METL – TP1
Neural Network Basics

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Evaluation: You are allowed an unlimited number of submissions in order to receive feedback. When you are satisfied with your work, you can ask for it to be graded. You can also ask for it to be graded upon a single submission, without receiving feedback. All your TPs must have been graded and must have received an average grade of at least 4/6 for you to register for the METL exam. Indicative deadline: March 4 2020 (this TP should take you two weeks).

1 Preliminary instructions

Mathematics as used in the field of machine learning is often filled with approximations or underspecifications which can hinder the comprehension of the notions at hand. The purpose of this TP is to make your life easier by first ***making the implicit explicit****. For our first TP, we go over some important mathematical notions regarding neural networks, as usually specified in the field, and rework them as cleanly as possible. To do so, we ask you to be as precise and clean as possible in all your mathematical developments and demonstrations. Notably:*

1. *Always specify the* ***domain*** *of the function at hand;*
2. *Always specify the* ***scope*** *of your variables;*
3. *Always specify the* ***nature*** *of your demonstration (by equivalence, reductio ad absurdum, proof by induction, etc.) and use the relevant mathematical symbols;*
4. *Always keep you demonstrations* ***short*** *and* ***simple****: limit verbosity, write down* ***all*** *the necessary steps, but* ***only*** *the necessary steps.*

2 Softmax

Consider the following (poorly defined) *softmax* function:

$$softmax(x) = \frac{e^x}{\sum_j e^{x_j}} \tag{1}$$

1. Cleanly redefine the softmax function;
2. Prove that softmax is invariant to constant offsets in the input, that is, for any input vector x and any constant c:

$$softmax(x) = softmax(x + c) \tag{2}$$

Note: In practice, we make use of this property and choose $c = -\max_i x_i$ when computing softmax probabilities for numerical stability, that is, we subtract the maximum element from all elements of x. Remember this in your implementation of softmax...

3. Given an input matrix of N rows and d columns, compute the softmax prediction for each row. Write your implementation in `softmax.py` and test your code by running:

   ```
   python3 softmax.py
   ```

   Note: The provided tests are not exhaustive. Later parts of the assignment will reference this code so it is important to have a correct implementation. Your implementation should also be efficient and vectorized whenever possible.

3 Gradient, Sigmoid, Forward, Backward

1. Derive the gradients of the sigmoid function and show that it can be rewritten as a function of the function value (i.e. in some expression where only $\sigma(x)$, but not x, is present). Assume that the input x is a scalar for this question. Recall the (yet again poorly defined) sigmoid function, which you will first properly redefine:

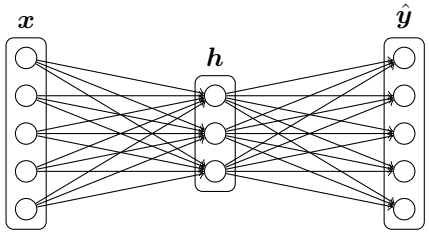
$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{3}$$

2. Derive the gradient with respect to the inputs of a softmax function when cross entropy loss is used for evaluation, i.e. find the gradients with respect to the softmax input vector θ, when the prediction is made by $\hat{y} = softmax(\theta)$. Recall the cross entropy function:

$$CE(y, \hat{y}) = -\sum_i y_i log(\hat{y}_i) \tag{4}$$

   where y is the one-hot label vector and $\hat{y}$ is the predicted probability vector for all classes. *Hint: you may want to consider the fact that many elements of y are zeros, and assume that only the k-th dimension of y is one.*

3. Derive the gradients with respect to the inputs x of a one-hidden-layer neural network. That is, find $\frac{\partial J}{\partial x}$ where J is the cost/loss function of the neural network. Consider a neural network that employs a sigmoid activation function for the hidden layer and a softmax for the output layer. Assume the one-hot label vector to be y and the cost/loss function to be cross entropy. You can denote the sigmoid gradient as $\sigma'(x)$.



   Recall that the forward propagation follows:

$$h = sigmoid(xW_1 + b_1) \qquad \hat{y} = softmax(hW_2 + b_2) \tag{5}$$

   Note that here we are assuming that the input vector (thus the hidden variables and output probabilities) is a row vector. When we apply the sigmoid function to a vector, we apply it to each of its elements. W_i and b_i $(i = 1, 2)$ are the weights and biases of the two layers.

4. How many parameters are there in this neural network, assuming the input to be D_x-dimensional, the output to be D_y-dimensional and there to be H hidden units?

5. Fill in the implementation for the sigmoid activation function and its gradient in `sigmoid.py` and test your implementation using:

   ```
   python3 sigmoid.py
   ```

   Again, thoroughly test your code as the provided tests may not be exhaustive.

6. To make debugging easier, we will now implement a gradient checker. Fill in the implementation of `gradcheck_naive` in `gradcheck.py` and test your code using:

   ```
   python3 gradcheck.py
   ```

   Hint: Use the centrale difference.[1] *Reminder: Why do we need to check the gradient?*[2]

7. Implement the forward and backward passes for a neural network with one sigmoid hidden layer. Fill in your implementation in `neural.py` and sanity check it by running:

   ```
   python3 neural.py
   ```

[1] *https://math.stackexchange.com/questions/2120946/why-is-central-difference-preferred-over-backward-and-f*
[2] *http://ufldl.stanford.edu/wiki/index.php/Gradient_checking_and_advanced_optimization*