Chapter 4

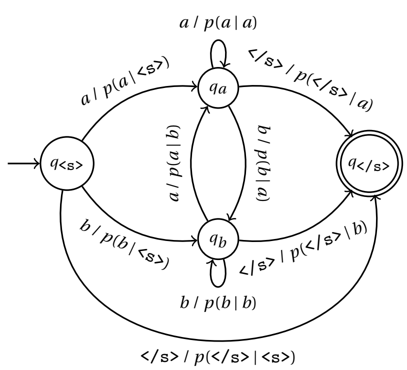
Recurrent Neural Networks

You can think of an RNN as a finite automaton whose transition function (δ) is defined by a neural network. It reads in a sequence of inputs, $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$, and computes a sequence of outputs, $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}$. (The superscripts are written with parentheses to make it clear that this isn't exponentiation.)

They're used for all kinds of language related things, like language modeling, speech, translation. They are often used as a kind of preprocessing step for a wide variety of tasks, because the **y**'s can be seen as a representation of the words that incorporates contextual information.

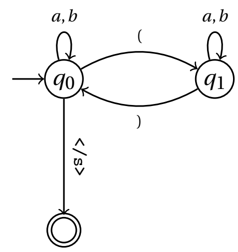
4.1 Motivation

Let's start with a bigram language model. Recall that there are states $q_{\texttt{<s>}}$ and $q_{\texttt{</s>}}$, and a state q_a for every $a \in \Sigma$. We show what the transitions look like for two symbols $a, b \in \Sigma$, but you can imagine what it would look like in general.



(4.1)

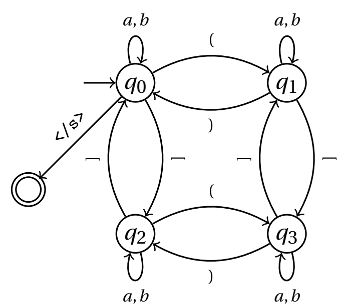
If you had to predict the next word in a sentence, you might use information from very far back in the string. To take a simple example, if there's a left parenthesis, it should be matched by a right parenthesis potentially very far away. Here's a finite automaton that keeps track of whether we're inside parentheses. Again, we just show transitions for two symbols $a, b \in \Sigma$, but you can imagine what it would look like in general.



(4.2)

Presumably, the probability of seeing a right parenthesis is low in q_0, but high in q_1. We can intersect the bigram automaton with this automaton, and we get a new automaton that models both bigrams and parentheses.

Now, we can make a similar automaton to keep track of left and right square brackets (sorry to focus on punctuation; there are plenty of long-distance phenomena in the words themselves, but none as clear-cut as punctuation). Intersect all three automata (bigram, parentheses, square brackets) together and we get an even bigger and more powerful automaton. I can't draw the whole thing, but here's what the intersection of the parentheses and square brackets automata looks like:



(4.3)

We could dream up all kinds of features, design an automaton for each one, and intersect them all together. But then we would have two problems.

The first problem is that coming up with ideas for structuring the state space is laborious. Can the model learn this automatically? The answer is actually yes – we haven't yet covered the methods to do this, but we could just make an automaton with a bunch of states and transitions between all of them, and the model could automatically figure out what to do with them.

The second, more serious, problem is that we are quickly going to end up with many states. If there are 30 features, even if they are all just on/off features like our parentheses feature, there are $2^{30} \approx 1$ billion states, and something like $2^{60} \approx 10^{18}$ probabilities that we have to estimate. Most of these are going to be really bad estimates, because some states will be visited very rarely or not at all.

RNNs make this easier. They have a state space that is just as big as in the above thought experiment, defined by *units* that correspond to what we called "features." But they define the transition function in a different way that has many fewer parameters and can therefore be estimated much better.

4.2 Example

Figure 4.2 shows a run of a simple RNN with 30 hidden units trained on the Wall Street Journal portion of the Penn Treebank, a common toy dataset for neural language models. When we run this model on a

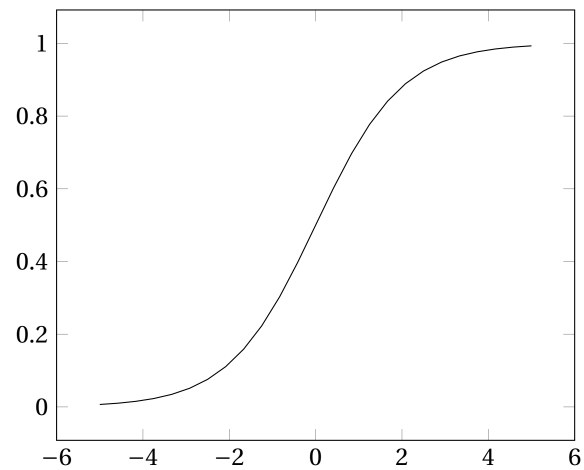


Figure 4.1: The sigmoid function is 0 for very negative values, 1 for very positive values, and smooth in between.

new sentence, we can visualize what each of its hidden units is doing at each time step. The units have been sorted by how rapidly they change.

The first unit seems to be unchanging; maybe it's useful for other units to compute their values. The second unit is blue on the start symbol, then becomes deeper and deeper red as the end of the sentence approaches. This unit seems to be measuring the position in the sentence and/or trying to predict the end of the sentence. The third unit is red for the first part of the sentence, usually the subject, and turns blue for the second part, usually the predicate. The rest of the units are unfortunately difficult to interpret. But we can see that the model is learning something about the large-scale structure of a sentence, without being explicitly told anything about sentence structure.

Other kinds of RNNs that perform better than this simple RNN have been shown to have units that perform various functions, including keeping track of parentheses (Karpathy, Johnson, and Fei-Fei, 2016).

4.3 Definition

These days most people do not implement RNNs themselves; they just one of many toolkits that do it for them. But for reference, here's a definition. A so-called *simple* RNN is defined as follows. The input to the RNN is a sequence of vectors, $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$. Typically, these are *one-hot* vectors: the vector has a component for each word in the vocabulary, with one component set to 1 and the other components set to 0. The output of the RNN is another sequence of vectors, $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}$, each of which is the RNN's estimate of $P(\mathbf{y}^{(i)} \mid \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)})$. To compute this, the RNN computes an intermediate sequence of vectors $\mathbf{h}^{(1)}, \ldots, \mathbf{h}^{(n)}$.

$$\mathbf{h}^{(0)} = \mathbf{0} \tag{4.4}$$

$$\mathbf{h}^{(i)} = \text{sigmoid}(\mathbf{A}\mathbf{h}^{(i-1)} + \mathbf{B}\mathbf{x}^{(i)} + \mathbf{c}) \tag{4.5}$$

where (see Figure 4.1)

$$\text{sigmoid}(z) = \frac{1}{1+\exp(-z)}. \tag{4.6}$$

Then the outputs are computed as:

$$\mathbf{y}^{(i)} = \text{softmax}(\mathbf{D}\mathbf{h}^{(i)} + \mathbf{e}), \tag{4.7}$$

where the softmax function takes the exp of every component and then normalizes them to sum to one:

$$\mathbf{s}^{(i)} = \mathbf{D}\mathbf{h}^{(i)} + \mathbf{e} \tag{4.8}$$

$$y_j^{(i)} = \frac{\exp s_j^{(i)}}{\sum_{j'} \exp s_{j'}^{(i)}}. \tag{4.9}$$

The vectors/matrices $\mathbf{A}, \mathbf{B}, \mathbf{c}, \mathbf{D}, \mathbf{e}$ are parameters of the model. Their components can be arbitrary real numbers, and they don't have any intuitive interpretation (like probabilities do). They will be learned during the training process, as described in the next subsection.

When using an RNN as a language model, we typically set the input and output sequences to be the same, but shifted by one time step:

$$\mathbf{x}^{(1)} = \texttt{<s>} \tag{4.10}$$

$$\mathbf{x}^{(i+1)} = w_i \qquad i = 1, \ldots, n \tag{4.11}$$

$$\mathbf{y}^{(i)} = w_i \qquad i = 1, \ldots, n \tag{4.12}$$

$$\mathbf{y}^{(n+1)} = \texttt{</s>} \tag{4.13}$$

In other words, at each time step, the network uses all the previous words to predict what the next word might be.

4.4 Training

We are given a set of training examples, each of which is a sequence of input vectors, $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}$, and a sequence of output vectors, $\mathbf{c}^{(1)}, \ldots, \mathbf{c}^{(n)}$ (the $\mathbf{c}$ stands for "correct"). Usually the $\mathbf{c}$ vectors are one-hot vectors. For each such training example, the RNN outputs a sequence of vectors, $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(n)}$.

During training, we try to find the parameters that maximize the following objective function (shown here for a single sentence; in general, we would sum over multiple sentences):

$$L = \log P(\mathbf{c}^{(1)} \cdots \mathbf{c}^{(n)}) \tag{4.14}$$

$$= \sum_{i=1}^{n} \mathbf{c}^{(i)} \cdot \log \mathbf{y}^{(i)} \tag{4.15}$$

where the log is elementwise and $\cdot$ is a vector dot product (inner product). Since each $\mathbf{c}^{(i)}$ is a one-hot vector, dotting it with another vector selects a single component from that other vector, which in this case is the log-probability of the ith word.

To maximize this function, there are lots of different methods. We're going to look at the easiest (but still very practical) method, *stochastic gradient ascent*.[1] It is also known as the method of steepest ascent. Imagine that the log-likelihood is an infinite, many-dimensional surface. Each point on the surface corresponds to a setting of the λ's, and the altitude of the point is the log-likelihood for that setting of the λ's. We want to find the highest point on the surface. We start at an arbitrary location (say, with all the λ's set to zero) and then repeatedly move a little bit in the steepest uphill direction.

Let $\boldsymbol{\lambda}$ be the vector of all the parameters of the model, and $\log L(\boldsymbol{\lambda})$ is the objective function, or the function we're maximizing. Gradient ascent looks like this:

initialize parameters $\boldsymbol{\lambda}$ to zero
repeat
  $\boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \eta \nabla \left(\log L(\boldsymbol{\lambda})\right)$
until done

The function $\nabla(\log L)$ is the gradient of $\log L$ and gives the direction, at $\boldsymbol{\lambda}$, that goes uphill the steepest. These days, it's uncommon to need to figure out what the gradient is by hand, because there are numerous automatic differentiation packages that do this for you.

The *learning rate* $\eta > 0$ controls how far we move at each step.

Question 1. What happens if η is too small? too big?

To guarantee convergence, η should decrease over time (for example, $\eta = 1/t$), but it's also common in practice to leave it fixed.

In *stochastic* gradient ascent, at each iteration of the above algorithm, L is the objective function for a single sentence, and we change to a new sentence at each iteration (typically, in random order).

One last trick is fairly important. When using SGA on RNNs, a common problem is known as the *vanishing gradient* problem and its evil twin, the *exploding gradient* problem. What happens is that L is a a very long chain of functions (n times a constant). When we differentiate L, then by the chain rule, the partial derivatives are products of the partial derivatives of the functions in the chain. Suppose these partial derivatives are small numbers (less than 1). Then the product of many of them will be a vanishingly small number, and the gradient update will not have very much effect.

Or, suppose these partial derivatives are large numbers (greater than 1). Then the product of many of them will explode into a very large number, and the gradient update will be very damaging. This is definitely the more serious problem, and preventing it is important. The simplest fix is just to check if the norm of the gradient is bigger than 5, and if so, scale it so that its norm is just 5.

[1] If we're minimizing a function, then we use stochastic gradient *de*scent, and this is the name that the method is more commonly known by.

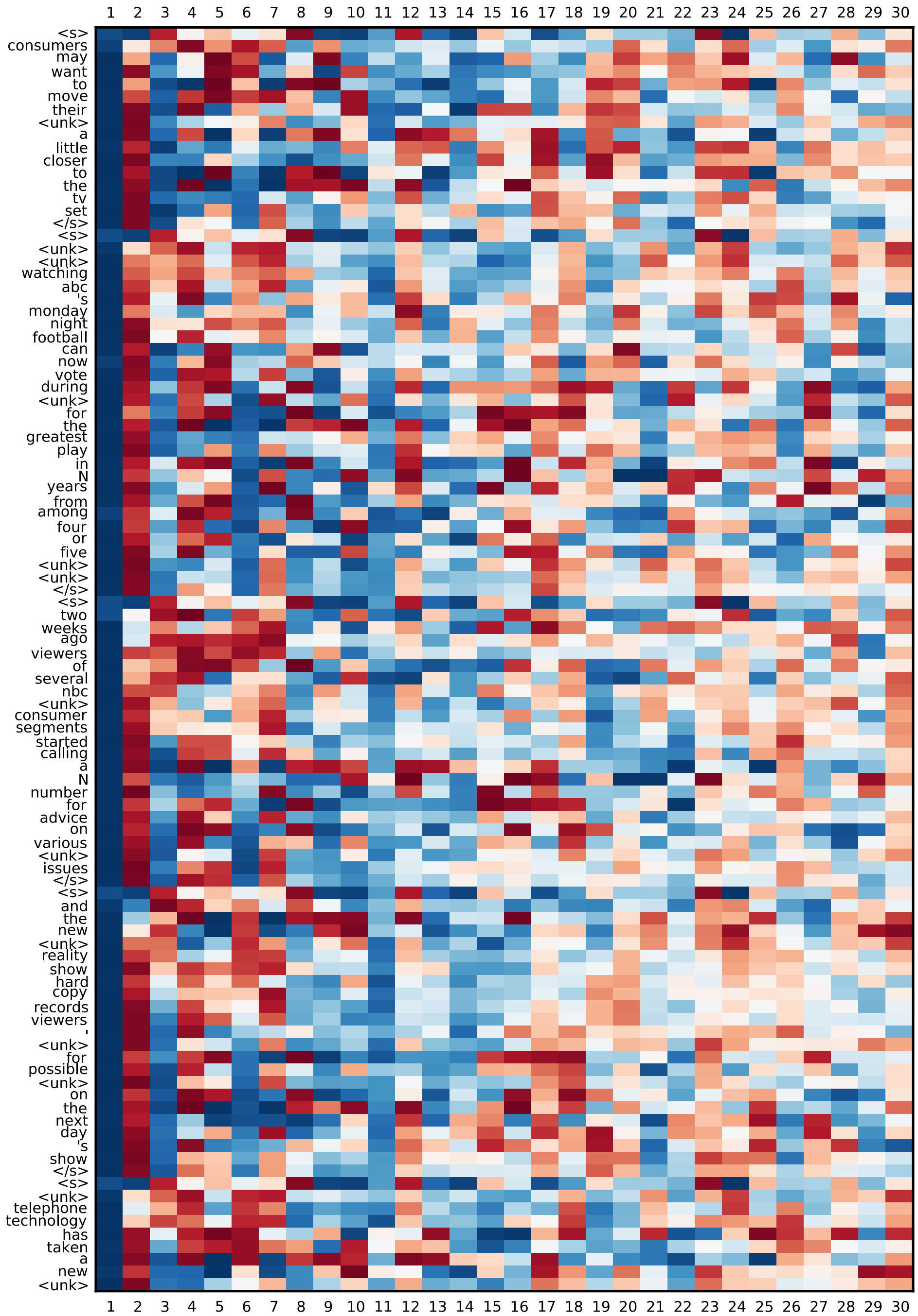


Figure 4.2: Visualization of a simple RNN language model on English text.

Bibliography

Karpathy, Andrej, Justin Johnson, and Li Fei-Fei (2016). “Visualizing and Understanding Recurrent Neural Networks”. In: *Proc. ICLR*.