Deep Learning and Temporal Data Processing

3 - Recurrent Neural Networks

Andrea Palazzi

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University of Modena and Reggio Emilia

Agenda



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Introduction

Recurrent Neural Networks



In **feedforward neural network** computation flows directly from input x through intermediate layers h to output y.

Conversely, some networks topology feature feedback connections, in other words model outputs are fed back into the model itself.

The term **recurrent neural networks** defines this family of models.

Recurrent Neural Networks

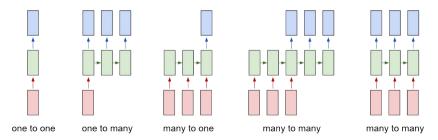


Recurrent neural networks (RNN) are specialized for processing sequences.

Similarly, we saw that convolutional neural networks feature specialized architecture for processing images.

RNNs boast a much wider API with respect to feedforward neural networks.

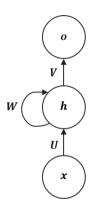
Indeed, these models can deal with sequences in the input, in the output or even both.



Vanilla RNN

Vanilla RNN





The vanilla RNN is provided with three sets of parameters:

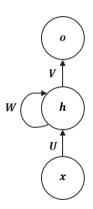
- U maps inputs to the hidden state
- W parametrizes hidden state transition
- V maps hidden state to output

System dynamics is as simple as:

$$\begin{cases} \boldsymbol{h}^{(t)} = \phi(\boldsymbol{W} \, \boldsymbol{h}^{(t-1)} + \boldsymbol{U} \, \boldsymbol{x}^{(t)}) \\ \boldsymbol{o}^{(t)} = \boldsymbol{V} \, \boldsymbol{h}^{(t)} \end{cases}$$
(1)

Intuition about Hidden State





The hidden state $h^{(t)}$ can be intuitively viewed as a *lossy* summary of the sequence of past inputs fed to the network, in which are stored the main task-relevant aspects of the past sequence of inputs up to time t.

Since the an input sequence of arbitrary length $(x^{(1)}, x^{(2)}, ..., x^{(t)})$ is mapped into a fixed size vector $\mathbf{h}^{(t)}$, this summary is necessarily lossy.

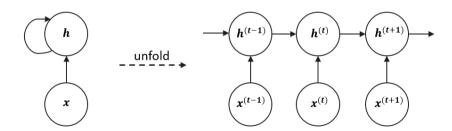
Training a RNN

Unfolding the Computational Graph



A recurrent computational graph can be unfolded into a sequential computational graph with a repetitive structure.

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



Backpropagation Through Time



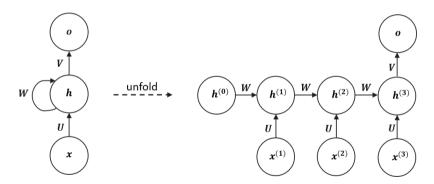
The capacity to **unfold** a **recurrent graph into** a **DAG** (Directed Acyclic Graph) allows to train recurrent neural network by means of standard backpropagation.

Because the gradient conceptually flows backward though time instead of though layers, this algorithm is usually referred to as **backpropagation through time** (BPTT).

Backpropagation Through Time



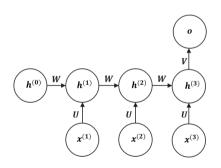
Let's make an example for an simple architecture which processes sequences of length au=3 and produces an output at the end of the sequence.



Backpropagation Through Time



Now, given a differentiable loss on final output L(y, o) let's compute the derivative of the objective L with respect to the weights V, W and U and see what happens.



•
$$\frac{\partial L}{\partial \mathbf{V}} = \frac{\partial L}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial \mathbf{V}}$$

•
$$\frac{\partial L}{\partial \mathbf{W}} = \frac{\partial L}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial \mathbf{h}^{(3)}} \sum_{k=0}^{3} \left(\frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{h}^{(k)}} \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}} \right)$$

•
$$\frac{\partial L}{\partial \mathbf{U}} = \frac{\partial L}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial \mathbf{h}^{(3)}} \sum_{k=0}^{3} \left(\frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{h}^{(k)}} \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{U}} \right)$$

Consideration: while $\frac{\partial L}{\partial \mathbf{V}}$ depends only on current state, $\frac{\partial L}{\partial \mathbf{W}}$ and $\frac{\partial L}{\partial \mathbf{U}}$ depend on all previous sequence states.

The Challenge of Long-Term Dependencies



Looking closer, we see that terms $\frac{\partial \pmb{h}^{(t)}}{\partial \pmb{h}^{(k)}}$ must be themselves computed through the chain rule. For example, we can obtain $\frac{\partial \pmb{h}^{(3)}}{\partial \pmb{h}^{(1)}} = \frac{\partial \pmb{h}^{(3)}}{\partial \pmb{h}^{(2)}} \frac{\partial \pmb{h}^{(2)}}{\partial \pmb{h}^{(1)}}$.

Turns out [3] that when using tanh and sigmoid activations, the 2-norm of these Jacobian matrices is upper bounded by 1 and 1/4 respectively. Thus, we can easily end up multiplying smaller and smaller numbers until the gradients become zero.

This problem is known as **vanishing gradient problem**, and causes serious trouble when trying to learn long-term dependencies in the input sequences, because contributions of "far-away" steps become zero.

The Challenge of Long-Term Dependencies



Depending on the network parameters and choice of activation functions, the opposite problem can arise. This is called **exploding gradient problem** and happens when gradients become bigger and bigger until numerical problems destroy the optimization process.

Both issues can be mitigated through proper weight initialization, accurate choice of activation functions and gradient clipping.

Note: these problems can also happen in deep feedforward networks: however, they are more common in recurrent architectures because these models are usually very deep (actually as deep as the length of the input sequence).

Advanced RNN Architectures

Advanced Recurrent Architectures



Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) are more complex recurrent architectures that have been proposed [2, 1] to overcome the issues in the gradient flow and to ease the learning of long-term dependencies.

Both these architectures feature advanced **learnable gating mechanisms** in order to explicitly learn long-term dependencies.

Long Short-Term Memory networks



Let's see how update equations look like for a LSTM model. Please notice that LSTM framework, notation is usually slightly different than form vanilla RNN.

$$\begin{cases} \mathbf{i} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_i + \mathbf{s}^{(t-1)} \mathbf{W}_i) \\ \mathbf{f} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_f + \mathbf{s}^{(t-1)} \mathbf{W}_f) \\ \mathbf{o} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_o + \mathbf{s}^{(t-1)} \mathbf{W}_o) \\ \mathbf{g} = \tanh(\mathbf{x}^{(t)} \mathbf{U}_g + \mathbf{s}^{(t-1)} \mathbf{W}_g) \\ \mathbf{c}_t = \mathbf{c}_{t-1} \odot \mathbf{f} + \mathbf{g} \odot \mathbf{i} \\ \mathbf{s}_t = \tanh(\mathbf{c}_t) \odot \mathbf{o} \end{cases}$$

$$(2)$$

Here \odot denotes element-wise multiplication. If this sounds complicated, in the following slides we'll parse each of these equations to make a sense out of it.

Long Short-Term Memory networks



$$\begin{cases}
\mathbf{i} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_i + \mathbf{s}^{(t-1)} \mathbf{W}_i) \\
\mathbf{f} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_f + \mathbf{s}^{(t-1)} \mathbf{W}_f) \\
\mathbf{o} = \sigma(\mathbf{x}^{(t)} \mathbf{U}_o + \mathbf{s}^{(t-1)} \mathbf{W}_o)
\end{cases} \tag{3}$$

These are the input, forget and output **gates** respectively. Each gate has the same dimension of the hidden state. Gates are multiplied element-wise with other functions of LSTM thus acting as **continuous**, **differentiable switches** thanks to the sigmoid activation function.

Input and output gates controls how much of the input let through and how much of the internal state exposing to the external, respectively. Conversely, forget gate controls how much memory form previous time step must be overwritten.

Credits

Credits



These slides heavily borrow from the following Stanford course:

• http://cs231n.stanford.edu/

if you want to deepen your knowledge of these concepts, I'd really suggest you to start from here!

Also, nice convolution animations are taken from here:

• https://github.com/vdumoulin/conv_arithmetic

References i



[1] K. Cho, B. Van Merriënboer, C. Gulcehre, D. Bahdanau, F. Bougares, H. Schwenk, and Y. Bengio.

Learning phrase representations using rnn encoder-decoder for statistical machine translation.

arXiv preprint arXiv:1406.1078, 2014.

[2] S. Hochreiter and J. Schmidhuber.

Long short-term memory.

Neural computation, 9(8):1735-1780, 1997.

References ii



[3] R. Pascanu, T. Mikolov, and Y. Bengio.

On the difficulty of training recurrent neural networks.

In International Conference on Machine Learning, pages 1310–1318, 2013.