Assignment 2. Recurrent Neural Networks

University of Amsterdam – Deep Learning Course

November 13, 2017

The deadline for this assignment is November $28^{\rm th}$ at 23:59.

In this assignment you will study and implement recurrent neural networks (RNNs). This type of neural network is best suited for sequential processing of data, such a sequence of characters, words or video frames. Its applications are mostly in neural machine translation, speech analysis and video understanding. These networks are very powerful and have found their way into many production environments. For example **Google's neural machine translation system** relies on Long-Short Term Networks (LSTMs).

The assignment consists of two parts. First, you will get familiar with vanilla RNNs and LSTMs on a simple toy problem. This will help you understand the fundamentals of recurrent networks. In the second part, you will use LSTMs for learning and generating text. We expect each student to hand in their code and individually write a report that gives the answers to each question.

1 Vanilla RNN versus LSTM

For the first task, you will compare vanilla Recurrent Neural Networks (RNN) with Long-Short Term Networks (LSTM). TensorFlow has a large amount of building blocks for recurrent neural networks. However, to get you familiar with the concept of recurrent connections, in this first part of this assignment you will implement a vanilla RNN and LSTM from scratch. The use of tf.contrib.rnn and tf.nn.dynamic_rnn is not allowed until the second part of this assignment.

(Total: 55 points)

1.1 Toy Problem: Palindrome Numbers

In this first assignment, we will focus on very simple sequential training data for understanding the memorization capability of recurrent neural networks. More specifically, we will study *palindrome* numbers. Palindromes are numbers which read the same backward as forward, such as:

 $\begin{array}{r}
 303 \\
 4224 \\
 175282571 \\
 682846747648286
\end{array}$

We can use a recurrent neural network to predict the next digit of the palindrome at every timestep. While very simple for short palindromes, this task becomes increasingly difficult for longer palindromes. For example when the network is given the input 68284674764828_ and the task is to predict the digit on the _ position, the network has to remember

information from 14 timesteps earlier. If the task is to predict the last digit only, the intermediate digits are irrelevant. However, they may affect the evolution of the dynamic system and possibly erase the internally stored information about the initial values of input. In short, this simple problem enables studying the memorization capability of recurrent networks.

For the coding assignment, please use the palindrome generator defined in utils.py.

1.2 Vanilla RNN in TensorFlow

The vanilla RNN is formalized as follows. Given a sequence of input vectors $\mathbf{x}^{(t)}$ for t = 1, ..., T, the network computes a sequence of hidden states $\mathbf{h}^{(t)}$ and a sequence of output vectors $\mathbf{p}^{(t)}$ using the following equations for timesteps t = 1, ..., T:

$$\mathbf{h}^{(t)} = \tanh(\mathbf{W}_{hx}\mathbf{x}^{(t)} + \mathbf{W}_{hh}\mathbf{h}^{(t-1)} + \mathbf{b}^{h})$$
 (1)

$$\mathbf{p}^{(t)} = \mathbf{W}_{oh} \mathbf{h}^{(t)} + \mathbf{b}_o \tag{2}$$

As you can see, there are several trainable weight matrices and bias vectors. \mathbf{W}_{hx} denotes the input-to-hidden weight matrix, \mathbf{W}_{hh} is the hidden-to-hidden (or recurrent) weight matrix, \mathbf{W}_{oh} represents the hidden-to-output weight matrix and the \mathbf{b}_h and \mathbf{b}_o vectors denote the biases. For the first timestep t=1, the expression $\mathbf{h}^{(t-1)}=\mathbf{h}^{(0)}$ is replaced with a special vector \mathbf{h}_{init} that is commonly initialized to a vector of zeros. The output value $\mathbf{p}^{(t)}$ depends on the state of the hidden layer $\mathbf{h}^{(t)}$ which in its turn depends on all previous state of the hidden layer. Therefore, a recurrent neural network can be seen as a (deep) feedforward network with shared weights.

To optimize the trainable weights, the gradients of the RNN are computed via back-propagation through time (BPTT). The goal is to calculate the gradients of the loss \mathcal{L} with respect to the model parameters \mathbf{W}_{hx} , \mathbf{W}_{hh} and \mathbf{W}_{oh} (biases omitted). Similar to training a feed-forward network, the weights and baises are updated using SGD or one of its variants. Different from feed-forward networks, recurrent networks can give output logits $\hat{\mathbf{y}}^{(t)}$ at every timestep. In this assignment the outputs will be given by the softmax function, i.e. $\hat{\mathbf{y}}^{(t)} = \operatorname{softmax}(\mathbf{p}^{(t)})$. For the task of predicting the final palindrome number, we compute the standard cross-entropy loss only over the last timestep:

$$\mathcal{L} = -\sum_{k=1}^{K} \mathbf{y}_k \log \hat{\mathbf{y}}_k \tag{3}$$

Where k runs over the number of classes (K = 10 because we have ten digits). In this expression, \mathbf{y} denotes a one-hot vector of length K containing true labels.

Question 1.1 (10 points)

Recurrent neural networks can be trained using backpropagation through time. Similar to feed-forward networks, the goal is to compute the gradients of the loss w.r.t. \mathbf{W}_{oh} , \mathbf{W}_{hh} and \mathbf{W}_{hx} . Write down an expression for the gradient $\frac{\partial \mathcal{L}^{(T)}}{\partial \mathbf{W}_{oh}}$ in terms of the variables in Equations 1 and 2. Do the same for $\frac{\partial \mathcal{L}^{(T)}}{\partial \mathbf{W}_{hh}}$. What difference do you observe in temporal dependence of the two gradients. Study the latter gradient and explain what problems might occur when training this recurrent network for a large number of timesteps.

Question 1.2 (10 points)

Implement the vanilla recurrent neural network as specified by the equations above in the file vanilla_rnn.py. For the *forward* pass you will need to use the tf.scan operation and plain matrix multiplications. You do not need to implement the *backward* pass yourself, but instead you can rely on automatic differentiation and use the RMSProp optimizer for tuning the weights. For the optimization part we have prepared the code in train.py.

Question 1.3 (5 points)

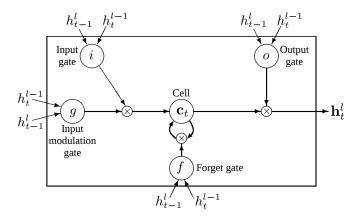
As the recurrent network is implemented, you are ready to experiment with the memorization capability of the vanilla RNN. Given a palindrome of length T, use the first T-1 digits as input and make the network predict the last digit. The network is successful if it correctly predicts the last digit and thus was capable of memorizing a small amount of information for T timesteps.

Start with short palindromes (T=5), train the network until convergence and record the accuracy. Repeat this by gradually increasing the sequence length and create a plot that shows the accuracy versus palindrome length. As a sanity check, make sure that you obtain an accuracy of at least 90% for T=5 with the default parameters provided in train.py.

Question 1.4 (5 points)

To improve optimization of neural networks, many variants of stochastic gradient descent have been proposed. Two popular optimizers are RMSProp and Adam and/or the use of momentum. In practice, these methods are able to converge faster and obtain better local minima. In your own words, write down the benefits of such methods in comparison to vanilla stochastic gradient descent. Your answer needs to touch upon the concepts of momentum and adaptive learning rate.

Figure 1. A graphical representation of LSTM memory cells (Zaremba et al. (ICLR, 2015))



1.3 Long-Short Term Network (LSTM) in TensorFlow

As you have observed after implementing the previous questions, training a vanilla RNN for remembering its inputs for an increasing number of timesteps is difficult. The problem is that the influence of a given input on the hidden layer (and therefore on the output layer), either decays or blows up exponentially as it unrolls the network. In practice, the vanishing gradient problem is the main shortcoming of vanilla RNNs. As a result, training a vanilla RNNs to learn tasks containing delays of more than 10 timesteps between relevant input and target is difficult. To overcome this problem, many different RNN architectures have been suggested. The most widely used variant is the Long-Short Term Network (LSTMs). An LSTM (Figure 1) introduces a number of gating mechanisms to improve gradient flow for better training. Before continuing, please read the following blogpost: Understanding LSTM Networks.

In this assignment we will use the following LSTM definition:

$$\mathbf{g}^{(t)} = \tanh(\mathbf{W}_{gx}\mathbf{x}^{(t)} + \mathbf{W}_{gh}\mathbf{h}^{(t-1)} + \mathbf{b}_{g})$$
(4)

$$\mathbf{i}^{(t)} = \sigma(\mathbf{W}_{ix}\mathbf{x}^{(t)} + \mathbf{W}_{ih}\mathbf{h}^{(t-1)} + \mathbf{b}_i)$$
 (5)

$$\mathbf{f}^{(t)} = \sigma(\mathbf{W}_{fx}\mathbf{x}^{(t)} + \mathbf{W}_{fh}\mathbf{h}^{(t-1)} + \mathbf{b}_f)$$
(6)

$$\mathbf{o}^{(t)} = \sigma(\mathbf{W}_{ox}\mathbf{x}^{(t)} + \mathbf{W}_{oh}\mathbf{h}^{(t-1)} + \mathbf{b}_o)$$
 (7)

$$\mathbf{c}^{(t)} = \mathbf{g}^{(t)} \odot \mathbf{i}^{(t)} + \mathbf{c}^{(t-1)} \odot \mathbf{f}^{(t)}$$
(8)

$$\mathbf{h}^{(t)} = \tanh(\mathbf{c}^{(t)}) \odot \mathbf{o}^{(t)} \tag{9}$$

$$\mathbf{p}^{(t)} = \mathbf{W}_{out}\mathbf{h}^{(t)} + \mathbf{b}_{out} \tag{10}$$

$$\hat{\mathbf{y}}^{(t)} = \operatorname{softmax}(\mathbf{p}^{(t)}). \tag{11}$$

In these equations \odot is element-wise multiplication and $\sigma(\cdot)$ is the sigmoid function. The first six equations are the LSTM's core part whereas the last two equations are just the linear output mapping. Note that the LSTM has more weight matrices than the vanilla RNN. As the forward pass of the LSTM is relatively intricate, writing down the correct gradients for the LSTM would involve a lot of derivatives. Fortunately, LSTMs can easily be implemented in TensorFlow and automatic differentiation takes care of the derivatives.

Question 1.5 (10 points)

- (a) The LSTM extends the vanilla RNN cell by adding four gating mechanisms. Those gating mechanisms are crucial for successfully training recurrent neural networks. The LSTM has an *input modulation gate* $\mathbf{g}^{(t)}$, *input gate* $\mathbf{i}^{(t)}$, *forget gate* $\mathbf{f}^{(t)}$ and *output gate* $\mathbf{o}^{(t)}$. For each of these gates, write down a short paragraph on their purpose, explicitly discuss the non-linearity they use and motivate why this is a good choice.
- (b) Given the LSTM cell as defined by the equations above and an input sample $\mathbf{x} \in \mathbb{R}^{T \times d}$ where T denotes the sequence length and d is the feature dimensionality. Let n denote the number of units in the LSTM and m represents the batch size. Write down the formula for the *total number* of trainable parameters in the LSTM as defined above.

Question 1.6 (15 points)

Implement the LSTM network as specified by the equations above in the file 1stm.py. For the forward pass you are required to use the tf.scan operation and plain matrix multiplications. You do not need to implement the backward pass yourself, but instead you can rely on automatic differentiation and use the RMSProp optimizer for tuning the weights. For the optimization part we have prepared the code in train.py.

Using the palindromes as input, perform the same experiment you have done in Question 1.3. Train the network until convergence. You might need to adjust the learning rate when increasing the sequence length. The initial parameters in the prepared code provide a starting point. Again, create a plot of your results by gradually increasing the sequence length. Write down a comparison with the vanilla RNN and think of reasons for the different behavior. As a sanity check, your LSTM should obtain near-perfect accuracy for T = 5.

$\mathbf{2}$ Recurrent Nets as Generative Model (Total: 45 points)

In this assignment you will build an LSTM for generation of text. By training an LSTM to predict the next character in a sentence, the network will learn local structure in text. You will train a two-layer LSTM on sentences from a book and use the model to generate new next. Before starting, we recommend reading the blog post The Unreasonable Effectiveness of Recurrent Neural Networks.

Given a training sequence $\mathbf{x} = (x^1, \dots, x^T)$, a recurrent neural network can use its output vectors $\mathbf{p} = (p^1, \dots, p^T)$ to obtain a sequence of predictions $\hat{\mathbf{y}}^{(t)}$. In the first part of this assignment you have used the recurrent network as sequence-to-one mapping, here we use the recurrent network as sequence-to-sequence mapping. The total cross-entropy loss can be computed by averaging over all timesteps using the target labels $\mathbf{y}^{(t)}$.

$$\mathcal{L}^{(t)} = -\sum_{k=1}^{K} \mathbf{y}_k^{(t)} \log \hat{\mathbf{y}}_k^{(t)}$$

$$\mathcal{L} = \frac{1}{T} \sum_{t} \mathcal{L}^{(t)}$$
(12)

$$\mathcal{L} = \frac{1}{T} \sum_{t} \mathcal{L}^{(t)} \tag{13}$$

Again, k runs over the number of classes (vocabulary size). In this expression, \mathbf{v} denotes a one-hot vector of length K containing true labels. Using this sequential loss, you can train a recurrent network to make a prediction at every timestep. The LSTM can be used to generate text, character by character that will look similar to the original text. Just like multi-layer perceptrons, LSTM cells can be stacked to create deeper layers for increased expressiveness. Each recurrent layer can be unrolled in time.

For training you can use a large text corpus such as publicly available books. We provide a number of books in the assets directory. However, you are also free to download other books, we recommend Project Gutenberg as good source. Make sure you download the books in plain text (.txt) for easy file reading in Python. We provide the TextDataset class for loading the text corpus and drawing batches of example sentences from the text.

The files train_text.py and model.py provide a starting point for your implementation. The sequence length specifies the length of training sentences which also limits the number of timesteps for backpropagation in time. When setting the sequence length to 30 steps, the gradient signal will never backpropagate more than 30 timesteps. As a result, the network cannot learn text dependencies longer than this number of characters.

Question 2.1 (45 points)

Implement a two-layer LSTM network to predict the next character in a sentence by training on sentences from a book. Train the model on sentences of length T=30 from your book of choice. Define the total loss as average of cross-entropy loss over all timesteps (Equation 13).

Make the network generate new sentences of length T=30 now and then by randomly setting the first character of the sentence. Report 5 text samples generated by the network over evenly spaced intervals during training. Carefully study the text generated by your network. What changes do you observe when the training process evolves?

We recommend reading **TensorFlow's documentation on RNNs** before you start. Study the code and its outputs for dataset.py to sample sentences from the book to train with. Also, have a look at the parameters defined in train.py and implement the corresponding TensorFlow code to make the features work. We obtained good results with the default parameters as specified, but you may need to tune them depending on your own implementation.

Since the network may need training for some hours until convergence, it is advised to run training on the SurfSara cluster. Also, you might want to save the trained weights now and then so you can resume training later or generate new text using the model.

Bonus Question 2.3 (10 points)

Given the trained network, make your model generate sentences longer than T=30 characters. In order to do so, you need to save the LSTM's hidden state and memory state after unrolling the network for 30 timesteps and then passing it as input for the next 30 characters. In particular, it could be fun to make your network finish some sentences that make relate to the book that your are training on. For example, if you are training on Grimm's Fairytales, you could make the network finish the sentence "Sleeping beauty is ...". Be creative and test the capabilities of your model.

Report

We expect each student to write a small report about recurrent neural networks with explicitly answering the questions in this assignment. Please clearly mark each answer by a heading indicating the question number. Again, use the NIPS LATEX template as was provided here: https://goo.gl/P9TxPA.

Deliverables

Create ZIP archive containing your report and all Python code. Please preserve the directory structure as provided in the Github repository for this assignment. Give the ZIP file the following name: lastname_assignment2.zip where you insert your lastname. Please submit your deliverable through Blackboard. We cannot guarantee a grade for the assignment if the deliverables are not handed in according to these instructions.

The deadline for this assignment is November 28th at 23:59.