1 TensorFlow and Backpropagation

A TensorFlow computation is described by a directed graph. Fig. 1 shows a typical TensorFlow computation graph. In the graph, each node has zero or more inputs and outputs. For example, the $\text{MatMul}$ node in the left bottom has inputs $W$ and $x$ and it outputs $Wx$. Tensors (arbitrary dimensionality arrays such as vectors or matrices) flow along the edge of graph, e.g. the output of $\text{MatMul}$ is fed into $\text{Add}$.

![TensorFlow graph](image)

Figure 1: TensorFlow graph

The left part of the figure represents the computation graph of forward propagation. The
computation it represents is:

\[ h = \text{ReLU}(Wx + b_1) \]  
\[ \hat{y} = \text{softmax}(Uh + b_2) \]  
\[ J = \text{CE}(y, \hat{y}) = -\sum_i y_i \log \hat{y}_i \]  

Here ReLU (rectified linear unit) performs element-wise rectified linear function:

\[ \text{ReLU}(z) = \max(z, 0) \]

The dimensions of the matrices are:

\[ W \in \mathbb{R}^{m \times n} \quad x \in \mathbb{R}^n \quad b_1 \in \mathbb{R}^m \quad U \in \mathbb{R}^{k \times m} \quad b_2 \in \mathbb{R}^k \]

1) (8 points) Use backpropagation to calculate these four gradients

\[ \frac{\partial J}{\partial b_2} \quad \frac{\partial J}{\partial U} \quad \frac{\partial J}{\partial b_1} \quad \frac{\partial J}{\partial W} \]

*Hint: You can use the following notation:*

\[ 1\{x > 0\} = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x \leq 0. \end{cases} \]

*Using it on a matrix would perform an element-wise operation, e.g.*

\[ 1\begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} > 0 \} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \]
2) The right part of the figure represents the computation graph of backpropagation. Each gradient operation node in this part (e.g. dMatMul) takes as input not only the partial gradients computed already along the backpropagation path, but also, optionally, the inputs and outputs of the corresponding operation node in the forward propagation to calculate gradients. Here, the MatMul node in the bottom left corresponds to dMatMul node in the bottom right, and the ReLU node corresponds to the dReLU node. Briefly explain why the corresponding inputs and/or outputs of the forward operation node are sometimes needed when backpropagating to calculate gradient. Give an example for each case.

(1 point) Explanation:

(i) (2 points) Case 1: The input of the corresponding operation node is needed

(ii) (2 points) Case 2: The output of the corresponding operation node is needed

3) (2 points) The CE node (softmax cross-entropy) in the graph expects unscaled inputs (they are not yet exponentiated), since it performs a softmax internally for efficiency. Give a reason why this is more efficient than a separate softmax and cross-entropy layer.
2 Word2Vec

1) Recall the loss function for GloVe:

\[
J(\theta) = \frac{1}{2} \sum_{i=1}^{W} \sum_{j=1}^{W} f(P_{ij})(u_i^T v_j - \log P_{ij})^2
\]

where \( P_{ij} \) (a scalar) is the probability that word \( j \) appears in the context of word \( i \),
\( f : \mathbb{R} \to \mathbb{R} \) is a function that gives a weight to each \( (i, j) \) pair based on its probability \( P_{ij} \),
\( u_i \) is a column vector of shape \( (d \times 1) \) representing the output vector for word \( i \), and
\( v_j \) is a column vector of shape \( (d \times 1) \) representing the input vector for word \( j \).

(i) (2 points) Calculate the gradient of the loss function with respect to input and output vectors:
\[
\frac{\partial J(\theta)}{\partial u_i} \quad \text{and} \quad \frac{\partial J(\theta)}{\partial v_j}.
\]

(ii) (2 points) Show what the function \( f(x) \) looks like by drawing it.
(iii) (2 points) Explain in one or two sentences why should $f(x)$ have the form that you have drawn.

(iv) (2 points) Give one advantage of GloVe over Skipgram/CBOW models.

2) (2 points) What are two ways practitioners deal with having two different sets of word vectors $U$ and $V$ at the end of training both Glove and word2vec?
3 DeepNLP in Practice

You are consulting for a healthcare company. They provide you with clinical notes of the first encounter that each patient had with their doctor regarding a particular medical episode. There are a total of 12 million patients and clinical notes. Figure 2 shows a sample clinical note. At the time that each clinical note was written, the underlying illnesses associated with the medical episode were unknown to the doctor. The company provides you with the true set of illnesses associated with each medical episode and asks you to build a model that can infer these underlying illnesses using only the current clinical note and all previous clinical notes belonging to the patient. The set of notes provided to you span 10 years; each patient therefore can have multiple clinical notes (medical episodes) in that period.

![Sample clinical note](source USMLE)

Each note can contain any number of tokens (see Figure 2). Some tokens (e.g. ”Meds”) occur more frequently than others in the collection of notes provided to you.

You call your former CS224D TA for advice. He tells you to first create a distributed representation of each patient note by combining the distributed representations of the words contained in the note.

1) (2 points) Given the sample note provided in Figure 2, how would you map the various tokens into a distributed vector representation?
2) (2 points) You have the option of representing each note as the summation of its constituent word vectors or as the average of its word vectors. Both seem reasonable. What’s your best course of action? Briefly justify your selection.

3) (2 points) Your former TA tells you that you must normalize (magnitude-wise) your word-vectors before you perform the operation you decided to do in 2). Assuming you might try a standard neural network model, for which nonlinearities might that matter more?

4) (2 points) You now have a distributed representation of each patient note (note-vector). You assume that a patient’s past medical history is informative of their current illness. As such, you apply a recurrent neural network to predict the current illness based on the patient’s current and previous note-vectors. Explain why a recurrent neural network would yield better results than a feed-forward network in which your input is the summation (or average) of past and current note-vectors?
5) (2 points) A patient may have any number of illnesses from a list of 70,000 known medical illnesses. The output of your recurrent neural network will therefore be a vector with 70,000 elements. Each element in this output vector represents the probability that the patient has the illness that maps to that particular element. Your former TA tells you that illnesses are not mutually exclusive i.e. having one illness does not preclude you from having any other illnesses. Given this insight, is it better to have a sigmoid non-linearity or a softmax non-linearity as your output unit? Why?

6) (4 points) You try to figure out a better way to reduce the training and testing time of your model. You perform a run time analysis and observe that the computational bottleneck is in your output unit: the number of target illnesses is too high. Your former TA tells you that each illness in the list of 70,000 illnesses belongs to one of 300 classes (e.g. a migraine belongs to the neurological disorder class). He shares with you a dictionary which maps each illness to its corresponding class. How can you use this information to reduce the time complexity of your model? Include your forward propagation equations in your answer.
7) (2 points) Your model now trains (and predicts) several times faster. You achieve a precision score of 72% on positive cases (true positives) and a precision score of 68% on negative cases (true negatives). Confident with your initial results, you decide to make a more complex model. You implement a bidirectional deep recurrent neural network over the chronologically ordered patient note-vectors. Your new results are stellar. Your positive precision is 95% and your negative precision is 92%. You boast to your TA that you have built an AI doctor. You coin the name Dr. AI for your model. Unfortunately, your TA tells you that you have made a mistake. What is the mistake?

8) (2 points) Which level(s) of the linguistic hierarchy were you tackling here?
4  **LSTMs, GRUs, and Recursive Networks**

1) Problematic Gradients

(a) (3 points) ______ suffer(s) from the vanishing gradient problem. Circle all that apply and JUSTIFY YOUR ANSWER.

   (i) 1-Layer Feed-forward NN (i.e., the NN from problem set 1)
   (ii) Very Deep Feed-forward NN
   (iii) Recurrent NN
   (iv) Word2vec CBOW
   (v) Word2vec Skip-Gram

Circle True/False for the following and briefly JUSTIFY YOUR ANSWER:

(b) (2 points) (True/False) Adding more hidden layers will solve the vanishing gradient problem for a 2 layer neural network.

(c) (2 points) (True/False) Adding $L_2$-regularization will help with vanishing gradients.

(d) (2 points) (True/False) Clipping the gradient (cutting off at a threshold) will solve the exploding gradients problem.
2) Here are the defining equations for a LSTM cell.

\[
\begin{align*}
    i_t &= \sigma \left( W^{(i)} x_t + U^{(i)} h_{t-1} \right) \\
    f_t &= \sigma \left( W^{(f)} x_t + U^{(f)} h_{t-1} \right) \\
    o_t &= \sigma \left( W^{(o)} x_t + U^{(o)} h_{t-1} \right) \\
    \tilde{c}_t &= \tanh \left( W^{(c)} x_t + U^{(c)} h_{t-1} \right) \\
    c_t &= f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \\
    h_t &= o_t \odot \tanh (c_t)
\end{align*}
\]

Recall that \( \odot \) denotes element-wise multiplication and that \( \sigma \) denotes the sigmoid function.

Circle True/False for the following and briefly JUSTIFY YOUR ANSWER:

(a) (2 points) (True/False) If \( x_t \) is the 0 vector, then \( h_t = h_{t-1} \).

(b) (2 points) (True/False) If \( f_t \) is very small or zero, then error will not be back-propagated to earlier time steps.

(c) (2 points) (True/False) The entries of \( f_t, i_t, o_t \) are non-negative.

(d) (2 points) (True/False) \( f_t, i_t, o_t \) can be viewed as probability distributions. (i.e., their entries are non-negative and their entries sum to 1.)
3) (3 points) Here are the defining equations for a GRU cell.

\[
\begin{align*}
    z_t &= \sigma \left( W^{(z)} x_t + U^{(z)} h_{t-1} \right) \\
    r_t &= \sigma \left( W^{(r)} x_t + U^{(r)} h_{t-1} \right) \\
    \tilde{h}_t &= \tanh \left( W x_t + r_t \circ U h_{t-1} \right) \\
    h_t &= z_t \circ h_{t-1} + (1 - z_t) \circ \tilde{h}_t
\end{align*}
\]

Recall that $\circ$ denotes element-wise multiplication and that $\sigma$ denotes the sigmoid function. $h_t$ and $x_t$ are column vectors. Assume that the $h_t$ are of dimension $d_h$ and that the $x_t$ are of dimensions $d_x$. What are the dimensions of $W^{(z)}$, $U^{(z)}$, $W^{(r)}$, $U^{(r)}$, $W$, and $U$? Define clearly which numbers are rows and columns.
4) (3 points) Fig. 3 illustrates a deep recurrent network. Assume that each circle in this model denotes a GRU-cell (as in the previous question). Assume that GRU parameters are shared for each layer in the deep RNN.

![Deep RNN Diagram](image)

Figure 3: Deep RNN

Let $W^{(z)}_i, U^{(z)}_i, W^{(r)}_i, U^{(r)}_i, W_i, U_i$ denote the parameters for the $i$-th hidden layer (the $h^i_t$ nodes above). Assume that $x_t$ is of dimension $d_x$ and that the $h^i_t$ are of dimension $d_h$. What are the dimensions for $W^{(z)}_2, U^{(z)}_2, W^{(r)}_2, U^{(r)}_2, W_2$, and $U_2$ (note that these should **not all** be the same as those for the previous answer). Hint: the output of a lower level’s cell becomes the input to the next higher layer.
5  Hyper-Parameter Tuning

1) (2 points) In our objective functions, we usually regularize the weight parameters of the softmax but not its biases. Explain why.

2) (3 points) In 2-3 short sentences, describe why we initialize the weights in our model to be i) small and ii) random numbers. Hint: Think of the softmax and tanh nonlinearities.
3) Your training error and cost are high and your validation cost and error are almost equal to it. Answer the following questions:

(i) (2 points) What does this mean for your model?

(ii) (1 point) What actions would you take?

4) (3 points) Explain why we use $\frac{f(x+h)-f(x-h)}{2h}$ and not $\frac{f(x+h)-f(x)}{h}$ to estimate the numerical gradient of $f$. Remember that for a smooth function, $f : \mathbb{R} \rightarrow \mathbb{R}$, its Taylor series expanded around $a$ is $\sum_{n=0}^{\infty} \frac{f^{(n)}(a)(x-a)^n}{n!}$
Use this page for scratch work.