# CS 224d: Assignment #2

*Updated Tuesday 28th April, 2015 at 1:49pm*

**Due date: 4/30 11:59 PM PST** (You are allowed to use three (3) late days maximum for this assignment)

This handout consists of several homework problems, as well as instructions on the "deliverables" associated with the coding portions of 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 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://cs224d.stanford.edu/assignments.html. When you are ready to submit, please follow the instructions on the course website.

**Note on Logistics:** In response to feedback from the first assignment, Assignment 2 relies much less on notebook grading. Instead, we've provided a list of "deliverables" for the programming sections. Some of these are short-answer questions; put these in your written portion. For the rest, we give you code snippets that create the correct output; just run the corresponding cells, and include the files they create in your submission `.zip` file.

## 0 Warmup: Boolean Logic

A famous result from the early days of AI (see `https://en.wikipedia.org/wiki/Perceptrons_(book)`) proved that a linear classifier, such as a single layer of a neural network, cannot compute even simple functions such as binary XOR. We will show by example that a two-layer neural network, however, is perfectly capable of learning this pattern.

(a) Let $x \in \{0, 1\}$ and $y \in \{0, 1\}$. Express the XOR ($\oplus$) function as the composition of other boolean logic operations (NOT, AND, OR, implication, etc.). Argue graphically (i.e. plot or sketch ($x, y$, class $= f(x, y)$) for $x \in \{0, 1\}$ and $y \in \{0, 1\}$) that the operations you use in your composition *are* possible to compute with an ordinary (single-layer) linear classifier.

(b) Assume that each neuron has a step-function activation, i.e $h_i(x, y) = \theta(w_{i1}x + w_{i2}y + b_i)$, where:

$$\theta(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Find weights that allow $h_i(x, y)$ to compute the single-layer functions from (a). Your classifier can have real-valued weights; only the data need be binary. (*Hint: which operation is given by $\theta(x + y - 0.5)$?*)

(c) Open the IPython notebook `part0-XOR.ipynb` and follow the instructions, using what you derived in (a) and (b) to implement a very simple 2-layer network that can compute (i.e. classify) binary XOR.

# 1 Deep Networks for Named Entity Recognition

*This section is based on an assignment originally created for CS 224N. A more detailed writeup can be found at* `http://nlp.stanford.edu/~socherr/pa4_ner.pdf`*, and may be of use as a refresher.*

In this section, we'll get to practice backpropagation and training deep networks to attack the task of Named Entity Recognition: predicting whether a given word, in context, represents one of four categories:

- Person (`PER`)
- Organization (`ORG`)
- Location (`LOC`)
- Miscellaneous (`MISC`)

We formulate this as a 5-class classification problem, using the four above classes and a null-class (`O`) for words that do not represent a named entity (most words fall into this category).

The model is a 2-layer neural network, with an additional representation layer similar to what you saw with `word2vec`. Rather than averaging or sampling, here we explicitly represent context as a "window" consisting of a word concatenated with its immediate neighbors:

$$x^{(t)} = [Lx_{t-1},\ Lx_t,\ Lx_{t+1}] \in \mathbb{R}^{3d} \tag{1}$$

where the input $x_{t-1}, x_t, x_{t+1}$ are one-hot vectors (really, just indices) into a word-representation matrix $L \in \mathbb{R}^{d \times |V|}$ [1], with each column $L_i$ as the vector for a particular word $i = x_t$. We then compute our prediction as:

$$h = \tanh(Wx^{(t)} + b_1) \tag{2}$$

$$\hat{y} = \text{softmax}(Uh + b_2) \tag{3}$$

And evaluate by cross-entropy loss

$$J(\theta) = -\sum_{k=1}^{5} y_k \log \hat{y}_k \tag{4}$$

where $y \in \mathbb{R}^5$ is a one-hot label vector. To compute the loss for the training set, we sum (or average) this $J(\theta)$ as computed with respect to each training example.

For this problem, we let $d = 50$ be the length of our word vectors, which are concatenated into a window of width $3 \times 50 = 150$. The hidden layer has a dimension of 100, and the output layer $\hat{y}$ has a dimension of 5.

(a) Compute the gradients of $J(\theta)$ with respect to all the model parameters:

$$\frac{\partial J}{\partial U} \quad \frac{\partial J}{\partial b_2} \quad \frac{\partial J}{\partial W} \quad \frac{\partial J}{\partial b_1} \quad \frac{\partial J}{\partial L_i}$$

where

$$U \in \mathbb{R}^{5x100} \quad b_2 \in \mathbb{R}^5 \quad W \in \mathbb{R}^{100x150} \quad b_1 \in \mathbb{R}^{100} \quad L_i \in \mathbb{R}^{50}$$

[1] In the code, we'll implement this with word vectors as *rows* for efficiency, and so you can access $L_i$ as `L[i]`. See `nerwindow.py` for more details.

In the spirit of backpropagation, you should express the derivative of activation functions (tanh, softmax) in terms of their function values (as with sigmoid in Assignment 1). This identity may be helpful:

$$\tanh(z) = 2\ \text{sigmoid}(2z) - 1$$

Furthermore, you should express the gradients by using an "error vector" propagated back to each layer; this just amounts to putting parentheses around factors in the chain rule, and will greatly simplify your analysis. All resulting gradients should have simple, closed-form expressions in terms of matrix operations. (*Hint: you've already done most of the work here as part of Assignment 1.*)

(b) To avoid parameters from exploding or becoming highly correlated, it is helpful to augment our cost function with a Gaussian prior: this tends to push parameter weights closer to zero, without constraining their direction, and often leads to classifiers with better generalization ability.

If we maximize log-likelihood (as with the cross-entropy loss, above), then the Gaussian prior becomes a quadratic term [2] (L2 regularization):

$$J_{reg}(\theta) = \frac{\lambda}{2}\left[\sum_{i,j} W_{ij}^2 + \sum_{i'j'} U_{i'j'}^2\right] \tag{5}$$

and we optimize the combined loss function

$$J_{full}(\theta) = J(\theta) + J_{reg}(\theta) \tag{6}$$

Update your gradients from part (a) to include the additional term in this loss function (i.e. compute $\frac{dJ_{full}}{dW}$, etc.).

(c) In order to avoid neurons becoming too correlated and ending up in poor local minimina, it is often helpful to randomly initialize parameters. Empirically, the following has been found to work well:

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

$$\epsilon = \frac{\sqrt{6}}{\sqrt{m+n}} \tag{7}$$

Implement the function `random_weight_matrix(m,n)` in `misc.py` to perform this initialization. A cell is provided to test this code in `part1-NER.ipynb`.

(d) Open the notebook `part1-NER.ipynb` and follow the instructions to implement the NER window model, using the gradients you derived in (a) and (b). You'll also want to take a look at the example classifier in `softmax_example.py` for a guide on how to implement your model using our starter code.

**Deliverables:**

- Working implementation of the NER window model, in `nerwindow.py`. (We'll look at, and possibly run this code for grading.)
- In your writeup (i.e. where you're writing the answers to the written problems), *briefly* state the optimal hyperparameters you found for your model: regularization, dimensions, learning rate (including time-varying, such as annealing), SGD batch size, etc.

[2] **Optional (not graded):** The interested reader should prove that this is indeed the maximum-likelihood objective when we let $W_{ij} \sim N(0, 1/\lambda)$ for all $i, j$.

(e) In the notebook, follow the instructions to plot learning curves for your best model, and for a comparison of learning rates.

**Deliverables:**

- Plot of the learning curve for your best model, in `ner.learningcurve.best.png`.
- Plot comparing $\alpha = 0.01$ to $\alpha = 0.1$ in `ner.learningcurve.comparison.png`.

(f) In the notebook, follow the instructions to evaluate your model's performance on the dev set, and compute predictions on the test data. Note that the test set has only dummy labels; we'll compare your predictions against the ground truth after you submit.

Note that you should compute F1 scores by a weighted average across all classes *except* `"O"`, since this null class is not of interest for practical applications. The function `eval_performance()` in `nerwindow.py` will do this for you.

**Deliverables:**

- Report, in your writeup, the performance of your model on the dev set (as output by `eval_performance()`).
- List of predicted labels for the `test` set, one per line, in the file `test.predicted`.

### 1.1 Deep Networks: Probing Neuron Responses

Still in the `part1-NER.ipynb` notebook, follow the instructions to "probe" the responses of the hidden and output neurons in your network. You should report the following in your writeup:

(a) Top-10 word lists for the center word, on 5 hidden layer neurons of your choice.

(b) Top-10 word lists for the center word, on model output for `PER`, `ORG`, `LOC`, and `MISC`.

(c) Top-10 word lists for the first word (preceding the center word), on model output for `PER`, `ORG`, `LOC`, and `MISC`.

For each, give a *brief* (no more than 2 sentence) comment on what the model appears to learn.

## 2 Recurrent Neural Networks: Language Modeling

In this section, you'll implement your first recurrent neural network (RNN[3]) and use it to build a language model.

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 words $x_1, \ldots, x_t$, a language model predicts the following word $x_{t+1}$ by modeling:

$$P(x_{t+1} = v_j \mid x_t, \ldots, x_1)$$

where $v_j$ is a word in the vocabulary.

Your job is to implement a recurrent neural network language model, which uses feedback information in the hidden layer to model the "history" $x_t, x_{t-1}, \ldots, x_1$. Formally, the model[4] is, for $t = 1, \ldots, n-1$:

[3] We'll start talking about *recursive* neural networks soon and also call these RNNs - but it turns out that recurrent nets are just a special case of recursive nets, so there's actually nothing ambiguous!

[4] 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`

$$h^{(t)} = \text{sigmoid}\left(Hh^{(t-1)} + Lx^{(t)}\right) \tag{8}$$

$$\hat{y}^{(t)} = \text{softmax}\left(Uh^{(t)}\right) \tag{9}$$

$$\bar{P}(x_{t+1} = v_j \mid x_t, \ldots, x_1) = \hat{y}_j^{(t)} \tag{10}$$

where $h^{(0)} = h_0 \in \mathbb{R}^{D_h}$ is some initialization vector for the hidden layer and $Lx^{(t)}$ is the product of $L$ with the one-hot vector $x^{(t)}$ representing index of the current word [5]. The parameters are:

$$H \in \mathbb{R}^{D_h \times D_h} \quad L \in \mathbb{R}^{D_h \times |V|} \quad U \in \mathbb{R}^{|V| \times D_h} \tag{11}$$

where $L$ is the input word representation matrix and $U$ is the output word representation matrix, and $D_h$ is the dimension of the hidden layer.

The output vector $\hat{y}^{(t)} \in \mathbb{R}^{|V|}$ is a probability distribution over the vocabulary, and we optimize the (unregularized) cross-entropy loss:

$$J^{(t)}(\theta) = -\sum_{j=1}^{|V|} y_j^{(t)} \log \hat{y}_j^{(t)} \tag{12}$$

where $y^{(t)}$ is the one-hot vector corresponding to the target word (which here is equal to $x_{t+1}$). As in Part 1, this is a point-wise loss, and we sum (or average) the cross-entropy loss across all examples in a sequence, across all sequences[6] in the dataset in order to evaluate model performance.

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

$$\text{PP}^{(t)}\left(\hat{y}^{(t)}, y^{(t)}\right) = \frac{1}{\bar{P}(x_{t+1}^{\text{pred}} = x_{t+1} \mid x_t, \ldots, x_1)} = \frac{1}{\sum_{j=1}^{|V|} y_j^{(t)} \cdot \hat{y}_j^{(t)}} \tag{13}$$

i.e. the inverse probability of the correct word, according to the model distribution $\bar{P}$. Show how you can derive perplexity from the cross-entropy loss (*Hint: remember that $y^{(t)}$ is one-hot!*), and thus argue that minimizing the (arithmetic) mean cross-entropy loss will also minimize the (geometric) mean perplexity across the training set. ***This should be a very short problem - not too perplexing!***

For a vocabulary of $|V|$ words, what would you expect perplexity to be if your model predictions were completely random? Compute the corresponding cross-entropy loss for $|V| = 2000$ and $|V| = 10000$, and keep this in mind as a baseline.

(b) As you did in part 1, compute the gradients with for all the model parameters at a single point in time $t$:

$$\frac{\partial J^{(t)}}{\partial U} \qquad \frac{\partial J^{(t)}}{\partial L_{x^{(t)}}} \qquad \left.\frac{\partial J^{(t)}}{\partial H}\right|_{(t)}$$

where $L_{x^{(t)}}$ is the column of $L$ corresponding to the current word $x^{(t)}$, and $\big|_{(t)}$ denotes the gradient for the appearance of that parameter at time $t$. (Equivalently, $h^{(t-1)}$ is taken to be fixed, and you need not backpropagate to earlier timesteps just yet - you'll do that in part (c)).

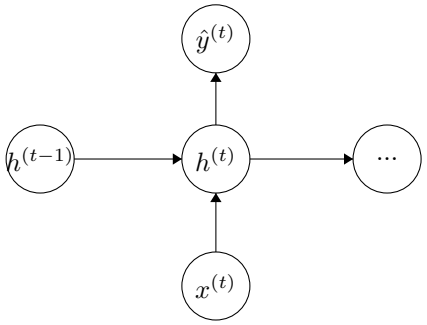
Additionally, compute the derivative with respect to the *previous* hidden layer value:

[5] As in Part 1, in the code it is more convenient to represent $L$ as a *"tall"* matrix and access rows as `L[x[t]]`.

[6] We implement this for you in `compute_mean_loss` in `rnnlm.py`.

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

(c) Below is a sketch of the network at a single timestep:




Draw the "unrolled" network for 3 timesteps, and compute the backpropagation-through-time gradients:

$$\frac{\partial J^{(t)}}{\partial L_{x^{(t-1)}}} \qquad \frac{\partial J^{(t)}}{\partial H}\Big|_{(t-1)}$$

where $\big|_{(t-1)}$ denotes the gradient for the appearance of that parameter at time $(t-1)$. Because parameters are used multiple times in feed-forward computation, we need to compute the gradient for each time they appear.

You should use the backpropagation rules from Lecture 5 [7] to express these derivatives in terms of an error term $\delta^{(t)}$, such that you can re-use expressions for $t-2$, $t-3$, and so on.

Note that the true gradient with respect to a training example requires us to run backpropagation all the way back to $t=0$. In practice, however, we generally truncate this and only backpropagate for a fixed number $\tau \approx 3-5$ timesteps.

(d) Given $h^{(t-1)}$, how many operations are required to perform one step of forward propagation to compute $J^{(t)}(\theta)$? How about backpropagation for a single step in time? For $\tau$ steps in time? Express your answer in big-O notation in terms of the dimensions $D_h$ and $|V|$ of the matricies $L$, $H$, and $U$ (Equation 11). What is the slow step?

**Bonus:** 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.

(e) Implement the above model in `rnnlm.py`. You'll need to implement just three functions, for now:

- `__init__()` (not much to do here)
- `_acc_grads()`
- `compute_seq_loss()`

Data loaders and other starter code is provided in the `part2-RNNLM.ipynb` notebook, and you should use this to verify your implementation.

[7] `http://cs224d.stanford.edu/lectures/CS224d-Lecture5.pdf`

*Be sure to read the instructions carefully in the starter code!* They describe the data format and how to run your model over a sequence. Particuarly, you should *sum* the pointwise costs $J^{(t)}(\theta)$ over a sequence. When accumulating gradients, you should also add up all the gradients you compute for $J^{(t)}(\theta)$ for each target word in the sequence. (This is basically minibatch SGD.)

(f) Train a model on the `ptb-train` data, consisting of the first 20 sections of the WSJ corpus of the Penn Treebank. For speed, we recommend using a small vocabulary of 2000-5000 words.

As in Part1, you should tune your model to maximize generalization performance (minimize cross-entropy loss) on the dev set. We'll evaluate your model on an unseen, but similar set of sentences.

**Deliverables:**

- In your writeup, include the best hyperparameters you used (training schedule, number of iterations, learning rate, backprop timesteps), and your perplexity score on the `ptb-dev` set.
- Model parameters saved as `rnnlm.U.npy`, `rnnlm.H.npy`, and `rnnlm.L.npy`; we'll use these to test your model.

(g) The networks that you've seen in Assignment 1 and in Part1 of this assignment are discriminative models: they take data, and make a prediction. The RNNLM model you've just implemented is a *generative* model, in that it actually models the distribution of the *data* sequence $x_1, \ldots, x_n$. This means that not only can we use it to evaluate the likelihood of a sentence, but we can actually use it to generate one!

In `rnnlm.py`, implement the `generate_sequence()` function. This should run the RNN forward in time, beginning with the index for the start token `<s>`, and sampling a new word $x_{t+1}$ from the distribution $\hat{y}^{(t)}$ at each timestep. Then feed this word in as input at the next step, and repeat until the model emits an `end` token (index of `</s>`).

***Note:*** *this should not require a lot of coding - our solution is less than 15 lines, and most of this is copied from* `compute_seq_loss()`.

**Deliverables:**

- Include 2-3 generated sentences in your writeup. See if you can generate something humorous!
- Your code, in `rnnlm.py`; we'll run this to test using the parameters from (f).
- **Bonus:** Implement the unigram-filling described in the notebook.

***Completely optional, not graded:*** If you want to experiment further with language models, you're welcome to load up your own texts and train on them - sometimes the results can be quite entertaining! (See `http://kingjamesprogramming.tumblr.com/` for a great one[8] trained on a mix of the King James Bible and the Structure and Interpretation of Computer Programs.)

**Extra Credit:** For extra credit, implement the extension you described in Part 2, part (d). Write your code in the `ExtraCreditRNNLM` class in `rnnlm.py`, and include the following in your submission:

- Description of the extensions you implemented (3-4 sentences max).
- Dev set perplexity and optimal hyperparameters as in Part 2 (f).
- Comparison of training speed between your extension and the original model (3-4 sentences max).

[8] This one just uses a simple n-gram Markov model, but there's no reason an RNNLM can't compete!

- Relevant model parameters saved as `extracredit.U.npy`, `extracredit.H.npy`, etc. (these may be different from the usual RNNLM parameters, depending on your implementation). If your saved parameters exceed 15 MB, let the TAs know before submitting through the usual system.