CS 224n: Assignment #2

Due date: 2/8 11:59 PM PST (You are allowed to use 3 late days maximum for this assignment)

These questions require thought, but do not require long answers. Please be as concise as possible.

? We encourage students to discuss in groups for assignments. However, each student must finish the problem set and programming assignment individually, and must turn in her/his assignment. We ask that you abide the university Honor Code and that of the Computer Science department, and make sure that all of your submitted work are done by yourself.

Please review any additional instructions posted on the assignment page at http://cs224n.stanford.edu/assignments.html. When you are ready to submit, please follow the instructions on Piazza.

1 Tensorflow Softmax (25 points)

In this question, we will implement a linear classifier with loss function

$$J(\mathbf{W}) = CE(\mathbf{y}, \operatorname{softmax}(\mathbf{x}\mathbf{W} + \mathbf{b}))$$

Where x is a vector of features, W is the model's weight matrix, and b is a bias term. We will use Tensor-Flow's automatic differentiation capability to fit this model to provided data.

(a) (5 points, coding) Implement the softmax function using TensorFlow in q1_softmax.py. Remember that

$$\operatorname{softmax}(\boldsymbol{x})_i = \frac{e^{\boldsymbol{x}_i}}{\sum_i e^{x_i}}$$

Note that you may **not** use tf.nn.softmax or related built-in functions. You can run basic (nonexhaustive tests) by running python ql_softmax.py.

(b) (5 points, coding) Implement the cross-entropy loss using TensorFlow in q1_softmax.py. Remember that

$$CE(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{i=1}^{N_c} y_i \log(\hat{y}_i)$$

where $y \in \mathbb{R}^{N_c}$ is a one-hot label vector and N_c is the number of classes. This loss is summed over all examples in a minibatch. Note that you may **not** use TensorFlow's built-in cross-entropy functions for this question. You can run basic (non-exhaustive tests) by running python ql_softmax.py.

(c) (5 points, coding/written) Carefully study the Model class in model.py. Briefly explain the purpose of placeholder variables and feed dictionaries in TensorFlow computations. Fill in the implementations for add_placeholders and create_feed_dict in q1_classifier.py.

Hint: Note that configuration variables are stored in the Config class. You will need to use these configuration variables in the code.

- (d) (5 points, coding) Implement the transformation for a softmax classifier in the function add_prediction_op in q1_classifier.py. Add cross-entropy loss in the function add_loss_op in the same file. Use the implementations from the earlier parts of the problem (already imported for you), not TensorFlow built-ins.
- (e) (5 points, coding/written) Fill in the implementation for add_training_op in q1_classifier.py. Explain in a few sentences what happens when the model's train_op is called (what gets computed during forward propagation, what gets computed during backpropagation, and what will have changed after the op has been run?). Verify that your model is able to fit to synthetic data by running python q1_classifier.py and making sure that the tests pass.

Hint: Make sure to use the learning rate specified in Config.

2 Neural Transition-Based Dependency Parsing (50 points)

In this section, you'll be implementing a neural-network based dependency parser. A dependency parser analyzes the grammatical structure of a sentence, establishing relationships between "head" words and words which modify those heads. Your implementation will be a *transition-based* parser, which incrementally builds up a parse one step at a time. At every step it maintains a partial parse, which is represented as follows:

- A stack of words that are currently being processed.
- A buffer of words yet to be processed.
- A list of *dependencies* predicted by the parser.

Initially, the stack only contains ROOT, the dependencies lists is empty, and the buffer contains all words of the sentence in order. At each step, the parse applies a *transition* to the partial parse until its buffer is empty and the stack is size 1. The following transitions can be applied:

- SHIFT: removes the first word from the buffer and pushes it onto the stack.
- LEFT-ARC: marks the second (second most recently added) item on the stack as a dependent of the first item and removes the second item from the stack.
- RIGHT-ARC: marks the first (most recently added) item on the stack as a dependent of the second item and removes the first item from the stack.

Your parser will decide among transitions at each state using a neural network classifier. First, you will implement the partial parse representation and transition functions.

(a) (6 points, written) Go through the sequence of transitions needed for parsing the sentence "I parsed this sentence correctly". The dependency tree for the sentence is shown below. At each step, give the configuration of the stack and buffer, as well as what transition was applied this step and what new dependency was added (if any). The first three steps are provided below as an example.



stack	buffer	new dependency	transition
[ROOT]	[I, parsed, this, sentence, correctly]		Initial Configuration
[ROOT, I]	[parsed, this, sentence, correctly]		SHIFT
[ROOT, I, parsed]	[this, sentence, correctly]		SHIFT
$[{\rm ROOT,\ parsed}]$	[this, sentence, correctly]	$\operatorname{parsed} \to I$	LEFT-ARC

- (b) (2 points, written) A sentence containing n words will be parsed in how many steps (in terms of n)? Briefly explain why.
- (c) (6 points, coding) Implement the __init__ and parse_step functions in the PartialParse class in q2_parser_transitions.py. This implements the transition mechanics your parser will use. You can run basic (not-exhaustive) tests by running python q2_parser_transitions.py.
- (d) (6 points, coding) Our network will predict which transition should be applied next to a partial parse. We could use it to parse a single sentence by applying predicted transitions until the parse is complete. However, neural networks run much more efficiently when making predictions about batches of data at a time (i.e., predicting the next transition for a many different partial parses simultaneously). We can parse sentences in minibatches with the following algorithm.

Algorithm 1 Minibatch Dependency Parsing

Input: sentences, a list of sentences to be parsed and model, our model that makes parse decisions

Initialize partial_parses as a list of partial parses, one for each sentence in sentences Initialize unfinished_parses as a shallow copy of partial_parses while unfinished_parses is not empty do

Take the first batch_size parses in unfinished_parses as a minibatch

Use the model to predict the next transition for each partial parse in the minibatch

Perform a parse step on each partial parse in the minibatch with its predicted transition

Remove the completed (empty buffer and stack of size 1) parses from unfinished_parses end while

Return: The dependencies for each (now completed) parse in partial_parses.

Implement this algorithm in the minibatch_parse function in q2_parser_transitions.py. You can run basic (not-exhaustive) tests by running python q2_parser_transitions.py.

Note: You will need minibatch_parse to be correctly implemented to evaluate the model you will build in part (h). However, you do not need it to train the model, so you should be able to complete most of part (h) even if minibatch_parse is not implemented yet.

We are now going to train a neural network to predict, given the state of the stack, buffer, and dependencies, which transition should be applied next. First, the model extracts a feature vector representing the current state. We will be using the feature set presented in the original neural dependency parsing paper: A Fast and Accurate Dependency Parser using Neural Networks¹. The function extracting these features has been implemented for you in parser_utils. This feature vector consists of a list of tokens (e.g., the last word in the stack, first word in the buffer, dependent of the second-to-last word in the stack if there is one, etc.). They can be represented as a list of integers

$$[w_1, w_2, ..., w_m]$$

where m is the number of features and each $0 \le w_i < |V|$ is the index of a token in the vocabulary (|V| is the vocabulary size). First our network looks up an embedding for each word and concatenates them into a single input vector:

$$oldsymbol{x} = [oldsymbol{E}_{w_1}, ..., oldsymbol{E}_{w_m}] \in \mathbb{R}^{dm}$$

¹Chen and Manning, 2014, http://cs.stanford.edu/people/danqi/papers/emnlp2014.pdf

where $E \in \mathbb{R}^{|V| \times d}$ is an embedding matrix with each row E_i as the vector for a particular word i. We then compute our prediction as:

$$egin{aligned} & m{h} = \mathrm{ReLU}(m{x}m{W} + m{b}_1) \ & \hat{m{y}} = \mathrm{softmax}(m{h}m{U} + m{b}_2) \end{aligned}$$

(recall that ReLU(z) = max(z, 0)). We will train the model to minimize cross-entropy loss:

$$J(\theta) = CE(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{i=1}^{N_c} y_i \log \hat{y}_i$$

To compute the loss for the training set, we average this $J(\theta)$ across all training examples.

(e) (4 points, coding) In order to avoid neurons becoming too correlated and ending up in poor local minimina, it is often helpful to randomly initialize parameters. One of the most frequent initializations used is called Xavier initialization².

Given a matrix A of dimension $m \times n$, Xavier initialization selects values A_{ij} uniformly from $[-\epsilon, \epsilon]$, where

$$\epsilon = \frac{\sqrt{6}}{\sqrt{m+n}}$$

Implement the initialization in xavier_weight_init in q2_initialization.py. You can run basic (nonexhaustive tests) by running python q2_initialization.py. This function will be used to initialize W and U.

(f) (2 points, written) We will regularize our network by applying Dropout³. During training this randomly sets units in the hidden layer h to zero with probability p_{drop} and then multiplies h by a constant γ (dropping different units each minibatch). We can write this as

$$h_{drop} = \gamma d \circ h$$

where $\mathbf{d} \in \{0,1\}^{D_h}$ (D_h is the size of \mathbf{h}) is a mask vector where each entry is 0 with probability p_{drop} and 1 with probability $(1 - p_{drop})$. γ is chosen such that the value of \mathbf{h}_{drop} in expectation equals \mathbf{h} :

$$\mathbb{E}_{p_{drop}}[\boldsymbol{h}_{drop}]_i = h_i$$

for all $0 < i < D_h$. What must γ equal in terms of p_{drop} ? Briefly justify your answer.

(g) (4 points, written) We will train our model using the Adam⁴ optimizer. Recall that standard SGD uses the update rule

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} J_{minibatch}(\boldsymbol{\theta})$$

where θ is a vector containing all of the model parameters, J is the loss function, $\nabla_{\theta} J_{minibatch}(\theta)$ is the gradient of the loss function with respect to the parameters on a minibatch of data, and α is the learning rate. Adam uses a more sophisticated update rule with two additional steps⁵.

 $^{^2{\}rm This}$ is also referred to as Glorot initialization and was initially described in http://jmlr.org/proceedings/papers/v9/glorot10a/glorot10a.pdf

³Srivastava et al., 2014, https://www.cs.toronto.edu/ hinton/absps/JMLRdropout.pdf

⁴Kingma and Ma, 2015, https://arxiv.org/pdf/1412.6980.pdf

⁵The actual Adam update uses a few additional tricks that are less important, but we won't worry about them for this problem.

(i) First, Adam uses a trick called *momentum* by keeping track of m, a rolling average of the gradients:

$$m \leftarrow \beta_1 m + (1 - \beta_1) \nabla_{\boldsymbol{\theta}} J_{minibatch}(\boldsymbol{\theta})$$

 $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha m$

where β_1 is a hyperparameter between 0 and 1 (often set to 0.9). Briefly explain (you don't need to prove mathematically, just give an intuition) how using m stops the updates from varying as much. Why might this help with learning?

(ii) Adam also uses adaptive learning rates by keeping track of v, a rolling average of the magnitudes of the gradients:

$$m \leftarrow \beta_1 m + (1 - \beta_1) \nabla_{\boldsymbol{\theta}} J_{minibatch}(\boldsymbol{\theta})$$

$$\boldsymbol{v} \leftarrow \beta_2 \boldsymbol{v} + (1 - \beta_2) (\nabla_{\boldsymbol{\theta}} J_{minibatch}(\boldsymbol{\theta}) \circ \nabla_{\boldsymbol{\theta}} J_{minibatch}(\boldsymbol{\theta}))$$

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \circ \boldsymbol{m} / \sqrt{\boldsymbol{v}}$$

where \circ and / denote elementwise multiplication and division (so $z \circ z$ is elementwise squaring) and β_2 is a hyperparameter between 0 and 1 (often set to 0.99). Since Adam divides the update by \sqrt{v} , which of the model parameters will get larger updates? Why might this help with learning?

(h) (20 points, coding/written) In q2_parser_model.py implement the neural network classifier governing the dependency parser by filling in the appropriate sections. We will train and evaluate our model on the Penn Treebank (annotated with Universal Dependencies).Run python q2_parser_model.py to train your model and compute predictions on the test data (make sure to turn off debug settings when doing final evaluation).

Hints:

- When debugging, pass the keyword argument debug=True to the main method (it is set to true by default). This will cause the code to run over a small subset of the data, so the training the model won't take as long.
- This code should run within 1 hour on a CPU.
- When running with debug=True, you should be able to get a loss smaller than 0.2 and a UAS larger than 65 on the dev set (although in rare cases your results may be lower, there is some randomness when training). When running with debug=False, you should be able to get a loss smaller than 0.08 on the train set and an Unlabeled Attachment Score larger than 87 on the dev set. For comparison, the model in the original neural dependency parsing paper gets 92.5 UAS. If you want, you can tweak the hyperparameters for your model (hidden layer size, hyperparameters for Adam, number of epochs, etc.) to improve the performance (but you are not required to do so).

Deliverables:

- Working implementation of the neural dependency parser in q2_parser_model.py. (We'll look at, and possibly run this code for grading).
- Report the best UAS your model achieves on the dev set and the UAS it achieves on the test set.
- List of predicted labels for the test set in the file q2_test.predicted.
- (i) **Bonus** (2 points). Add an extension to your model (e.g., 12 regularization, an additional hidden layer) and report the change in UAS on the dev set. Briefly explain what your extension is, what UAS the resulting model gets on the dev and test sets, and why the extension helps (or hurts!) the

model. Some extensions may require tweaking the hyperparameters in Config to make them effective. For both bonus points, your extended model should get better UAS than the baseline model without an extension. You should turn in your extension with your code, but your extension should be turned off by default. An easy way of doing this is add an extension boolean to your model's Config that is set to False when you turn in the code. If your extension does not improve over your baseline, do not turn in those predictions when you submit q2_test.predicted, use the baseline's ones instead (we will make sure these predictions produce a good UAS when grading)!

3 Recurrent Neural Networks: Language Modeling (25 points)

In this section, you'll analyze a recurrent neural network (RNN) used for language modeling.

Language modeling is a central task in NLP, and language models can be found at the heart of speech recognition, machine translation, and many other systems. Given a sequence of words (represented as one-hot vectors) $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(t)}$, a language model predicts the next word $\boldsymbol{x}^{(t+1)}$ by modeling:

$$P(\mathbf{x}^{(t+1)} = \mathbf{w}_j \mid \mathbf{x}^{(t)}, \dots, \mathbf{x}^{(1)})$$

where \boldsymbol{w}_i is a word in the vocabulary.

Your job is to compute the gradients of a recurrent neural network language model, which uses a hidden layer to represent the "history" $\boldsymbol{x}^{(t)}, \boldsymbol{x}^{(t-1)}, \dots, \boldsymbol{x}^{(1)}$ of previous words. Formally, the model⁶ is:

$$egin{aligned} oldsymbol{e}^{(t)} &= oldsymbol{E} oldsymbol{x}^{(t)} \\ oldsymbol{h}^{(t)} &= \operatorname{sigmoid} \left(oldsymbol{W}_h oldsymbol{h}^{(t-1)} + oldsymbol{W}_e e^{(t)} + oldsymbol{b}_1
ight) \\ \hat{oldsymbol{y}}^{(t)} &= \operatorname{softmax} \left(oldsymbol{U} oldsymbol{h}^{(t)} + oldsymbol{b}_2
ight) \\ ar{P}(oldsymbol{x}^{(t+1)} = oldsymbol{w}_i \mid oldsymbol{x}^{(t)}, \dots, oldsymbol{x}^{(1)})) &= \hat{oldsymbol{y}}_i^{(t)} \end{aligned}$$

where $\mathbf{h}^{(0)} = \mathbf{h}_0 \in \mathbb{R}^{D_h}$ is some initialization vector for the hidden layer and $\mathbf{E}\mathbf{x}^{(t)}$ is the product of \mathbf{E} with the one-hot vector $\mathbf{x}^{(t)}$ representing the current word. Essentially, the first equation embeds the current word, the second equation produces a new hidden state given the current word's embedding and previous hidden state, and the last equation predicts what the next word will be. The parameters are:

$$E \in \mathbb{R}^{d \times |V|}$$
 $W_h \in \mathbb{R}^{D_h \times D_h}$ $W_e \in \mathbb{R}^{D_h \times d}$ $b_1 \in \mathbb{R}^{D_h}$ $U \in \mathbb{R}^{|V| \times D_h}$ $b_2 \in \mathbb{R}^{|V|}$ (1)

where E is the embedding matrix, W_e the input word representation matrix, W_h the hidden state transformation matrix, and U is the output word representation matrix. b_1 and b_2 are biases. d is the embedding size, |V| is the vocabulary size, and D_h is the hidden layer size.

The output vector $\hat{y}^{(t)} \in \mathbb{R}^{|V|}$ is a probability distribution over the vocabulary. The model is trained by minimizing the (un-regularized) cross-entropy loss:

$$J^{(t)}(\theta) = CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}) = -\sum_{j=1}^{|V|} y_j^{(t)} \log \hat{y}_j^{(t)}$$

 $^{^6}$ This model is adapted from a paper by Toma Mikolov, et al. from 2010: http://www.fit.vutbr.cz/research/groups/speech/publi/2010/mikolov_interspeech2010_IS100722.pdf

where $y^{(t)}$ is the one-hot vector corresponding to the target word (which here is equal to $x^{(t+1)}$). We average the cross-entropy loss across all examples (i.e., words) in a sequence to get the loss for a single sequence.

(a) (4 points, written) Conventionally, when reporting performance of a language model, we evaluate on *perplexity*, which is defined as:

$$PP^{(t)}\left(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)}\right) = \frac{1}{\bar{P}(\boldsymbol{x}_{\text{pred}}^{(t+1)} = \boldsymbol{x}^{(t+1)} \mid \boldsymbol{x}^{(t)}, \dots, \boldsymbol{x}^{(1)})} = \frac{1}{\sum_{i=1}^{|V|} y_i^{(t)} \cdot \hat{y}_i^{(t)}}$$

i.e. the inverse probability of the correct word, according to the model distribution \bar{P} .

- (i) (2 points) Show how you can derive perplexity from the cross-entropy loss (*Hint: remember that* $y^{(t)}$ is one-hot!). This should be a very short problem not too perplexing!
- (ii) (1 point) Now use this relationship between perplexity and cross-entropy to show that minimizing the geometric mean perplexity, $\left(\prod_{t=1}^T PP(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)})\right)^{1/T}$, is equivalent to minimizing the arithmetic mean cross-entropy loss, $\frac{1}{T}\sum_{t=1}^T CE(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)})$, across the training set. (Hint: for any positive function f, minimizing $\log(f)$ is equivalent to minimizing f itself)
- (iii) (1 point) Suppose you have a vocabulary of |V| words and your "language model" works by picking the next word uniformly at random from the vocabulary (mathematically, $\bar{P}(\boldsymbol{x}^{(t+1)} = \boldsymbol{w}_j \mid \boldsymbol{x}^{(t)}, \dots, \boldsymbol{x}^{(1)})) = 1/|V|$ for every word \boldsymbol{w}_j in the vocabulary). What would the perplexity $PP(\boldsymbol{y}^{(t)}, \hat{\boldsymbol{y}}^{(t)})$ for a single word to be? Compute the corresponding cross-entropy loss when |V| = 10000.
- (b) (7 points, written) Compute the gradients of the loss J (the cross-entropy loss) with respect to the following model parameters at a single point in time t (to save a bit of time, you don't have to compute the gradients with the respect to the biases b_1 and b_2):

$$\frac{\partial J^{(t)}}{\partial \boldsymbol{U}} \qquad \frac{\partial J^{(t)}}{\partial \boldsymbol{e}^{(t)}} \qquad \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_e} \bigg|_{(t)} \qquad \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h} \bigg|_{(t)}$$

where $|_{(t)}$ denotes the gradient for the appearance of that parameter at time t (in other words, $h^{(t-1)}$ is taken to be fixed, so you don't need to take it's derivative when applying the chain rule and backpropagate to earlier timesteps - you'll do that in part (c)).

Additionally, compute the derivative with respect to the *previous* hidden layer value:

$$\frac{\partial J^{(t)}}{\partial \boldsymbol{h}^{(t-1)}}$$

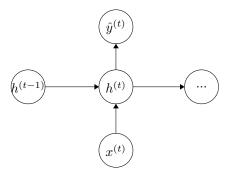
Hint: you may want to define the following variables:

$$oldsymbol{z}^{(t)} = oldsymbol{W}_h oldsymbol{h}^{(t-1)} + oldsymbol{W}_e oldsymbol{e}^{(t)} + oldsymbol{b}_1 \ oldsymbol{ heta}^{(t)} = oldsymbol{U} oldsymbol{h}^{(t)} + oldsymbol{b}_2$$

and define (and compute the value of) the following error terms:

$$\begin{aligned} \boldsymbol{\delta}_{1}^{(t)} &= \frac{\partial J}{\partial \boldsymbol{\theta}^{(t)}} \\ \boldsymbol{\delta}_{2}^{(t)} &= \frac{\partial J}{\partial \boldsymbol{z}^{(t)}} = \boldsymbol{\delta}_{1}^{(t)} \frac{\partial \boldsymbol{\theta}^{(t)}}{\partial \boldsymbol{h}^{(t)}} \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{z}^{(t)}} \end{aligned}$$

(c) (7 points, written) Below is a sketch of the network at a single timestep:



Draw the "unrolled" network for 3 timesteps (your picture should show $h^{(t-3)}$ to $h^{(t)}$. Next, compute the following backpropagation-through-time gradients:

$$\left. \frac{\partial J^{(t)}}{\partial \boldsymbol{e}^{(t-1)}} \qquad \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_e} \right|_{(t-1)} \qquad \left. \frac{\partial J^{(t)}}{\partial \boldsymbol{W}_h} \right|_{(t-1)}$$

where $|_{(t-1)}$ denotes the gradient for the appearance of that parameter at time (t-1). Use the error term $\gamma^{(t-1)} = \frac{\partial J^{(t)}}{\partial h^{(t-1)}}$ to represent the derivative you computed in the previous part (it should show up in three gradients you compute).

We have to compute multiple gradients with respect to parameters like W_e because they are used multiple times in the feed-forward computation. The final gradient for the parameters will be the sum of all their gradients over time (e.g., the gradient $\frac{\partial J^{(t)}}{\partial W_e} = \sum_{i=0}^t \frac{\partial J^{(t)}}{\partial W_e}|_{(i)}$).

- (d) (3 points, written) Given $h^{(t-1)}$, how many operations are required to perform backpropagation for a single timestep (i.e., compute the terms you found in part (b)). Express your answer in big-O notation in terms of the dimensions d, D_h and |V| (Equation 1). Don't worry about the gradients you didn't compute (with respect to b_1 and b_2), they actually don't change the answer!
 - (Hint: You only have to worry about matrix multiplications, the other operations do not change the big-O runtime. Multiplying a vector by an n by m matrix takes O(nm) operations.)
- (e) (3 points, written) Now suppose you have a sequence of T words. How many operations are required to compute the gradient of the loss with respect to the model parameters across the entire sequence $(\sum_{t=1}^{T} J^{(t)}(\theta))$? Assume we backpropagate through time all the way to t=0 for each word.

Hint: Look at the computational graph you drew in part (c). Will we have to pass an error signal (upstream gradient) into $h^{(0)}$ T times (once for the loss from every word), or can we be more efficient that that? Therefore, how many times will we have to do the single timestep (your answer to (d)) computations?

(f) (1 point, written) Which term in your big-O expressions is likely the largest? Which layer in the RNN is that term from?

Bonus (1 point, written) Given your knowledge of similar models (i.e. word2vec), suggest a way to speed up this part of the computation. Your approach can be an approximation, but you should argue why it's a good one. The paper "Extensions of recurrent neural network language model" (Mikolov, et al. 2013) may be of interest here.