Chapter 1

Sequence Modeling: Recurrent and Recursive Nets

Recurrent Neural Networks or RNNs are a family of neural networks for processing sequential data.

Rumelhart et al, 1986a — Learning Representations by Back Propagating Errors

> We describe a new learning procedure, back-propagation, for networks of neurone-like units. The procedure repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector. As a result of the weight adjustments, internal 'hidden' units which are not part of the input or output come to represent important features of the task domain, and the regularities in the task are captured by the interactions of these units. The ability to create useful new features distinguishes back-propagation from earlier, simpler methods such as the perceptron-convergence procedure.

A RNN is a network that is specialized for processing a sequence of values $x^{(1)}, ..., x^{(\tau)}$. RNNs can scale to much longer sequences than would be practical for networks without sequence based specialization, and they can also process sequences of variable length.

To go from multilayer networks to recurrent networks, we need to take advantage of parameter sharing. This makes it possible to extend and apply the model to examples of different forms and generalize across them.

Such sharing is important when a specific piece of information can occur at multiple positions within the sequence.

A related idea is the use of convolution across a 1D temporal space. This approach is the basis for time delay neural networks. The convolution operation allows a network to share parameters across time, but it is shallow. The output of convolution is a sequence where each member of the output is a function of a small number of neighboring members of the input. The idea of parameter sharing in this case manifests in the application of the same convolution kernel at each time step.

Recurrent networks share parameters in a different way. Each member of the output is a function of the previous members of the output. Each output member is produced using the same update rule applied to the previous outputs. This formulation results in the sharing of parameters through a very deep computational graph.

This chapter extends the idea of a computational graph to include cycles which represent the influence of the present value of a variable on its own value at a future time step.

For more information on recurrent neural networks than is available in this chapter, look into Alex Graves — Supervised Sequence Labelling with Recurrent Neural Networks

1.1 Unfolding Computational Graphs

In this section we explain the idea of **unfolding** a recursive or recurrent computation into a computational graph that has a repetitive structure, typically corresponding to a chain of events. Unfolding this graph results in the sharing of parameters across a deep network structure.

Consider the classical form of a dynamical system:

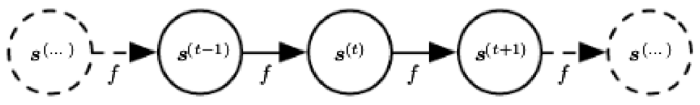
$$s^{(t)} = f(s^{(t-1)}; \theta)$$

where $s^{(t)}$ is the state of the system. This is recurrent because the definition of s at time t refers back to the same definition at time $t-1$.

For a finite number of steps, we can unfold the graph by applying the definition $\tau - 1$ times. For example, if we unfold above 3 times:

$$s^{(3)} = f(s^{(2)}; \theta) = f(f(s^{(1)}; \theta)\theta)$$

By unfolding this repeatedly, we yield an expression that does not involve recurrence. Such an expression can now be represented by a traditional directed acyclic computational graph.



Many recurrent networks also define their hidden units using recursive functions, such as

$$h^{(t)} = f(h^{(t-1)}, x^{(t)}; \theta)$$

Typical RNNs will add extra architectural features such as output layers that read information out of the state h to make predictions. When the network is trained to perform a task that requires predicting the future from the past, the network typically learns to use $h^{(t)}$ as a kind of lossy summary of the task relevant aspects of the past sequence of inputs up to t. This summary is in general necessarily lossy since it maps an arbitrary length sequence $(x^{(t)}, x^{(t-1)}, ..., x^{(2)}, x^{(1)})$ to a fixed length vector $h^{(t)}$.

For example, if we were to use an RNN to predict the next word given the previous words, it may not be necessary to store all of the information in the input sequence up to time t, but instead only enough information to predict the rest of the sentence. The most demanding situation is when we ask $h^{(t)}$ to be rich enough to allow one to approximately recover the input sequence, as in autoencoder frameworks.

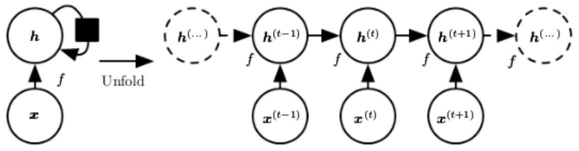


Figure 10.2: A recurrent network with no outputs. This recurrent network just processes information from the input $\boldsymbol{x}$ by incorporating it into the state $\boldsymbol{h}$ that is passed forward through time. *(Left)*Circuit diagram. The black square indicates a delay of a single time step. *(Right)*The same network seen as an unfolded computational graph, where each node is now associated with one particular time instance.

What we call unfolding is the operation that maps a circuit (as in the left side of above) to a computational graph with repeated pieces (as in the right side). The unfolded graph now has a size that depends on the sequence length.

The unfolding process has two major advantages:

1. Regardless of the sequence length, the learned model always has the same input size, because it is specified in terms of transition from one state to another state, rather than specified in terms of a variable length history of states.

2. It is possible to use the same transition function f with the same parameters at each step

2 follows because we can represent the unfolded recurrence after t steps with a function g:

$$h^{(t)} = g^{(t)}(x^{(t)}, x^{(t-1)}, ..., x^{(2)}, x^{(1)}) = f(h^{(t-1)}x^{(t)}; \theta)$$

The function $g^{(t)}$ takes the whole past sequence as input and produces the current state, but the unfolded recurrent structure allows us to factorize $g^{(t)}$ into repeated applications of a function f.

The two advantages above allow us to learn a single model f that operates on all time steps and all sequence lengths, rather than needing to learn a separate model $g^{(t)}$ for all possible time steps. Learning a single, shared model allows generalization to sequence lengths that did not appear in the training set and allows the model tobe estimated with far fewer training examples than would be required without parameter sharing.

1.2 Recurrent Networks

Now that we know of graph unrolling and parameter sharing, we can design a wide variety of networks. Some examples of design patterns for RNNs include the following:

- RNNs that produce an output at each time step and have recurrent connections between hidden units
- RNNs that produce an output at each time step and have recurrent connections only from the output at one time step to the hidden units at the next time step
- RNNs with recurrent connections between hidden units that read an entire sequence and then produce a single output

Any function computable by a Turing machine can be computed by a recurrent network of a finite size.

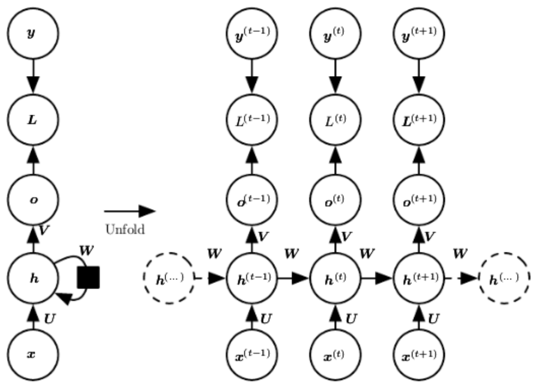


Figure 10.3: The computational graph to compute the training loss of a recurrent network that maps an input sequence of $\boldsymbol{x}$ values to a corresponding sequence of output $\boldsymbol{o}$ values. A loss L measures how far each $\boldsymbol{o}$ is from the corresponding training target $\boldsymbol{y}$. When using softmax outputs, we assume $\boldsymbol{o}$ is the unnormalized log probabilities. The loss L internally computes $\hat{\boldsymbol{y}} = \text{softmax}(\boldsymbol{o})$ and compares this to the target $\boldsymbol{y}$. The RNN has input to hidden connections parametrized by a weight matrix $\boldsymbol{U}$, hidden-to-hidden recurrent connections parametrized by a weight matrix $\boldsymbol{W}$, and hidden-to-output connections parametrized by a weight matrix $\boldsymbol{V}$. Equation 10.8 defines forward propagation in this model. *(Left)*The RNN and its loss drawn with recurrent connections. *(Right)*The same seen as an time-unfolded computational graph, where each node is now associated with one particular time instance.

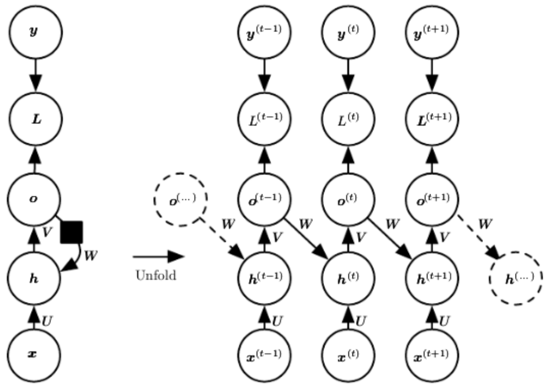


Figure 10.4: An RNN whose only recurrence is the feedback connection from the output to the hidden layer. At each time step t, the input is $\boldsymbol{x}_t$, the hidden layer activations are $\boldsymbol{h}^{(t)}$, the outputs are $\boldsymbol{o}^{(t)}$, the targets are $\boldsymbol{y}^{(t)}$ and the loss is $L^{(t)}$. *(Left)*Circuit diagram. *(Right)*Unfolded computational graph. Such an RNN is less powerful (can express a smaller set of functions) than those in the family represented by figure 10.3. The RNN in figure 10.3 can choose to put any information it wants about the past into its hidden representation $\boldsymbol{h}$ and transmit $\boldsymbol{h}$ to the future. The RNN in this figure is trained to put a specific output value into $\boldsymbol{o}$, and $\boldsymbol{o}$ is the only information it is allowed to send to the future. There are no direct connections from $\boldsymbol{h}$ going forward. The previous $\boldsymbol{h}$ is connected to the present only indirectly, via the predictions it was used to produce. Unless $\boldsymbol{o}$ is very high-dimensional and rich, it will usually lack important information from the past. This makes the RNN in this figure less powerful, but it may be easier to train because each time step can be trained in isolation from the others, allowing greater parallelization during training, as described in section 10.2.1.

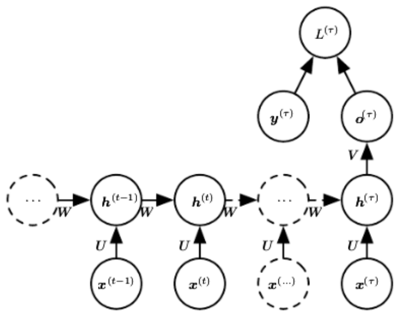


Figure 10.5: Time-unfolded recurrent neural network with a single output at the end of the sequence. Such a network can be used to summarize a sequence and produce a fixed-size representation used as input for further processing. There might be a target right at the end (as depicted here) or the gradient on the output $\boldsymbol{o}^{(t)}$ can be obtained by back-propagating from further downstream modules.