# Automatic Reverse-Mode Differentiation

TAs: Karandeep Johar, Bhuwan Dhingra

Out 11/3/2016
Due 11/17/2016 via Autolab

**Prerequisite:** Please ensure you have first read Prof Cohen's notes on Automatic Reverse Mode Differentiation[1].

**Guidelines for Answers:** Please answer to the point. Please state any additional assumptions you make while answering the questions. You need to submit a tar file containing source files and a pdf version of report separately to autolab. Please make sure you write the report legibly for grading.

**Rules for Student Collaboration:** The purpose of student collaboration in solving assignments is to facilitate learning, not to circumvent it. Studying the material in groups is strongly encouraged. It is allowed to seek help from other students in understanding the material needed to solve a homework problem, provided no written notes are taken or shared during group discussions. The actual solutions must be written and implemented by each student alone, and the student should be ready to reproduce their solution upon request. You may ask clarifying questions on Piazza. However, under no circumstances should you reveal any part of the answer publicly on Piazza or any other public website. Any incidents of plagiarism or collaboration without full disclosure will be handled severely.

**Rules for External Help:** Some of the homework assignments used in this class may have been used in prior versions of this class, or in classes at other institutions. Avoiding the use of heavily tested assignments detracts from the main purpose of these assignments, which is to reinforce the material and stimulate thinking. Because some of these assignments may have been used before, solutions to them may be available online or from other people. It is explicitly forbidden to use any such sources or to consult people who have

[1] `http://www.cs.cmu.edu/~wcohen/10-605/notes/autodiff.pdf`

solved these problems before. You must solve the homework assignments completely on your own. We will mostly rely on your wisdom and honor to follow this rule. However, if a violation is detected, it will be dealt with harshly.

- Did you receive any help whatsoever from anyone in solving this assignment? Yes/No
- If you answered yes, give full details:______________________________
  (e.g. "Jane explained to me what is asked in Question 3.4" )
- Did you give any help whatsoever to anyone in solving this assignment? Yes/No
- If you answered yes, give full details:______________________________
  (e.g. "I pointed Joe to section 2.3 to help him with Question 2" )

# 1 Overview

In this assignment we will use an automatic differentiation system to implement two neural network architectures for character level entity classification, using `python` and `numpy`. The architectures we will implement are:

- A feedforward network or Multilayer Perceptron (MLP)
- A Long Short Term Memory (LSTM) network followed by a feedforward layer

Character level entity classification refers to determining the type of an entity given the characters which appear in its name as features. For example, given the name “`Antonio_Veciana`” you might guess that it is a `Person`, and given the name “`Anomis_esocampta`” you might guess that it is a `Species`. We will be classifying the following 5 `DBPedia` categories - `Person`, `Place`, `Organisation`, `Work`, `Species`.

# 2 Neural Architectures

## 2.1 Mutlilayer Perceptron

MLP is a simple neural network architecture consisting of multiple layers, each of which apply a linear transformation followed by non-linear mapping to their inputs:

$$o_i = f(x^T w_i + b_i)$$

Here $x \in \mathbb{R}^{d_{in}}$ is the layer input and $o_i \in \mathbb{R}$ is the $i$-th output of the layer. $w_i$, $b_i$ are layer parameters which will be optimized during learning. The number of outputs at each layer is called the *dimension* of that layer and we denote it by $d_{out}$. We would like to use vector/matrix multiplications wherever possible to utilize their fast implementation in `numpy`, and combine the above for all $i$ as:

$$o = f(x^T W + b)$$

$W = [w_1, w_2, \ldots, w_{d_{out}}] \in \mathbb{R}^{d_{in} \times d_{out}}$ stacks all the weight vectors horizontally, and $\mathbf{b} \in \mathbb{R}^{d_{out}}$ holds all the biases. The non-linearity $f$ is applied elementwise.

To further speed-up the computation we can process a minibatch of inputs together. Let $X \in \mathbb{R}^{N \times \mathbb{R}^{d_{in}}}$ be a matrix holding $N$ examples row-wise. We can compute the layer outputs for all of these together:

$$O = f(XW + B) \tag{1}$$

$B = \mathbf{1} \otimes b^T \in \mathbb{R}^{N \times d_{out}}$ is a "broadcasted" version of the bias of appropriate dimensions. For this assigment we will use `numpy` for all matrix operations, which takes care of broadcasting automatically (see here[2] for details), hence we can use the vector $b$ directly. The nonlinearity we will use is the `Rectified Linear Unit (ReLU)`:

$$f(x) = \begin{cases} x & x > 0 \\ 0 & x \leq 0 \end{cases}$$

For vectors the nonlinearity is applied element-wise, and we can again use numpy broadcasting for this. In multi-layer networks, output of the layer $k$ is passed as input to layer $k+1$:

$$O^{(k+1)} = f(O^{(k)} W^{(k)} + b^{(k)}) \tag{2}$$

We can set output size of the last layer of the MLP to produce a vector the same size as the number of labels $C$ in our dataset. The operations described thus far map inputs to positive reals, but for classification tasks

[2] `https://docs.scipy.org/doc/numpy/user/basics.broadcasting.html`

we are interested in obtaining a *distribution* over class labels. This is usually done by passing the output of MLP through a `softmax` layer:

$$p_j = \frac{e^{o_j}}{\sum_{j'=1}^{C} e^{o_{j'}}} \tag{3}$$

Note that $p$ defines a valid distribution, and elements of $o$ which have a high relative value will have a high probability in $p$. The above equation computes $p$ for a single $o$, but in your code you should use `numpy` operations to compute a minibatch of distributions $P$ from a minibatch of outputs $O$.

Lastly, we need to define a loss function which measures how far the output distribution $p_i$ for example $i$ is from its target distribution $t_i$. We will use the cross-entropy loss for this:

$$l_i = -\sum_{j=1}^{C} t_i^{(j)} \log p_i^{(j)} \tag{4}$$

For single-label classification, $t_i$ is an $C$-dimensional one-hot vector encoding the correct label for this example. The objective function we will optimize is the average of losses across a minibatch:

$$L = \frac{1}{N} \sum_{i=1}^{N} l_i \tag{5}$$

Now we can take gradients of $L$ wrt to the parameters of the network and perform Stochastic Gradient Descent (SGD).

To summarize, the first architecture you will implement for this assignment consists of an MLP with one hidden layer, followed by a softmax layer (3) and cross-entropy loss (4). Given an input minibatch $X$ and their associated targets $T$, the output $P$ and loss $L$ are computed as:

$$\begin{aligned} O^{(1)} &= \text{relu}(XW^{(1)} + b^{(1)}) \\ O^{(2)} &= \text{relu}(O^{(1)}W^{(2)} + b^{(2)}) \\ P &= \text{softmax}(O^{(2)}) \\ L &= \text{mean}(\text{cross-entropy}(T, P)) \end{aligned}$$

## 2.2 Long Short Term Memory

The MLP is a powerful model – with enough hidden units it can approximate any function, but it is not the most appropriate model when the input is a sequence. For sequences, the input size of the MLP and consequently size of $W^{(1)}$, will increase linearly with the size of the length of the sequence and might get prohibitively large. Instead, we would like to have a model which can loop over the input sequence, and starting from an initial state iteratively updates this state based on the input at that time step. LSTMs are one example of such a model [3].

Lets say we have a sequence of inputs $x_1, x_2, \ldots, x_M \in \mathbb{R}^{d_{in}}$, an initial *cell state* $c_0 = \mathbf{0} \in \mathbb{R}^{d_{out}}$ and an initial *output* $h_0 = \mathbf{0} \in \mathbb{R}^{d_{out}}$. At time $t$ the LSTM does the following updates:

$$\begin{aligned}
i_t &= \sigma(x_t^T W_i + h_{t-1}^T U_i + b_i) \\
f_t &= \sigma(x_t^T W_f + h_{t-1}^T U_f + b_f) \\
o_t &= \sigma(x_t^T W_o + h_{t-1}^T U_o + b_o) \\
\tilde{c}_t &= tanh(x_t^T W_c + h_{t-1}^T U_c + b_c) \\
\\
c_t &= f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \\
h_t &= o_t \odot tanh(c_t)
\end{aligned}$$

Here $W_* \in \mathbb{R}^{d_{in} \times d_{out}}$, $U_* \in \mathbb{R}^{d_{out} \times d_{out}}$, $b_* \in \mathbb{R}^{d_{out}}$ are parameters, $\odot$ is an element-wise product and $\sigma$ is the sigmoid function (applied element-wise):

$$\sigma(x)_i = \frac{1}{1 + e^{-x_i}} \tag{6}$$

**Note:** The above equations are shown for single inputs $x$ for clarity. In your implementation you must use minibatches $X$ of $N$ examples at a time, the same way as we did for the MLP. This amounts to replacing $x_t^T$ with matrices $X_t$ of size $N \times d_{in}$, and $h_t^T$, $c_t^T$ with matrices $H_t$, $C_t$ of size $N \times d_{out}$.

Now we are ready to implement the second architecture for this assignment. We will replace the first layer of MLP in the previous section with an LSTM layer. Let LSTM$(X_1, X_2, \ldots, X_M)$ be a function which loops over the sequence $X_1, \ldots, X_M$, performs the updates described above, and returns the final output $H_M$. Then, given inputs $X_1, \ldots, X_M$, the output $P$ and loss $L$

[3] An excellent introduction to LSTMs can be found at `http://colah.github.io/posts/2015-08-Understanding-LSTMs/`

are computed as follows:

$$\begin{aligned}
H_M &= \text{LSTM}(X_1, X_2, \ldots, X_M) \\
O^{(2)} &= \text{relu}(H_M W^{(2)} + b^{(2)}) \\
P &= \text{softmax}(O^{(2)}) \\
L &= \text{mean}(\text{cross-entropy}(T, P))
\end{aligned}$$

### 2.3 Learning

Parameters of the above networks can be trained using minibatch SGD. Once the loss function $L$ is defined we can take its derivative wrt to any parameter $w_{ij}$ and update it as follows:

$$w_{ij}^{(k)} \leftarrow w_{ij}^{(k-1)} - \lambda \frac{dL}{dw_{ij}} \tag{7}$$

$\lambda$ is the learning rate.

## 3 Autodiff Implementation

In the starter code the following files are given -

- `xman.py` – classes for expression manager, registers and operations
- `utils.py` – classes for data preprocessing and forming minibatches (more on this below)
- `functions.py` – function definitions and their gradients are declared here
- `mlp.py` – you need to implement the mlp here
- `lstm.py` – you need to implement the lstm here
- `autograd.py` – class for forward and backward propagation over a defined set of registers

Here we briefly outline the steps needed to implement a model using the package provided with the handout.

## 3.1 Declare operations, their functions and gradients

First we must declare all the primitive operations our function uses in the XManFunctions class. For example, to declare relu, add the following lines to f class:

```
class f(XManFunctions):
    @staticmethod
    def relu(a):
        return XManFunctions.registerDefinedByOperator('relu',a)
```

add, mul and subtract are decalred by default in XManFunctions.

Next we need to define functions for both the forward and backward pass for each of the operators in our definition. The following example shows the definitions for add:

```
import numpy as np
# forward pass
EVAL_FUNS = {
    'add':      lambda x1,x2: x1+x2,
}

def _derivAdd(delta,x1):
if delta.shape!=x1.shape:
    # broadcast, sum along axis=0
    return delta.sum(axis=0)
else: return delta

# backward pass
BP_FUNS = {
    'add':     [lambda delta,out,x1,x2: _derivAdd(delta,x1),
                     lambda delta,out,x1,x2: _derivAdd(delta,x2)],
    }
```

Lets take a closer look at what is happening here. EVAL_FUNS is a dictionary whose keys are the names of the operators as declared in the previous section and values are the actual functions themselves (usually defined using lambda calculus). BP_FUNS is another dictionary with the same set of keys as EVAL_FUNS, but whose value for a key is a list of functions each computing its gradient wrt one of its inputs.

In the above example `BP_FUNS['add'][0]` computes the derivative wrt `x1`, and `BP_FUNS['add'][1]` computes the derivative wrt `x2`. As input each of these functions receives:

- `delta` - partial derivative of the output of this operation
- `out` - output of this operation in the forward pass. This can be sometimes useful for computing the derivative. For example, for the sigmoid nonlinearity $\sigma'(x) = \sigma(x)(1 - \sigma(x))$.
- `x1`,`x2`,... - all inputs to the operation

Some things to be careful about:

1. Remember that our functions need to run in minibatch mode, where they receive matrices as input and produce matrices as output
2. Ensure that the shape of a gradient matches the shape of the input wrt it is computed
3. Be careful about `numpy` broadcasting. An example of this is shown in `_derivAdd`. In numpy if we add a $N \times d$ matrix and a size $d$ vector, the vector is broadcasted to the size of the matrix. In this case the gradient coming back will be size $N \times d$, and needs to be summed along the first dimension for the vector (but not for the matrix!). This happens for example when we write $XW + b$.

## 3.2 Describe the Model

Once the primitive operations are defined, we can go ahead and define the model. First we need to declare registers to hold inputs and parameters, suppose there is one input `x` and two parameters `W` and `b`:

```
x = f.input(name='x', default=np.random.rand(1,10))
W = f.param(name='W', default=a*np.random.uniform(10,10))
b = f.param(name='b', default=0.1*np.random.uniform(10,))
```

You **must** specify the `name` and `default` fields for each register. `name` is used during the forward and backward passes to bind values to the correct register (more on this later), and `default` is used as initialization for parameters and for performing gradient checks on the inputs.

**Note on initialization of parameters:** As discussed in class, it is important to initialize parameters such that intermediate values in the network do not lie in the saturated regions of the non-linearity. One good heuristic is to sample the weights for $W$ of size $d_{in} \times d_{out}$ from a uniform distribution $\mathcal{U}[-a, a]$ whose scale $a$ is given by:

$$a = \sqrt{\frac{6}{d_{in} + d_{out}}} \tag{8}$$

This is called glorot initialization[4]. Bias terms can be initialized at a scale of 0.1.

Now write the model in terms of primitive operations:

```
xm = XMan()
xm.o1 = f.relu( f.mul(x,W) + b )
...
my_xman = xm.setup()
```

We can construct the Wengert list for any register in `my_xman` by calling `operationSequence()`.

```
wengert_list = my_xman.operationSequence(my_xman.loss)
```

Another useful method in the `XMan` class is `inputDict()`, which returns a dictionary containing default values associated with its registers. You can also overwrite these defaults by passing in keyword arguments:

```
# argument names should match register declaration
valueDict = my_xman.inputDict(x=np.random.rand(1,10)))
                               # overwrites default value of 'x'
```

## 3.3 Forward / Backward Pass

Next we need to propagate data and parameters through the Wengert list to get the outputs, and backpropagate gradients to get the updates for all parameters. The `Autograd` class in `autograd.py` provides helper functions to do this.

[4] `http://jmlr.org/proceedings/papers/v9/glorot10a/glorot10a.pdf`

```
ad = Autograd(my_xman)
valueDict = ad.eval(wengert_list, valueDict) # forward pass
gradients = ad.bprop(wengert_list, valueDict, loss=np.float_(1.))
                                               # backward pass
```

The last argument specifies gradient of the loss which will be backpropagated. `gradients` is a dictionary whose keys are register names and gradients as values. These can be used to apply updates to the parameters.

### 3.4 Gradient Checking

How do check if the our implementation is correct? One way to do that is gradient checking. Recall from calculus:

$$\frac{dJ(\theta)}{d\theta} = \lim_{\epsilon \to 0} \frac{J(\theta + \epsilon) - J(\theta - \epsilon)}{2\epsilon} \tag{9}$$

Thus for any specific value of a parameter $\theta$ we can numerically approximate the right hand side above by evaluating the output of the network at $\theta + \epsilon$ and $\theta - \epsilon$. For small $\epsilon$ the numerical gradient should match the one computed using autodiff. You can use $\epsilon = 10^{-4}$ and check if gradients match upto 3 decimal places.

## 4 Data

For this assignment you need to predict the category label of a DBPedia entity based on its title. The data format is **different** than the earlier assignments. The data contains two columns separated by tab, with the title in the first column and label in second.

```
Lloyd_Stinson   Person
Lobogenesis_centrota    Species
Loch_of_Craiglush   Place
```

We will encode entities for input to the networks by converting characters to a one-hot representation. Suppose we have a dictionary mapping each character in the data to an index `chardict = {'a':1,'b':2...}` and the total number of characters in the dataset is $V$, then we will represent `'a'` as a $V$-dimensional vector $[1, 0, 0, \ldots, 0]$, and `'b'` as another $V$-dimensional vector $[0, 1, 0, \ldots, 0]$. A string of characters will be encoded to a matrix whose each row is a $V$-dimensional vector.

For both MLP and LSTM we will fix the maximum length of an entity to $M$, longer entities will be truncated to this length, and shorter ones will be padded with white-space. We have provided you with code that preprocesses the data and divides it into minibatches in utils.py. You can,

```
from utils import *
# load data and preprocess
dp = DataPreprocessor()
data = dp.preprocess(<training_file>, <validation_file>,
       <testing_file>)
# minibatches
mb_train = MinibatchLoader(data.training, batch_size, max_len,
           len(data.chardict), len(data.labeldict))
mb_valid = MinibatchLoader(data.validation, batch_size, max_len,
           len(data.chardict), len(data.labeldict))
mb_test = MinibatchLoader(data.test, batch_size, max_len,
           len(data.chardict), len(data.labeldict))
```

`max_len` is the maximum length $M$. You can then iterate over the data using,

```
for (idxs,e,l) in mb_train:
    # idxs - ids of examples in minibatch
    # e - entities in one-hot format
    # l - corresponding output labels also in one-hot format
```

After every epoch (full sweep through `mb_train`) the data is shuffled for the next epoch. `idxs` has shape $N$, e has shape $N \times M \times V$ and l has shape $N \times C$ where $N$ is the batch size. Confirm that this makes sense to you.

For input to the MLP we will input all the one-hot encodings together to the network, so you will need to flatten `e` to a $N \times MV$ size matrix whose each row consists of the encoding of all characters in the entity concatenated together. You can use `numpy.reshape` for this.

For input to the LSTM, we will create a sequence of inputs $X_1, \ldots, X_M$ from `e`. Each of these would be a $N \times V$ matrix holding the batch inputs from time-step 1 through $M$.

To reduce the experimental load we will only use the tiny, small and smaller datasets. Again, they are in increasing size so that you can debug your code on more managable data sizes.

The data and minibatchLoader class converts the raw text in the files into first a dictionary and uses that to encode the input and the output labels into a one-hot vector format.

A validation file (*.valid files) is provided to prevent overfitting. You should evaluate the loss function on both the train and validation dataset and decide based on the loss vs number of epochs curve when you want to stop the training. Rmemeber you should not do backpropagation on the validation dataset. For reporting the results you use test (*.test) files.
You can get the data from

```
https://drive.google.com/open?id=0B58rr945j04BcGctanY1UHVFZVE
```

For the evaluation on Autolab we will run your code on a separate training and testing dataset with a specific set of params as command line arguments.

## 5 Deliverables

You majorly need to write the code for the build for the classes MLP and LSTM in mlp.py and lstm.py.

You need to write your function definitions and their derivatives in functions.py. Make sure that you call the final predicted labels as outputs and the loss function as loss. You should also remember to initialize the default parameters. Otherwise you'd get zero score on our gradient checking code. We will run your code using the command

```
python mlp.py --max_len 10 --num_hid 50
               --batch_size 16 --dataset autolab
               --epochs 0.05 --init_lr 0.05
               --output_file output
python lstm.py --max_len 10 --num_hid 50
               --batch_size 16 --dataset autolab
               --epochs 0.05 --init_lr 0.5
               --output_file output
```

We would be checking your code for gradient correctness, Mean Loss on the output, Memory and speed compared to the benchmark code written by us.

Your final output probabilities should be stored in the file specified by –output-file in npy format using np.save() in the same row order as the input test file. Tar the following files for submission.

- mlp.py (This file would contain the MLP class and the main file with the default params)
- lstm.py (This file would contain the LSTM class and the main class with the default params)
- functions.py (This file contains the function definitions and their gradients)
- Any other helper files
- report.pdf

Tar the files directly using the command below. Do NOT put the above files in a folder and then tar the folder. You do not need to upload the saved temporary files.

```
tar -cvf hw5.tar lstm.py mlp.py functions.py report.pdf
```

# 6 Questions

1. Plot the average training time per epoch for both MLP and LSTM for batch size $N = \{16, 32, 64\}$. Use default values for all other hyperparameters. What trends do you observe for the two architectures? Are they similar? Why or why not?

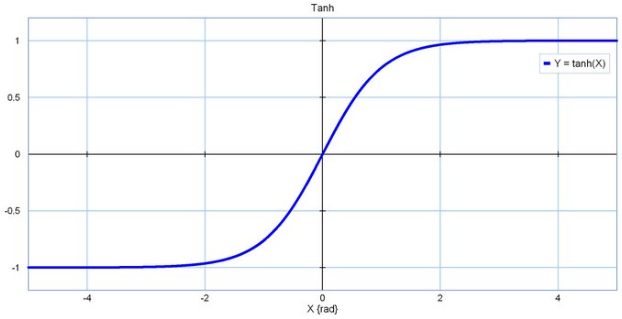
2. Plot the average training time per epoch for both MLP and LSTM for maximum input length $M = \{10, 15, 20\}$. What trends do you observe for the two architectures? Are they similar? Why or why not?

3. Given feature vectors for tokens in a query $q_1, q_2, \dots q_M$ and feature vectors for tokens in a document $d_1, d_2, \dots d_N$, where $q_i, d_j \in \mathbb{R}^n \quad \forall i, j$, the *soft-attention* distribution of $i$th query token over the document is given by:

$$\alpha_j^{(i)} = \frac{\exp q_i^T d_j}{\sum_{j'} \exp q_i^T d_{j'}} \qquad j = 1, \dots N \tag{10}$$

   Given a $M \times n$ matrix $Q$ and an $N \times n$ matrix $D$ holding all the query and document feature vectors respectively, write the steps needed to compute all the attention distributions for $i = 1, \dots M$, using only matrix operations. You can use broadcasting, and assume efficient implementaions of `row-sum` and `exp` are given.

4. Consider a single-layer MLP without bias which computes $f = \tanh(\sum_{i=1}^{1000} x_i w_i)$ where $x_i, w_i \geq 0 \quad i = 1, \ldots 1000$. Recall that $\tanh(x)$ looks like:



We initialize the weights $w_i \sim \mathcal{U}[0, a]$. Choose the scale $a$ for the following inputs:

- One-hot – $x_i = 1$ for $i = i_0$ and $x_i = 0$ for $i \neq i_0$.
- Small – $x_i \in [0, 1]$ for all $i$.
- Big – $x_i \in [1000, 1001]$ for all $i$.

# 7 Marking breakdown

- Code Correctness (gradient check)[5] - 30 points
- Code Accuracy (loss on held-out test set) - 20 points
- Code Speed and Memory usage - 20 points
- Report Questions - 30 points

[5] **Reminder** - You must name the loss register as “`loss`” for our gradient checking to work