DSCI 572: Supervised Learning II

Muhammad Abdul-Mageed

muhammad.mageed@ubc.ca

Deep Learning & NLP Lab

The University of British Columbia

Table of Contents

- 1 Recurrent Neural Networks
 - Definition
 - Parameters Sharing
 - RNNs as Computational Graphs
 - RNNs as Generative Models
 - An Example RNN

Intro. to RNNs

RNNs (Rumelhart et al., 1986)

- A family of networks classically specializing in sequential data
- RNNs have the advantage of sharing parameters
- Parameter sharing: each member of the output is a function of the previous members of the output.

Parameters Sharing

- Advantage of parameter sharing: makes it possible to apply the model to examples of different forms (e.g., different lengths).
- Especially important when a piece of information occurs at different positions in time:

Example

- "In Vancouver I live".
- "I live in Vancouver".

Comparison to Feedforward Net

- A fully connected feedforward network would have separate parameters for each input feature, needing to learn all the rules of the language separately at each position
- By comparison, a recurrent neural network shares the same weights across several time steps

RNNs: Computational Graphs With Cycles

- Operate on sequences of $x^{(t)}$ with the time step t ranging from 1 to τ .
- The time step can be the position of an item in the sequence.
- Can also be applied backward
- An extension of the idea of a computational graph, to include cycles
- Cycles represent the influence of the present value of a variable on its own value at a future time step

Unfolding Computational Graphs I

Consider the classical form of a dynamical system, with a state s^(t):

1: A Dynamical System

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

- For example, unfolding 3 times would give:

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

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

• The equation is recurrent because the definition of s at time t refers back to the same definition at time t-1.

Unfolding Computational Graphs II

- By repeatedly unfolding, we acquire an expression that does not involve recurrence.
- Can now be expressed by a traditional directed acyclic graph.

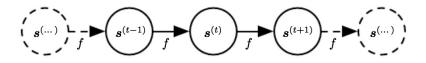


Figure: Each node represents the state at time t, and the function f maps the state at time t to the state at t+1. The same parameters are used for all time steps. [From Goodfellow et al., 2016]

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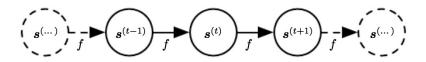


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RNNs as Computational Graphs

• Consider a dynamical system driven by an external signal $x^{(t)}$, where we observe the state now contains information about the whole past sequence:

2: Dynamical System With External Signal

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

• Treating the **state** as the **hidden units** of the network:

3: Hidden State of RNN

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



An RNN (Without Output)

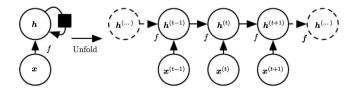


Figure: [From Goodfellow et al., 2016]

More on Unfolding

- Unfolding is the operation that maps a circuit as in the left side of the figure 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.

RNNs as Generative Models

RNNs as Lossy Summarizers

- Typical RNNs would add extra architectural features such as output layers that read information from the state h to make predictions.
- Can be trained to **predict the future from the past** (e.g., predict the next word in a sequence).
- In these cases, 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.
- Summary is necessarily **lossy**, since it maps an **arbitrary length** sequence $(x^{(t)}, x^{(t-1)}, x^{(t-2)}, \dots, x^{(2)}, x^{(1)})$ to a fixed length vector $h^{(t)}$.

RNNs as Lossy Summarizers Cont.

Lossy Summarization Illustrated

- Summary might selectively keep some aspects of the past sequence with more precision than other aspects, depending on the training criterion
- Consider the case of statistical language modeling where the purpose is to predict the next word
- May not be necessary to keep all information up to time step t to predict next word
- Most demanding case is when we ask network to predict whole sequence (auto-encoders)

Unfolded Recurrence after t steps

 The unfolded recurrence after t steps can be represented with a function g^(t):

4: A Function g

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

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

- The function g(t) takes the whole past sequence $(x^{(t)}, x^{(t-1)}, x^{(t-2)}, \dots, x^{(2)}, x^{(1)})$ as input and produces the current state.
- The unfolded recurrent structure allows us to factorize $g^{(t)}$ into repeated application of a function f.

Learning a Single, Shared Model

 Two factors make it possible to learn a single model f that operates on all time steps and all sequence lengths:

Learning a Single Model

- Regardless of the sequence length, the learned model always has the same input size. Why?
 - 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 every time step.

Advantages of Learning a Single, Shared Model

- Allows generalization to sequence lengths that did not appear in the training set
- Allows the model to be estimated with far fewer training examples than would be required without parameter sharing.

Mapping input seq x to output seq o

 Produce an output at each time step, with recurrent connections between hidden units

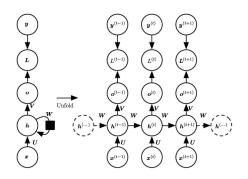


Figure: Three weight matrixes: U: input-to-hidden connections, W: hidden-to-hidden recurrent connections, V: hidden-to-output connections. Loss L compares how far each o is from its target o. Loss internally computes $\hat{o} = softmax(o)$ [From Goodfellow et al., 2016]

Mapping input seq **x** to output seq **o** Cont.

Notes on Previous Figure

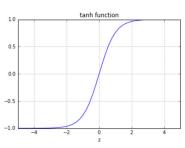
- Let's assume we will use a hyperbolic tangent (tanh) as an activation function.
- Figure does not specify what form the output and loss function take.
- Assume output is discrete (e.g., when the network predicts words or characters).
- Naturally, regard the output o as giving the unnormalized log probabilities of each possible value of the discrete variable (e.g., each word or character).
- Apply the softmax as a post-processing step to obtain a vector \hat{y} of normalized probabilities over the output.

Hyperbolic Tangent Function I

5: Hyperbolic Tangent

$$\tanh(z) = \frac{\sinh z}{\cosh z} = \frac{e^z - e^{-z}}{e^z + e^{-z}} = \frac{e^{2z} - 1}{e^{2z} + 1} = \frac{1 - e^{-2z}}{1 + e^{-2z}}$$

 Strongly neg inputs map to neg outputs; only zero-valued inputs map to near-zero outputs.



Hyperbolic Tangent Function II

```
1 import numpy as np
  2 np.set printoptions(formatter={'float': '{: 0.3f}'.format})
 4 z = np.arange(-5, 5, .2)
 5 t = np.tanh(z)
 6 print("Input: values in x\n {}".format(z))
 7 t=np.tanh(z)
 8 # Note: Its output is always between -1 and 1
 9 print("\nOutput: Tangent Hyperbolic values\n
                                                {}".format(t))
Input: values in x
   [-5.000 -4.800 -4.600 -4.400 -4.200 -4.000 -3.800 -3.600 -3.400 -3.200
 -3.000 -2.800 -2.600 -2.400 -2.200 -2.000 -1.800 -1.600 -1.400 -1.200
-1.000 -0.800 -0.600 -0.400 -0.200 0.000 0.200 0.400 0.600 0.800
 1.000 1.200 1.400 1.600 1.800 2.000 2.200 2.400 2.600 2.800
 3.000 3.200 3.400 3.600 3.800 4.000 4.200 4.400 4.600 4.8001
Output: Tangent Hyperbolic values
   [-1.000 -1.000 -1.000 -1.000 -1.000 -0.999 -0.999 -0.999 -0.998 -0.997
-0.995 -0.993 -0.989 -0.984 -0.976 -0.964 -0.947 -0.922 -0.885 -0.834
 -0.762 -0.664 -0.537 -0.380 -0.197 0.000 0.197 0.380 0.537 0.664
 0.762 0.834 0.885 0.922 0.947 0.964 0.976 0.984 0.989 0.993
 0.995 0.997 0.998 0.999 0.999 0.999 1.000 1.000 1.000 1.0001
```

RNN Update Equations I

• Forward propagation begins with a specification of the initial state $h^{(0)}$. Then, for each time step from t=1 to $t=\tau$, we apply the following update equations:

6: RNN Equations

$$\begin{aligned} \mathbf{a}^{(t)} &= \mathbf{b} + \mathbf{W} \ \mathbf{h}^{(t-1)} + \mathbf{U} \ \mathbf{x}^{(t)} \\ \mathbf{h}^{(t)} &= \tanh(\mathbf{a}^{(t)}) \\ \mathbf{o}^{(t)} &= \mathbf{c} + \mathbf{V} \ \mathbf{h}^{(t)} \\ \hat{\mathbf{y}}^{(t)} &= \textit{softmax}(\mathbf{o}^{(t)}) \end{aligned}$$

 where the parameters are the bias vectors b and c along with the weight matrices U, V, and W, respectively for input-to-hidden, hidden-to-output and hidden-to-hidden connections.

RNN Update Equations II

Mapping Sequences of Same Length

- This RNN maps an input sequence to an output sequence of the same length.
- The total loss for a given sequence of x values paired with a sequence of y values would then be just the sum of the losses over all the time steps.
- For example, if $L^{(t)}$ is the negative log-likelihood of $y^{(t)}$ given $x^{(1)}, \ldots, x^{(t)}$, then: See next slide...

RNN Loss

7: RNN Loss

$$L = (x^{(1)}, \dots, x^{(\tau)}, y^{(1)}, \dots, y^{(\tau)})$$

$$= \sum_{t} L^{(t)}$$

$$= -\sum_{t} \log p_{model}(y^{(t)}|x^{(1)}, \dots, x^{(t)})$$

Expensive Gradient

- Computing the gradients for the loss described earlier involves a forward pass and a backward pass, with a **costly runtime**: $O(\tau)$
- Cannot be parallelized due to sequential process: Each time step may be computed only after the previous one

Back-propagation Through Time (BPTT)

BPTT

- States computed during forward pass must be stored until re-used during the backward pass
- So, the **memory cost is also** $O(\tau)$
- The back-propagation algorithm applied to this unrolled graph with $O(\tau)$ is called back-propagation Through Time (BPTT).
- To sum up, this network trained with recurrent connections between hidden units is **very powerful**, yet **expensive to train**.
- Are there other options? (Yes, as we will see...)