Note: intermediate steps were calculated using `numpy` and, in general, will not be shown.

1. Consider a network with three layers: 5 inputs, 3 hidden units and 2 outputs where all units use a sigmoid activation function.

(a) Initialize connection weights to 0.1 and biases to 0. Using the squared error loss, do a stochastic gradient descent update (with learning rate $\eta = 1$) for the following training example:

$$x = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \end{bmatrix}^T, \quad z = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$$

(b) Compute the MLP class for the query point $x_{new} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \end{bmatrix}^T$

As an initial note, the input amount in the input layer matches each sample's feature count, not the amount of training samples.

The Multi-Layer Perceptron (MLP) is a feed-forward neural network with one or more hidden layers between the input and output layers. To train an MLP, we need to define a loss function and optimize it using gradient descent. The loss function is a measure of how well the network performs on the training data. The goal is to minimize the loss function by adjusting the weights and biases of the network. Our training will go through a number of epochs, each one with three main phases:

(a) **Forward pass**: compute the output of the network for a given input

(b) **Backward pass**: compute the gradient of the loss function with respect to the weights and biases

(c) **Update**: update the weights and biases using the gradient

The question's statement gives us, for starters, the initial weights and biases for the network. Note that each weight matrix has j columns, one for each neuron in layer $\ell - 1$, and i lines, one for each neuron in layer ℓ. Each bias matrix has only one column, with i lines, here following the same logic as the one for the weight matrices.

$$w^{[1]} = \begin{bmatrix} 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \end{bmatrix}, \quad w^{[2]} = \begin{bmatrix} 0.1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0.1 \end{bmatrix}, \quad b^{[1]} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad b^{[2]} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

As we know, the forward propagation's successive **net** (z) and **layer output** x values are given by:

$$z^{[\ell]} = w^{[\ell]} x^{[\ell-1]} + b^{[\ell]}, \quad x^{[\ell]} = f(z^{[\ell]})$$

Here, of course, as stated in the question, we have $f(z) = \sigma(z)$, where $\sigma(z)$ is the sigmoid function. Let's start to propagate forwards:

$$z^{[1]} = w^{[1]} x^{[0]} + b^{[1]} = \begin{bmatrix} 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 0.2 \\ 0.2 \end{bmatrix}$$

$$x^{[1]} = f(z^{[1]}) = \sigma(z^{[1]}) = \begin{bmatrix} 0.549834 \\ 0.549834 \\ 0.549834 \end{bmatrix}$$

In a similar manner, we're also able to calculate both the net and the output of the second layer:

$$z^{[2]} = \begin{bmatrix} 0.16495 \\ 0.16495 \end{bmatrix}, \quad x^{[2]} = \begin{bmatrix} 0.541144 \\ 0.541144 \end{bmatrix}$$

Regarding the back pass, we need to compute the gradient of the loss function with respect to the weights and biases. The loss function is the squared error loss, which is given by $E = \frac{1}{2}\sum_{i=1}^{n}(x_i - z_i)^2$. The gradient of the loss function with respect to the weights and biases is given by:

$$\frac{\partial E}{\partial w^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}}\frac{\partial z^{[\ell]}}{\partial w^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}}(x^{[\ell-1]})^T, \quad \frac{\partial E}{\partial b^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}}\frac{\partial z^{[\ell]}}{\partial b^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}}$$

$$\frac{\partial z^{[\ell]}}{\partial w^{[\ell]}} = (x^{[l-1]})^T, \quad \frac{\partial z^{[\ell]}}{\partial b^{[\ell]}} = 1$$

Considering L as the last (output) layer:

$$\delta^{[L]} = \frac{\partial E}{\partial z^{[L]}} = \frac{\partial E}{\partial x^{[L]}} \circ \frac{\partial x^{[L]}}{\partial z^{[L]}} = \frac{\partial E}{\partial x^{[L]}} \circ f'(z^{[L]}) = (x^{[L]} - z) \circ \sigma(z^{[L]}) \circ (1 - \sigma(z^{[L]}))$$

$$\underset{l \neq L}{\delta^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}} = (\frac{\partial z^{[\ell+1]}}{\partial x^{[\ell]}})^T \delta^{[\ell+1]} \circ f'(z^{[\ell]}) = (w^{[\ell+1]})^T \delta^{[\ell+1]} \circ \sigma(z^{[\ell]}) \circ (1 - \sigma(z^{[\ell]}))$$

Note that the sigmoid function's derivative is a well known derivative, which you should know (or bring in your note sheet). Moreover, the error's derivative regarding $x^{[L]}$ is represented here without the Σ sign, since we're dealing with a single training example.

The following calculations for the updates were done using `numpy`, of course, since I'm sane:

$$\delta^{[2]} = \begin{bmatrix} -0.113937 \\ 0.13437 \end{bmatrix}, \quad \delta^{[1]} = \begin{bmatrix} 0.00050575 \\ 0.00050575 \\ 0.00050575 \end{bmatrix}$$

$$\frac{\partial E}{\partial w^{[2]}} = \delta^{[2]}(x^{[1]})^T = \begin{bmatrix} -0.0626465 & -0.0626465 & -0.0626465 \\ 0.0738812 & 0.0738812 & 0.0738812 \end{bmatrix}, \quad \frac{\partial E}{\partial b^{[2]}} = \delta^{[2]} \cdot 1 = \begin{bmatrix} -0.113937 \\ 0.13437 \end{bmatrix}$$

$$\frac{\partial E}{\partial w^{[1]}} = \delta^{[1]}(x^{[0]})^T = \begin{bmatrix} 0.00050575 & 0.00050575 & 0 & 0 & 0 \\ 0.00050575 & 0.00050575 & 0 & 0 & 0 \\ 0.00050575 & 0.00050575 & 0 & 0 & 0 \end{bmatrix}, \quad \frac{\partial E}{\partial b^{[1]}} = \delta^{[1]} = \begin{bmatrix} 0.00050575 \\ 0.00050575 \\ 0.00050575 \end{bmatrix}$$

$$w^{[2]} = w^{[2]} - \eta\frac{\partial E}{\partial w^{[2]}} = \begin{bmatrix} 0.162647 & 0.162647 & 0.162647 \\ 0.0261188 & 0.0261188 & 0.0261188 \end{bmatrix}, \quad b^{[2]} = b^{[2]} - \eta\frac{\partial E}{\partial b^{[2]}} = \begin{bmatrix} 0.113937 \\ -0.13437 \end{bmatrix}$$

$$w^{[1]} = w^{[1]} - \eta\frac{\partial E}{\partial w^{[1]}} = \begin{bmatrix} 0.0994943 & 0.0994943 & 0.1 & 0.1 & 0.1 \\ 0.0994943 & 0.0994943 & 0.1 & 0.1 & 0.1 \\ 0.0994943 & 0.0994943 & 0.1 & 0.1 & 0.1 \end{bmatrix}, \quad b^{[1]} = b^{[1]} - \eta\frac{\partial E}{\partial b^{[1]}} = \begin{bmatrix} -0.00050575 \\ -0.00050575 \\ -0.00050575 \end{bmatrix}$$

The second section of the exercise asks us to compute the MLP class for a sample $x_{new} = \begin{bmatrix}1 & 0 & 0 & 0 & 1\end{bmatrix}^T$. As such, we'll want to calculate the MLP's output for this sample, $x^{[2]}_{new}$ (considering the newly updated weights and biases). We'll only need to perform a forward pass, of course:

$$z^{[1]} = w^{[1]}x_{new} + b^{[1]} = \begin{bmatrix}0.198989\\0.198989\\0.198989\end{bmatrix}, \quad x^{[1]} = \sigma(z^{[1]}) = \begin{bmatrix}0.549584\\0.549584\\0.549584\end{bmatrix}$$

$$z^{[2]} = w^{[2]}x^{[1]} + b^{[2]} = \begin{bmatrix}0.382101\\-0.0913066\end{bmatrix}, \quad x^{[2]} = \sigma(z^{[2]}) = \begin{bmatrix}0.59438\\0.477189\end{bmatrix}$$

The MLP classifies the sample as belonging to the first class, since it matches $\text{argmax}(x^{[2]}_{new})$.

2. Consider a network with four layers: 4, 4, 3 and 3 neurons, respectively. where all units use a hyperbolic tangent activation function.

(a) Initialize connection weights and biases to 0.1. Using the squared error loss, do a stochastic gradient descent update (with learning rate $\eta = 1$) for the following training example:

$$x = \begin{bmatrix}1 & 0 & 1 & 0\end{bmatrix}^T, \quad z = \begin{bmatrix}0 & 1 & 0\end{bmatrix}^T$$

(b) Reusing the computation from the previous exercise, do a gradient descent update (with $\eta = 0.1$) for the batch with the training example from a) and the following:

$$x = \begin{bmatrix}0 & 0 & 10 & 0\end{bmatrix}^T, \quad z = \begin{bmatrix}0 & 0 & 1\end{bmatrix}^T$$

A batch gradient descent update is essentially the joint update of all the singular stochastic gradient descent updates, for each training sample. Therefore, there are two main ways to compute this kind of update: the *vanilla* way, where we simply sum the updates for each training sample, and the *vectorized* way, where all the computations are done at the same time via matrix operations - here, instead of summing the updates, we'll simply have both nets and layer outputs containing one column per training sample. Since the former way would be a bit boring (and is in the teacher's solutions), we'll go with the latter.

Combining the two training examples, we'll have the following $x^{[0]}$ (plus the targets and weight/bias matrices):

$$x^{[0]} = \begin{bmatrix}1 & 0 & 1 & 0\\0 & 0 & 10 & 0\end{bmatrix}^T, \quad z = \begin{bmatrix}0 & 1 & 0\\0 & 0 & 1\end{bmatrix}^T$$

$$w^{[1]} = \begin{bmatrix}0.1 & 0.1 & 0.1 & 0.1\\0.1 & 0.1 & 0.1 & 0.1\\0.1 & 0.1 & 0.1 & 0.1\\0.1 & 0.1 & 0.1 & 0.1\end{bmatrix}, \quad b^{[1]} = \begin{bmatrix}0\\0\\0\\0\end{bmatrix}, \cdots, w^{[3]} = \begin{bmatrix}0.1 & 0.1 & 0.1\\0.1 & 0.1 & 0.1\\0.1 & 0.1 & 0.1\end{bmatrix}, \quad b^{[3]} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

The forward pass is the exact same as before; note, of course, that if we were calculating each net/layer output for each training sample separately, each column would be the result of a forward pass for a single training sample. Note, in the net update equations, that the matrix sums are actually column-wise sums.

$$z^{[1]} = w^{[1]}x^{[0]} + b^{[1]} = \begin{bmatrix} 0.2 & 1 \\ 0.2 & 1 \\ 0.2 & 1 \\ 0.2 & 1 \end{bmatrix}, \quad x^{[1]} = \tanh(z^{[1]}) = \begin{bmatrix} 0.197375 & 0.761594 \\ 0.197375 & 0.761594 \\ 0.197375 & 0.761594 \\ 0.197375 & 0.761594 \end{bmatrix}$$

$$z^{[2]} = w^{[2]}x^{[1]} + b^{[2]} = \begin{bmatrix} 0.0789501 & 0.304638 \\ 0.0789501 & 0.304638 \\ 0.0789501 & 0.304638 \end{bmatrix}, \quad x^{[2]} = \tanh(z^{[2]}) = \begin{bmatrix} 0.0787865 & 0.295551 \\ 0.0787865 & 0.295551 \\ 0.0787865 & 0.295551 \end{bmatrix}$$

$$z^{[3]} = w^{[3]}x^{[2]} + b^{[3]} = \begin{bmatrix} 0.0236359 & 0.0886653 \\ 0.0236359 & 0.0886653 \\ 0.0236359 & 0.0886653 \end{bmatrix}, \quad x^{[3]} = \tanh(z^{[3]}) = \begin{bmatrix} 0.0236316 & 0.0884337 \\ 0.0236316 & 0.0884337 \\ 0.0236316 & 0.0884337 \end{bmatrix}$$

After having finished the forward pass, we can start computing the gradient of the loss function with respect to the weights and biases. For starters, it'll be worth noting that $f'(z) = 1 - \tanh^2(z)$, another common activation function derivative.

$$\delta^{[L]} = \frac{\partial E}{\partial z^{[L]}} = \frac{\partial E}{\partial x^{[L]}} \circ \frac{\partial x^{[L]}}{\partial z^{[L]}} = \frac{\partial E}{\partial x^{[L]}} \circ f'(z^{[L]}) = (x^{[L]} - z) \circ (1 - \tanh^2(z^{[L]}))$$

$$\underset{l \neq L}{\delta^{[\ell]}} = \frac{\partial E}{\partial z^{[\ell]}} = (\frac{\partial z^{[\ell+1]}}{\partial x^{[\ell]}})^T \delta^{[\ell+1]} \circ f'(z^{[\ell]}) = (w^{[\ell+1]})^T \delta^{[\ell+1]} \circ (1 - \tanh^2(z^{[\ell]}))$$

$$\delta^{[3]} = \begin{bmatrix} 0.0236183 & 0.0877421 \\ -0.975823 & 0.0877421 \\ 0.0236183 & -0.904437 \end{bmatrix}, \quad \delta^{[2]} = \begin{bmatrix} -0.0922822 & -0.0665279 \\ -0.0922822 & -0.0665279 \\ -0.0922822 & -0.0665279 \end{bmatrix}, \quad \delta^{[1]} = \begin{bmatrix} -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \end{bmatrix}$$

Now, we can compute the gradient of the loss function with respect to the weights and biases (the update step).

$$\frac{\partial E}{\partial w^{[3]}} = \delta^{[3]} x^{[2]T} = \begin{bmatrix} 0.0277931 & 0.0277931 & 0.0277931 \\ -0.0509494 & -0.0509494 & -0.0509494 \\ -0.265447 & -0.265447 & -0.265447 \end{bmatrix}, \quad \frac{\partial E}{\partial b^{[3]}} = \delta^{[3]} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.0236183 & 0.0877421 \\ -0.975823 & 0.0877421 \\ 0.0236183 & -0.904437 \end{bmatrix}$$

$$\frac{\partial E}{\partial w^{[2]}} = \begin{bmatrix} -0.0688815 & -0.0688815 & -0.0688815 & -0.0688815 \\ -0.0688815 & -0.0688815 & -0.0688815 & -0.0688815 \\ -0.0688815 & -0.0688815 & -0.0688815 & -0.0688815 \end{bmatrix}, \quad \frac{\partial E}{\partial b^{[2]}} = \begin{bmatrix} -0.0922822 & -0.0665279 \\ -0.0922822 & -0.0665279 \\ -0.0922822 & -0.0665279 \end{bmatrix}$$

$$\frac{\partial E}{\partial w^{[1]}} = \begin{bmatrix} -0.0266062 & 0 & -0.110426 & 0 \\ -0.0266062 & 0 & -0.110426 & 0 \\ -0.0266062 & 0 & -0.110426 & 0 \\ -0.0266062 & 0 & -0.110426 & 0 \end{bmatrix}, \quad \frac{\partial E}{\partial b^{[1]}} = \begin{bmatrix} -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \\ -0.0266062 & -0.008382 \end{bmatrix}$$

We're now in position to update the weights and biases.

$$w^{[3]} = w^{[3]} - \eta \frac{\partial E}{\partial w^{[3]}} = \begin{bmatrix} 0.0972207 & 0.0972207 & 0.0972207 \\ 0.105095 & 0.105095 & 0.105095 \\ 0.126545 & 0.126545 & 0.126545 \end{bmatrix}, \quad b^{[3]} = \begin{bmatrix} -0.00236184 & -0.00877421 \\ 0.0975823 & -0.00877421 \\ -0.00236184 & 0.0904437 \end{bmatrix}$$

$$w^{[2]} = \begin{bmatrix} 0.106888 & 0.106888 & 0.106888 & 0.106888 \\ 0.106888 & 0.106888 & 0.106888 & 0.106888 \\ 0.106888 & 0.106888 & 0.106888 & 0.106888 \end{bmatrix}, \quad b^{[2]} = \begin{bmatrix} 0.00922822 & 0.00665279 \\ 0.00922822 & 0.00665279 \\ 0.00922822 & 0.00665279 \end{bmatrix}$$

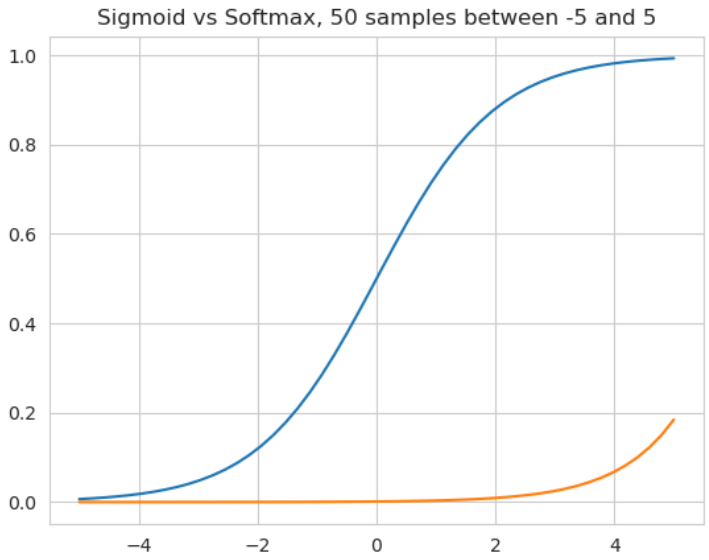
$$w^{[1]} = \begin{bmatrix} 0.102661 & 0.1 & 0.111043 & 0.1 \\ 0.102661 & 0.1 & 0.111043 & 0.1 \\ 0.102661 & 0.1 & 0.111043 & 0.1 \\ 0.102661 & 0.1 & 0.111043 & 0.1 \end{bmatrix}, \quad b^{[1]} = \begin{bmatrix} 0.00266062 & 0.0008382 \\ 0.00266062 & 0.0008382 \\ 0.00266062 & 0.0008382 \\ 0.00266062 & 0.0008382 \end{bmatrix}$$

3. Repeat the exact same exercise, but this time the **output units** have a softmax activation function, while the **error function** is now the cross-entropy loss function. What are the major differences between using squared error and cross-entropy?

The softmax activation function aims to scale numbers into probabilities: it's usually present in the output layer of a neural network, transforming the last layer's nets into a vector of probabilities. The softmax function is defined as follows (once again, write the derivative on your note sheet):

$$\text{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{n} \exp(z_j)}, \quad \frac{\partial \text{s}(z_i)}{\partial z_j} = \begin{cases} \text{s}(z_i) \cdot (1 - \text{s}(z_i)), & i = j \\ -\text{s}(z_i) \cdot \text{s}(z_j), & i \neq j \end{cases}$$

Even though the sigmoid's plot is, generally speaking, similar to the softmax's one, the two functions are not the same: for a given layer, the sum of the softmax's outputs is always equal to 1 (hence the notion of vectorizing probabilities), while the sigmoid sum does not have such restrictions.



Whenever we utilize the softmax activation function, we'll usually use the cross-entropy loss function, which is defined as follows:

$$E = -\sum_{i=1}^{n} z_i \log \hat{z}_i$$

The cross-entropy loss function essentially measures the distance between what the network thinks the output should be and what it actually is. We utilize it with the softmax activation function since our predictions actually represent probabilities (i.e they sum to 1). Here, the softmax should (ideally) perform better than the SSE, since it's more suited to the task at hand - SSE is more suited to regression problems.

Regarding the forward pass, here we can re-utilize every calculation from the previous exercise up until activating the last net: here, the activation function is the softmax, so we'll have to compute the softmax of the last net.

$$x^{[3]} = \text{softmax}(z^{[3]}) = \begin{bmatrix} 0.333333 & 0.333333 \\ 0.333333 & 0.333333 \\ 0.333333 & 0.333333 \end{bmatrix}$$

We'll need, now, to compute the error function's derivative with respect to both the weights and the biases. We'll start with the last layer's weights and biases.

$$\delta^{[3]} = \frac{\partial E}{\partial z^{[3]}} = \cdots = x^{[3]} - z = \begin{bmatrix} 0.333333 & 0.333333 \\ -0.666667 & 0.333333 \\ 0.333333 & -0.666667 \end{bmatrix}$$

$$\delta^{[2]} = (w^{[3]})^T \delta^{[3]} \circ \text{s'}(z^{[2]}) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \circ \text{s'}(z^{[2]}) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\delta^{[1]} = (w^{[2]})^T \delta^{[2]} \circ \text{s'}(z^{[1]}) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \circ \text{s'}(z^{[1]}) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

With $\delta^{[2]}$ and $\delta^{[1]}$ being the zero matrices, both weights and biases for their respective layers will not be updated (since the error's derivative with respect to them will be 0). Regarding the last layer's weights and biases, though:

$$\frac{\partial E}{\partial w^{[3]}} = \delta^{[3]} (x^{[2]})^T = \begin{bmatrix} 0.124779 & 0.124779 & 0.124779 \\ 0.0459927 & 0.0459927 & 0.0459927 \\ -0.170772 & -0.170772 & -0.170772 \end{bmatrix}$$

$$\frac{\partial E}{\partial b^{[3]}} = \delta^{[3]} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0.333333 & 0.333333 \\ -0.666667 & 0.333333 \\ 0.333333 & -0.666667 \end{bmatrix}$$

We're now in position to update the weights and biases (these calculations were performed for both samples instead of for only the first one, hence the different results in comparison with the teacher's solutions):

$$w^{[3]} = \begin{bmatrix} 0.0875221 & 0.0875221 & 0.0875221 \\ 0.0954007 & 0.0954007 & 0.0954007 \\ 0.117077 & 0.117077 & 0.117077 \end{bmatrix}, \quad b^{[3]} = \begin{bmatrix} -0.0333333 & -0.0333333 \\ 0.0666667 & -0.0333333 \\ -0.0333333 & 0.0666667 \end{bmatrix}$$