

Input: The number of clusters $k$;

Output: An FSA.

1: Train an RNN model $R$ and test on validation data $V$;
2: Record the hidden state point at every time step of every sequence in $V$;
3: Do clustering on the recorded hidden state points $H$;
4: Obtain alphabet $\Sigma$ according to (2);
5: Obtain set of states according to (3);
6: Obtain accepting states according to (4);
7: Calculate a matrix $N_s$ for each symbol $s$ in alphabet (e.g. 0 or 1 in binary alphabet);
8: Generate transition matrix $T$ according to (5).

1. indexing every cluster or state, associating each hidden state point to a state in FSA;
2. iterating through all hidden state points, and increasing $N_s(i, j)$ by one when $s$ incurs a transition from state $i$ to state $j$.

As a consequence, $N_s(i, j)$ represents the transition times from state $i$ to $j$ when inputting $s$. In this case, when inputting $s$, state $i$ may transit to several states. We intend to obtain a deterministic FSA for clear illustrating, so we only keep the biggest value which means abandoning the less frequent transitions in each row of $N_s$. Then the transition matrix $T$ can be quickly calculated as follows:

$$T(i, j) = \arg \max_k N_{s_j}(i, k)$$ (5)

We can draw an illustration of FSA according to $T$ and use $T$ to do classification. When doing classification, the state will keep jumping from one state to another in response to sequentially input symbols, until the end of the sequence. If the final state is an accepting state, the sequence is predicted to be positive by FSA.

The whole process of learning FSA from RNN is presented in Algorithm 1. We call our method LISOR (Learning with Interpretable Structure frOm Rnn) and present two concrete algorithms according to different clustering methods. The one based on k-means++ is named as “LISOR-k” while the other one based on k-means-x is called “LISOR-x”. By utilizing the tendency to form clustering of hidden state points, both LISOR-k and LISOR-x can learn a well generalized FSA from RNN models.
4. Experiments and Discussions

In this section, we conduct experiments on both artificial and real tasks and visualize the learned FSAs from corresponding RNN models. Besides that, in both tasks, we discuss that how we interpret the RNN models from FSAs, as well as show the accuracy when using the learned FSAs to do classification.

4.1. Artificial Tasks

In this section, we explore two artificial tasks. The goal of the experiments is to draw a visualized illustration of the learned FSAs and show how to interpret RNNs from the learned FSAs.

4.1.1. Settings

The first artificial task is to identify sequence 0110 in a group of length-4 sequences which only contain 0 and 1 (task “0110”). This is a simple task containing 16 distinct cases. We include 1000 instances in the training sets, with duplicated instances to improve accuracy. We use validation set containing all possible length 4 zero-one sequences without duplication to learn FSAs and randomly generate 100 instances to do testing.

The second task is to determine whether a sequence contains three consecutive zeros (task “000”). There is no limitation on the length of sequences, thus the task has infinite instance space and is more difficult than task “0110”. We randomly generate 3000 zero-one training instances whose lengths are also randomly decided. We also generate 500 validation and 500 testing instances.

For both these tasks we mainly study MGU, SRN, GRU and LSTM mentioned in Section 2. For all these four RNN models, we set the dimension of hidden state and the number of hidden layers to be 10 and 3 respectively. We conduct each experiment 5 times and report the average results.

4.1.2. Discussions on the Number of Clusters

According to Algorithm 1, in order to learn and visualize an FSA, we need to set the cluster number $k$ or equally, the number of states in FSA. Note that more clusters mean each cluster contains less hidden state points. A trivial example is that the number of clusters is equal to the number of hidden state points, then
Table 2: The number of clusters \((n_c)\) when the accuracy of FSA learned from four RNNs first achieves 1.0 on task “0110” by LISOR-k and LISOR-x. Note that the value is the smaller the better for higher efficiency and better interpretability. RNN models trained from different trials are with different initializations on parameters. We can see that on average FSA learned from MGU always achieves the accuracy 1.0 with the smallest number of clusters. The number of clusters is 65 means that the FSA's accuracy cannot meet 1.0 when \(n_c\) is up to 64 since we set \(n_c\) varying from 2 to 64. The smallest number of clusters in each trial and on average are bold.

| RNN Type | MGU | SRN | GRU | LSTM | RNN Type | MGU | SRN | GRU | LSTM |
|----------|-----|-----|-----|------|----------|-----|-----|-----|------|
| LISOR-k  |     |     |     |      | LISOR-x  |     |     |     |      |
| Trial 1  | 5   | 13  | 7   | 13   | Trial 1  | 5   | 13  | 8   | 15   |
| Trial 2  | 8   | 9   | 25  | 9    | Trial 2  | 8   | 9   | 65  | 10   |
| Trial 3  | 6   | 6   | 8   | 12   | Trial 3  | 6   | 6   | 8   | 12   |
| Trial 4  | 5   | 5   | 8   | 17   | Trial 4  | 5   | 5   | 8   | 65   |
| Trial 5  | 6   | 22  | 9   | 22   | Trial 5  | 6   | 20  | 9   | 24   |
| Average  | 6   | 11  | 11.2| 14.6 | Average  | 6   | 10.6| 19.6| 25.2 |

Table 3: The number of clusters \((n_c)\) when the accuracy of FSA learned from four RNNs first achieves 0.7 on task “000” by LISOR-k and LISOR-x. Note that the value is the smaller the better for higher efficiency and better interpretability. RNN models trained from different trials are with different initializations on parameters. We can see that on average FSA learned from MGU always achieves the accuracy 0.7 with the smallest number of clusters. The number of clusters is 201 means that the FSA's accuracy cannot meet 0.7 when \(n_c\) is up to 200 since we set \(n_c\) varying from 2 to 200. The smallest number of clusters in each trial and on average are bold.

| RNN Type | MGU | SRN | GRU | LSTM | RNN Type | MGU | SRN | GRU | LSTM |
|----------|-----|-----|-----|------|----------|-----|-----|-----|------|
| LISOR-k  |     |     |     |      | LISOR-x  |     |     |     |      |
| Trial 1  | 38  | 84  | 201 | 26   | Trial 1  | 31  | 52  | 156 | 25   |
| Trial 2  | 6   | 28  | 109 | 72   | Trial 2  | 6   | 27  | 137 | 60   |
| Trial 3  | 9   | 28  | 201 | 20   | Trial 3  | 9   | 18  | 201 | 26   |
| Trial 4  | 8   | 41  | 85  | 19   | Trial 4  | 8   | 39  | 91  | 22   |
| Trial 5  | 7   | 180 | 201 | 22   | Trial 5  | 7   | 145 | 201 | 39   |
| Average  | 13.6| 72.2| 159.4|31.8| Average  | 12.2| 56.2|157.2|34.4 |

the state transition in FSA resembles the way that hidden state points transit in RNNs. So the performance of FSA should be close to that of RNNs when \(k\) is large enough. Nevertheless, we hope the number of states in FSA to be as small as possible to prevent over-fitting, increase efficiency and reduce complexity so
as to be easily interpreted by human beings. Thus achieving high accuracy with small number of clusters is a good characteristic and we are attempting to make the number of clusters as small as possible with guaranteed classification performance.

In the task “0110”, we set the number of clusters $k$ varying from 2 to 64 (we accumulate $4 \times 16 = 64$ hidden points since we only have 16 sequences in validation data and each sequence contains 4 numbers). Table 2 gives the number of clusters required when the accuracy of FSAs learned from the four RNNs first achieves 1.0 which means perfectly identifying all 0110 sequences. We can see that among all four RNN models, FSA learned from MGU always achieves the accuracy 1.0 with the smallest number of clusters in each trial or on average. Specifically, on average, for LISOR-k the FSA learned from MGU firstly achieves accuracy 1.0 when the number of clusters is 6 followed by that of SRN at cluster number 11. The third one is the FSA learned from GRU with 11.2 clusters, and the final one is that of LSTM with 14.6. For LISOR-x, the corresponding numbers of clusters are 6, 10.6, 19.6 and 25.2, respectively. We can see that the cluster method k-means-x does not bring too many merits on this simple task compared to k-means++. It reduces the number of clusters of FSA learned from SRN but increases those of FSAs learned from GRU and LSTM. This phenomenon can be explained that due to the simpleness of this task, k-means++ already performs well enough, and thus k-means-x does not have space to improve.

In the task “000”, we set the number of clusters $k$ ranging from 2 to 200. Actually we have $500 \times n$ hidden state points where $n$ is the average length of all the 500 sequences, but we do not need that many since similar to the task “0110”, large number of clusters may not bring much to performance improvement but may make interpretation from FSA more difficult. This is a more complicated task than task “0110” and neither the original RNN models nor the learned FSA can reach accuracy 1.0 just like that of task “0110”. Thus we focus on the accuracy over 0.7, i.e., we will increase the number of clusters until the accuracy of the learned FSA model reaches an accuracy of 0.7. Thus we focus on the accuracy over 0.7. As can be seen from Table 2, on average for LISOR-k, FSA learned from MGU firstly achieves accuracy over 0.7 when there are 13.6 clusters. Then FSA learned from LSTM achieved this goal with 31.8 clusters followed by that of SRN at cluster number 72.2. The final one is FSA learned from GRU which achieves 0.7 when the number of clusters is 159.4. For LISOR-x, the corresponding numbers of clusters for FSA learned from MGU, SRN, GRU and LSTM are 12.2, 56.2, 157.2 and 34.4, respectively. We can see that cluster method k-means-x plays a role in this task which lowers the number of clusters of MGU, SRN and GRU.
Figure 3: FSAs learned from four RNNs trained on task “0110”. The number of clusters \( k \) is selected when FSA first reaches accuracy 1.0 as \( k \) increases. The 0110 route is marked by red color. Note that in (d) there are four isolated nodes from the main part. This is because we abandon the less frequent transitions when inputting a symbol to learn a deterministic FSA.

4.1.3. Graphical Illustration of FSA

In order to visualize the corresponding FSA for each RNN model, we focus on our first method LISOR-k as an example and choose the number of clusters \( k \) that most approaches the average number. In task “0110”, for LISOR-k, the average number of \( k \) that first achieves accuracy 1.0 for MGU, SRN, GRU and LSTM are 6, 11, 11.2 and 14.6. Thus we set the number of clusters for MGU to be 6 from trial 3, SRN to be 9 from trial 2, GRU to be 9 from trial 5, LSTM to be 13 from trial 1, respectively.

We then illustrate FSAs’ structure to give people a visual impression of the proposed LISOR’s output in Figure 3, drawn by Graphviz [EGK+04]. Here we use gray circle and double circle to represent start and accepting states, respectively. We mark paths of 0110 sequence by red color. As can be seen, for all length-4 zero-one sequences, only 0110 will eventually lead us to an accepting state by following the transitions in illustrated FSAs, and other sequences cannot reach the accepting state. We want to emphasize
We have first impression in section 4.1.2 that MGU can achieve guaranteed accuracy with smaller number of clusters. We will give more details results, i.e., how the accuracy of the learned FSA changes when the number of clusters is increasing.

4.1.4. Interpretation about Gate Effect

We have first impression in section 4.1.2 that MGU can achieve guaranteed accuracy with smaller number of clusters. We will give more details results, i.e., how the accuracy of the learned FSA changes when the number of clusters is increasing.

We also illustrate FSAs’ structure of “000” task in Figure 4. Similar to task “000”, we only focus on LISOR-k as an example and choose the number of clusters $k$ that most approaches the average number. For LISOR-k, the average number of $k$ that first achieves accuracy 0.7 for MGU, SRN, GRU and LSTM are 13.6, 72.2, 159.4 and 31.8. Thus we set the number of clusters for MGU to be 6 from trail 2, SRN to be 28 from trail 2, GRU to be 85 from trail 4, LSTM to be 19 from trail 4, respectively. We can see that the corresponding FSAs are much more complex than those of task “0110”. Due to the complexity of this task, different positive sequences will have different ways to reach the final accept state, thus we do not mark paths of transitions by positive sequences.

Figure 4: FSA learned from four different RNNs trained on task “000”. The number of clusters $k$ is selected when FSA first reaches accuracy 0.7 as $k$ increases.

that by following the flow of FSAs, transitions between states are caused directly by input word. We need not do any numerical calculation as we done in RNN models, thus making the whole process easier to be understandable.
Figure 5: Impact of the number of clusters on FSA’s accuracy when learning from MGU, SRN, GRU and LSTM. We can see that FSA learned from MGU can reach a satisfiable accuracy more quickly.

For task “0110”, the average accuracy tendencies of five trials are shown in (a) and (b), which correspond to algorithm LISOR-k and LISOR-x, respectively. Here we limited the number of clusters to be less than 24, since when it is larger than 24, the performance changes slightly. In Figure (a) and (b), all FSA models can reach high performance with small number of clusters since the task is not complex. When the number of clusters increase, FSA’s performance may be unstable due to the loss of information when we abandon less frequent transitions. We can see that the FSA learned from MGU always firstly achieves high accuracy and holds the lead.

For task “000”, the average accuracy tendencies of five trials are shown in Figure (c) and (d). As can be seen from Figure (c) and (d), all four FSAs’ accuracies increase with number of clusters increasing. MGU firstly achieved high accuracy and holds the lead.
In summary, we observe that the FSA learned from MGU reaches its best performance earlier than other RNN models when the number of clusters increases. Therefore, MGU is the most efficient when its learned FSA possesses more clear illustration and easier interpretability. Inspired by this phenomenon together with the fact that MGU contains less gates on the unit than GRU and LSTM, and also the fact that SRN contains no gates, we tend to treat the gate as a regularizer controlling the complexity of the learned FSAs, as well as the complexity of space of hidden state points, while no gate at all will lead to under-fitting. This conclusion motivates us to design other RNN models in the future, which necessarily contain gates, but contain only minimal number of gates as that of MGU.

4.1.5. Ensemble Results of Multiple FSAs

Generally, ensemble of multiple classifiers will improve the classification performance [Zho12]. In this section, we will show the ensemble accuracy results with the increasing of number of clusters of the learned

Figure 6: Comparison between the average accuracy of the 5 trials and the accuracy of the ensemble of MGU with the increasing of the number of clusters.
FSA. We focus on MGU since its learned FSA outperforms others from the previous experiment results. We train five MGUs with different initializations of parameters. After we got the corresponding FSAs, we give the final output using majority voting, i.e., only when 3 out of 5 FSAs vote for positive, the output will be positive. The results are shown in Figure 6. We can see that in both tasks, ensemble of multiple FSAs does improve classification performance. It shows that the ensemble of learned multiple structures will lead to better classification in our tasks. We further observe that on the more complex “000” task, the improvement is much larger than that on the easier task “0110”. We conjecture that ensemble of multiple FSAs is more suitable for complex tasks and will continue to use this strategy in more complex real tasks.

4.2. Real Task

In this section, we conduct our experiments on a practical task about sentiment analysis. We will mainly show the accuracy of our learned FSA from the four RNNs on real tasks. We then use the results of the best performed MGU as an example to show that the learned FSA indeed has semantic distinguishing ability.

4.2.1. Settings

In this task, we will use the IMDB dataset [MDP+11] to do sentiment analysis [PCH+17, MDP+11], which is a very common task in natural language processing. In this dataset, each instance is the comment for a movie and the task is to classify the given sentence into positive or negative sentiment.

To train the RNN models, we first use word2vec [MCCD13] to map each English word from film reviews into a 300 dimensions numerical vector. Then we train four different RNNs (MGU, SRN, GRU and LSTM) using these vectors as input. All RNN models’ dimension of hidden states and number of hidden layers are set to be 10 and 3 respectively, and we randomly select 2000 random-length film reviews as training data. After we get the trained RNN, we learn four different FSAs using 200 testing data. Note that we adopt a transductive setting, i.e. using the test data directly to learn FSAs to ensure all words in test data’s vocabulary be fully covered.

4.2.2. Discussion on the Number of Clusters

Note that this task is more complex than the artificial tasks, thus we cannot enumerate over all possible number of clusters (i.e., number of hidden states in RNNs). We have tried different number of clusters,
Figure 7: FSAs learned from MGU trained on sentiment analysis task. The FSA here is shrunk and the words between the same two states in the same direction are grouped into a word class. For example, the words in “word_class_0-1” all incur transitions from State 0 (S_0) to State 1 (S_1). We train five MGUs with different initializations. (a) is the result of trial 1 and trial 5 where the accepting state is State 1. (b) is the result of trial 2, 3 and 4 where the accepting state is State 0.

Table 4: Accuracy on sentiment analysis task when the number of cluster is 2. “Average” means the average accuracy results of the five structured FSAs. “Ensemble” means using ensemble technique to combine the five structured FSAs to improve the performance. LISOR-k and LISOR-x are our methods. In each method and each strategy, the highest accuracy is bold among the four RNNs.

| RNN Type | LISOR-k Average | LISOR-k Ensemble | LISOR-x Average | LISOR-x Ensemble |
|----------|----------------|------------------|----------------|------------------|
| MGU      | 0.701          | 0.740            | 0.740          | 0.850            |
| SRN      | 0.604          | 0.635            | 0.592          | 0.615            |
| GRU      | 0.662          | 0.660            | 0.699          | 0.780            |
| LSTM     | 0.669          | **0.750**        | 0.669          | 0.755            |

that is \( k \), from 2 to 20 and found that the smaller \( k \) is, the better the performance. We understand that if the number of clusters is large enough, FSA will perform better and have similar performance with corresponding RNN models. However, when \( k \) is small, our empirical results show that simple structure may lead to better performance. Thus in this part, we only exhibit the results when the number of clusters is 2. In this case, all the FSAs possess the simplest structure which is easy to understand as well as be visually illustrated. With same number of clusters, the FSA with higher accuracy is more practical.

4.2.3. Graphical Illustration of FSA

This task has much larger vocabulary size containing thousands of English words, which means the number of symbols (i.e., words) in \( \Sigma \) is not simply 2, which is adopted in the artificial tasks. Thus in order to show the graphical illustration of FSA, we shrink the edges in the same direction between two states into
one edge and illustrate the resulted FSA learned from MGU with two clusters in Figure 7. Other FSAs’
structures are similar and we omit them. In this way the words on a shrunk edge are naturally grouped
into a class named as “word_class”. We learned five FSAs from five different MGUs according to different
initializations. We find that their structures are the same but with different accepting state. As can be seen
from Figure 7, the accepting state of trial 1 and trial 5 are State 1 (S_1) while that of trial 2, 3 and 4 are
State 0 (S_0).

4.2.4. Accuracy Result

For each of MGU, SRN, GRU and LSTM, we train five different ones according to different initializations
and learn five corresponding FSAs from them. We show the average results of the five FSAs’ accuracy in
Table 4 for each RNN. We can see that, for both LISOR-k and LISOR-x, FSAs learned from MGU have
the highest accuracy compared to that of other three RNNs and LISOR-x performs better than LISOR-k,
which shows the effectiveness of k-means-x that utilizes the extra position feature. In order to show the
validity of multiple output structures, we adopt the same strategy as artificial tasks, i.e., combing the results
of the five FSAs by ensemble using majority voting. The ensemble classification results of FSAs learned
from MGU, SRN, GRU and LSTM are also shown in Table 4. As can be seen, for LISOR-k, the results of
ensemble method are almost better than the case without ensemble except GRU and FSA learned from
MGU exhibits competitive performance. For LISOR-x, the performances of ensemble are all better than
the cases without ensemble and the FSA learned from MGU outperforms other RNNs’ FSAs. LISOR-x is
better than LISOR-k in MGU, GRU and LSTM as well.

4.2.5. Semantic Interpretation

We try to find the semantic meaning behind the transitions between states in FSA. We still focus on MGU
due to its FSA’s best performance. The results are shown in Table 5 and Table 6. We consider the transition
from State 0 to State 1 in all the five learned FSAs. Table 5 shows the results on the 1th FSA and 5th FSA,
according to Figure 7 we realize that this is a transition leading to the accept state. Here the number in
the bracket shows the serial number of the FSA from which this word comes. We can see that transitions
leading to accepting state contains mainly “positive” words, for example, wonderful, spectacular, sweetness,
etc. We can also see that one FSA will only cover one part of the positive words, thus having limited
semantic meaning, while multiple structured FSA can make the semantic meaning more plentiful. The
Table 5: Transition words on one edge from State 0 leading to **acceptable** state (i.e., State 1 which contains **positive** film reviews), where most words are positive. Here the number in the bracket shows the serial number of the FSA from which this word comes.

| Positive                      | Negative                      |
|-------------------------------|-------------------------------|
|riffls(1) Wonderful(1) gratitude(1) diligent(1) spectacular(1) sweetness(1) exceptional(1) Best(1) feats(1) sexy(1) bravery(1) beautifully(1) immediacy(1) meditative(1) captures(1) incredible(1) virtues(1) excellent(1) shone(1) honor(1) pleasantly(1) lovingly(1) exhilarating(1) devotion(1) teaming(1) humanity(1) graceful(1) tribute(1) peaking(1) insightful(1) frenetic(1) romping(1) proudly(1) terrific(1) Haunting(1) sophisticated(1) strives(1) exemplary(1) favorite(1) professionalism(1) enjoyable(1) alluring(1) entertaining(1) sorrowful(1) Truly(1) noble(1) bravest(1) exciting(1) Hurray(1) wonderful(1) Miracle(1)... feelings(5) honest(5) nifty(5) smashes(5) ordered(5) revisit(5) moneyed(5) flamboyance(5) reliable(5) strongest(5) loving(5) useful(5) fascinated(5) carefree(5) recommend(5) Greatest(5) legendary(5) increasing(5) loyalty(5) respectable(5) clearer(5) priority(5) Hongsheng(5) notable(5) reminiscent(5) spiriting(5) astonishing(5) charismatic(5) lived(5) engaging(5) blues(5) pleased(5) subtly(5) versatile(5) favorites(5) remarkably(5) poignant(5) Breaking(5) heroics(5) promised(5) elite(5) confident(5) underrated(5) justice(5) glowing(5) ... adventure(1,5) victory(1,5) popular(1,5) adoring(1,5) perfect(1,5) mesmerizing(1,5) fascinating(1,5) extraordinary(1,5) AMAZING(1,5) timeless(1,5) delight(1,5) GREAT(1,5) nicely(1,5) awesome(1,5) fantastic(1,5) flawless(1,5) beguiling(1,5) famed(1,5) |
|downbeat(1) wicked(1) jailed(1) exceptionally(1) corruption(1) eccentric(5) troubled(5) cheats(5) coaxed(5) convicted(5) steals(5) painful(5) cocky(5) endures(5) annoyingly(5) dissonance(5) disturbing(5) goofiness(1,5) |

results on the 2th and 3th FSA are shown in Table 6, which is a transition leading to the unacceptable state. We can see that most of the activation words of this transition are negative, for example, dullest, unattractive, confusing, etc. We can also conclude that multiple structure can make the semantic meaning more abundant and plentiful.

5. Conclusion

It will be beneficial if we can learn an interpretable structure from the RNN models since there is still no clear understanding of the inner mechanism of RNN models. In this paper, realizing the similarity between RNNs and FSA, as well as the good interpretability of FSA, we try to learn FSA from RNN, and analyze RNNs from FSA’s point of view. After verifying that the hidden states of gated RNNs do form clusters, we propose two methods to learn FSAs from four kinds of RNNs, based on different clustering
Table 6: Transition words on one edge from State 0 leading to **unacceptable** state (i.e., State 1 which contains **negative** film reviews), where most words are negative. The number in the bracket shows the serial number of the FSA from which this word comes.

| Positive            | merry(2) advance(2) excused(2) beliefs(3) romancing(3) deeper(3) resurrect(3) whitewash(3) |
|---------------------|------------------------------------------------------------------------------------------|
| Negative            | shut(2) dullest(2) unattractive(2) Nothing(2) adulterous(2) stinkers(2) drunken(2) hurt(2) rigid(2) un-
|                     | able(2) confusing(2) risky(2) mediocre(2) nonexistent(2) idles(2) horrible(2) disobeys(2) bother(2)  |
|                     | scoff(2) interminably(2) arrogance(2) mislead(2) filthy(2) dependent(2) MISSED(2) asleep(2)       |
|                     | unfortunate(2) criticized(2) weary(2) corrupt(2) jeopardized(2) drivel(2) scraps(2) phony(2) prohib-
|                     | ited(2) foolish(2) reluctant(2) Ironically(2) fell(2) escape(2) ... fanciful(3) flawed(3) No(3)    |
|                     | corrupts(3) fools(3) limited(3) missing(3) pretense(3) drugs(3) irrational(3) cheesy(3) crappy(3) |
|                     | cheap(3) wandering(3) forced(3) warped(3) shoelift(3) concerns(3) intentional(3) Desperately(3)   |
|                     | dying(3) clich(3) bad(3) evil(3) evicted(3) dead(3) minor(3) drunk(3) loser(3) bothered(3) reek(3) |
|                     | tampered(3) inconsistencies(3) ignoring(3) Ward(3) doom(3) quit(3) goober(3) antithesis(3) fake(3) |
|                     | helplessness(3) surly(3) demoted(3) fault(3) worst(3) baffling(3) destroy(3) fails(3) Pity(3) pres-
|                     | sure(3) nuisance(3) farce(3) fail(3) worse(3) SPOLIER(3) egomaniacal(3) quandary(3) burning(3) |
|                     | drinker(3) blame(3) intimidated(3) perfidy(3) boring(3) conservative(3) forgetting(3) hostile(3)  |
|                     | ... unattractive(2,3) goof(2,3) lousy(2,3) stupidest(2,3) mediocrity(2,3) Badly(2,3) mediocre(2,3) |
|                     | waste(2,3) hypocrite(2,3) confused(2,3) vague(2,3) clumsily(2,3) stupid(2,3)                   |

strategies. We show the learned FSA graphically through illustration and explicitly give the transition route for human beings to follow. We also show how the number of gate affects the performance of RNNs, and the semantic meaning behind the numerical calculation in hidden units. We find that MGU with minimal gate can outperform other RNNs from the FSA's perspective. In the future, we plan to design other RNN models sharing the merit of minimal number of gate as MGU.

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