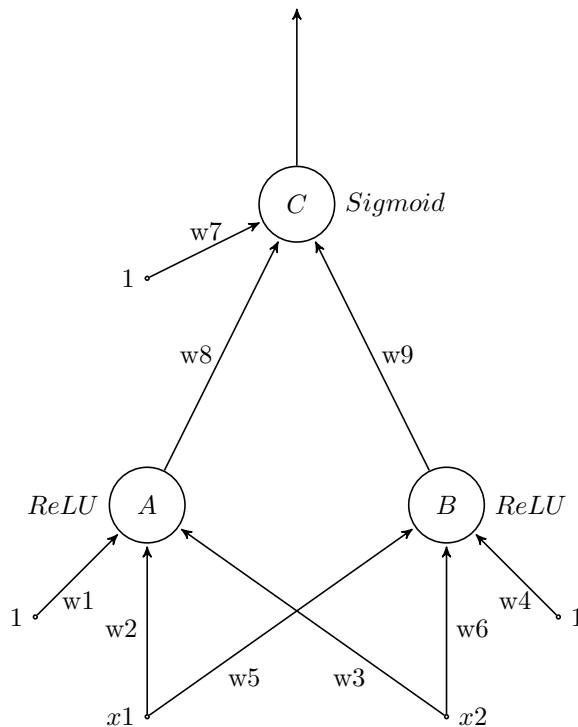# Question 1: Neural Network [100 points, evenly among parts]

We will build a neural network to perform binary classification. Each input item has two real-valued features $x = (x_1, x_2)$, and the class label y is either 0 or 1. Our neural network has a very simple structure:

There is one hidden layer with two hidden units A, B, and one output layer with a single output unit C. The input layer is fully connected to the hidden layer, and the hidden layer is fully connected to the output layer. Each unit also has a constant bias 1 input with the corresponding weight. See figure below. Units A are B are ReLU, namely

$$f_A(z) = f_B(z) = \max(z, 0).$$

Unit C is a sigmoid,

$$f_C(z) = \sigma(z) = \frac{1}{1 + e^{-z}}.$$

Write a program **Neural.java** with the following command line format:

`$java Neural FLAG [args]`

Where the optional arguments are real valued.

1. This neural network is fully defined by the nine weights $w_1, \ldots, w_9$. We will first focus on predictions *given* fixed weights.

   Remark: we will use both single index and double index to refer to a weight. Single index corresponds to the figure above. Double index, on the other hand, is used to describe the algorithm and denotes

the "from → to" nodes that the edge is connecting. For example, w_8 is the same as $w_{A,C}$, w_2 is the same as $w_{x_1,A}$, and w_1 is the same as $w_{1,A}$ where we used "1" to denote the constant bias input of one. These should be clear from the context.

Recall in a neural network for any unit j, it first collects input from lower units:

$$u_j = \sum_{i:i \to j} w_{ij} v_i$$

where v_i is the output of lower unit i. Specifically, if i is an input unit then $v_i = x_i$; if i is the bias then $v_i = 1$. The unit j then passes u_j through its nonlinear function $f_j()$ to produce its output v_j:

$$v_j = f_j(u_j).$$

When FLAG=100, arg1 ... arg9 are the weights $w_1, \ldots, w_9$, and arg10=x_1, arg11=x_2. Print $u_A, v_A, u_B, v_B, u_C, v_C$ on the same line separated by space. When printing real values, show 5 digits after decimal point by rounding (but do not round the actual variables). For example,

```
$java Neural 100 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 -1
0.00000 0.00000 0.30000 0.30000 0.97000 0.72512

$java Neural 100 1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 -0.2 1.7
2.18000 2.18000 1.43000 1.43000 1.34000 0.79249

$java Neural 100 4 3 2 1 0 -1 -2 -3 -4 -4 1
-6.00000 0.00000 0.00000 0.00000 -2.00000 0.11920
```

2. Given a training item $x = (x_1, x_2)$ and its label y, the error made by the neural network on the item is defined as
$$E = \frac{1}{2}(v_C - y)^2.$$

The partial derivative with respect to the output layer variable v_C is

$$\frac{\partial E}{\partial v_C} = v_C - y.$$

The partial derivative with respect to the intermediate variable u_C is

$$\frac{\partial E}{\partial u_C} = \frac{\partial E}{\partial v_C} f'_C(u_C).$$

Recall $f'_C(u_C) = \sigma'(u_C) = \sigma(u_C)(1 - \sigma(u_C)) = v_C(1 - v_C)$.

When FLAG=200, arg1 ... arg9 are the weights $w_1, \ldots, w_9$, arg10=x_1, arg11=x_2, and arg12=y. Print E, $\frac{\partial E}{\partial v_C}$, and $\frac{\partial E}{\partial u_C}$ on the same line separated by space. For example,

```
$java Neural 200 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 -1 1
0.03778 -0.27488 -0.05479
```

```
$java Neural 200 1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 -0.2 1.7 0
0.31402 0.79249 0.13032

$java Neural 200 4 3 2 1 0 -1 -2 -3 -4 -4 1 0
0.00710 0.11920 0.01252
```

3. The partial derivative with respect to hidden layer variable v_j is

$$\frac{\partial E}{\partial v_j} = \sum_{k:j \to k} w_{jk} \frac{\partial E}{\partial u_k}.$$

And

$$\frac{\partial E}{\partial u_j} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial u_j}.$$

Recall our hidden layer units are ReLU, for which

$$\frac{\partial v_j}{\partial u_j} = \frac{\partial \max(u_j, 0)}{\partial u_j} = \begin{cases} 1, & u_j \geq 0 \\ 0, & u_j < 0 \end{cases}$$

Note we define the derivative to be 1 when $u_j = 0$.

When FLAG=300, arg1 ... arg9 are the weights $w_1, \ldots, w_9$, arg10=x_1, arg11=x_2, and arg12=y. Print $\frac{\partial E}{\partial v_A}$, $\frac{\partial E}{\partial u_A}$, $\frac{\partial E}{\partial v_B}$, and $\frac{\partial E}{\partial u_B}$ on the same line separated by space.

```
$java Neural 300 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 -1 1
-0.04383 -0.04383 -0.04931 -0.04931

$java Neural 300 1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 -0.2 1.7 0
0.03910 0.03910 0.02606 0.02606

$java Neural 300 4 3 2 1 0 -1 -2 -3 -4 -4 1 0
-0.03755 0.00000 -0.05006 -0.05006
```

4. Now we can compute the partial derivative with respect to the edge weights:

$$\frac{\partial E}{\partial w_{ij}} = v_i \frac{\partial E}{\partial u_j}.$$

When FLAG=400, arg1 ... arg9 are the weights $w_1, \ldots, w_9$, arg10=x_1, arg11=x_2, and arg12=y. Print $\frac{\partial E}{\partial w_1}, \ldots \frac{\partial E}{\partial w_9}$ on the same line separated by space. For example,

```
$java Neural 400 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 -1 1
-0.04383 -0.04383 0.04383 -0.04931 -0.04931 0.04931 -0.05479 0.00000 -0.01644

$java Neural 400 1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 -0.2 1.7 0
0.03910 -0.00782 0.06647 0.02606 -0.00521 0.04431 0.13032 0.28411 0.18636

$java Neural 400 4 3 2 1 0 -1 -2 -3 -4 -4 1 0
0.00000 0.00000 0.00000 -0.05006 0.20025 -0.05006 0.01252 0.00000 0.00000
```

5. Now we perform one step of stochastic gradient descent. With step size η, we update the weights:

$$w_i = w_i - \eta \frac{\partial E}{\partial w_i}, \quad i = 1\ldots 9.$$

When FLAG=500, arg1 ... arg9 are the weights $w_1, \ldots, w_9$, arg10=x_1, arg11=x_2, arg12=y, and arg13=η. Print four lines:

(a) the old $w_1 \ldots w_9$

(b) the error E under the old w

(c) the updated $w_1 \ldots w_9$

(d) the error E after the update

For example,

```
$java Neural 500 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 -1 1 0.1
0.10000 0.20000 0.30000 0.40000 0.50000 0.60000 0.70000 0.80000 0.90000
0.03778
0.10438 0.20438 0.29562 0.40493 0.50493 0.59507 0.70548 0.80000 0.90164
0.03617

$java Neural 500 1 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 -0.2 1.7 0 0.1
1.00000 0.90000 0.80000 0.70000 0.60000 0.50000 0.40000 0.30000 0.20000
0.31402
0.99609 0.90078 0.79335 0.69739 0.60052 0.49557 0.38697 0.27159 0.18136
0.29972

$java Neural 500 4 3 2 1 0 -1 -2 -3 -4 -4 1 0 0.1
4.00000 3.00000 2.00000 1.00000 0.00000 -1.00000 -2.00000 -3.00000 -4.00000
0.00710
4.00000 3.00000 2.00000 1.00501 -0.02002 -0.99499 -2.00125 -3.00000 -4.00000
0.00371
```

6. Long long ago, in a galaxy far far away, 117 students took an AI class. We have a data set where x_1 is each student's score on homework 2, x_2 is their midterm score (both scaled to between 0 and 1), and the binary label y is whether they received an A at the end of semester ($y = 1$) or not ($y = 0$). We already randomly split the data set into a training set of $n = 67$ items, an evaluation set with 25 items, and a test set with 25 items. These files are denoted by the file names. We will train the neural network to predict if a student will receive an A at the end of semester.

We first define one "epoch" as going over the training items once in the natural order:

(a) FOR $j = 1$ TO n

(b) $w_i = w_i - \eta \frac{\partial E_j}{\partial w_i}, \quad i = 1\ldots 9$

(c)   PRINT w's evaluation set error

(d) END

where E_j is the error on the j-th training item. In other words, this is stochastic gradient descent (except that we go over training items in order rather than randomly, but we shall ignore the difference for now). Step (c) computes the evaluation set error as follows:

$$\sum_{k=1}^{25} \frac{1}{2}(v_C(x_k, w) - y_k)^2$$

where (x_k, y_k) is an evaluation set item, and we used the notation $v_C(x_k, w)$ to mean the neural network output when the input is x_k and the weights are w.

When FLAG=600, arg1 ... arg9 are the initial weights $w_1, \ldots, w_9$, arg10=η. Run one epoch (i.e. going over the 67 training items once). For each training item, print three lines:

(a) x_1, x_2, y

(b) the updated $w_1 \ldots w_9$

(c) the evaluation set error under the updated w

Therefore, you will print $67 * 3 = 201$ lines in total. For example,

```
$java Neural 600 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.1
0.98000 0.87000 1.00000
0.10049 0.20048 0.30043 0.40055 0.50054 0.60048 0.70062 0.80034 0.90087
7.18915
0.92000 0.88000 0.00000
0.09486 0.19530 0.29548 0.39422 0.49471 0.59491 0.69358 0.79648 0.89110
7.12401
...
0.81000 0.75000 0.00000
-0.13841 0.01138 0.16820 0.06903 0.24590 0.41273 0.22295 0.73651 0.52301
3.93300
0.94000 0.69000 0.00000
-0.13841 0.01138 0.16820 0.06135 0.23868 0.40744 0.20827 0.73651 0.51442
3.87761
```

7. We now run T epochs. For clarity, we will only print evaluation set error at the end of each epoch. When FLAG=700, arg1 ... arg9 are the initial weights $w_1, \ldots, w_9$, arg10=η, arg11=T. At the end of each epoch, print w, then on a separate line the evaluation set error.

```
$java Neural 700 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.1 3
-0.13841 0.01138 0.16820 0.06135 0.23868 0.40744 0.20827 0.73651 0.51442
3.87761
-0.15422 0.01050 0.18620 -0.10760 0.12065 0.33611 -0.14930 0.73903 0.41698
2.99174
-0.18275 0.01188 0.22380 -0.19706 0.06861 0.31792 -0.35328 0.74892 0.41936
2.71163
```

8. FLAG=800 has the same input as FLAG=700. But we will stop as soon as evaluation set error starts to increase after completing a whole epoch. If evaluation set error decreases or stays the same, we will step after T epochs. Print the number of epochs that actually happened, the final w, and the evaluation set error on different lines. Now you have a well-trained neural network. For a test item x, you can make a binary classification prediction by thresholding the network output at $1/2$ (predict positive class if the output is exactly $1/2$). Compute the test set classification accuracy (note: not the squared error) and print it, too.

```
$java Neural 800 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.1 10000
788
-3.51459 1.20379 4.45346 -2.72310 0.93258 3.44859 -3.99435 2.11219 1.63381
0.87178
0.96000

$java Neural 800 -0.8 0.5 0 -1 0 -0.7 -0.7 0.9 0.1 0.1 10000
2
-0.80000 0.50000 0.00000 -1.00000 0.00000 -0.70000 -0.65318 0.90000 0.10000
2.56847
0.72000
```