UNIVERSITY COLLEGE LONDON
DEPARTMENT OF SPACE AND CLIMATE PHYSICS

Candidate Code: HYXC3

Programme Title: MSc Scientific Computing

Module Code: SPCE0038

Module Title: Machine Learning with Big Data

End Assessment

In submitting this coursework, I assert that the work presented is entirely my own except where properly marked and cited.

Date of Submission:	11/05/20

Question 1

1(a)

With reference to the diagram of the basic *logistic unit* on the following page:

The input vector $\mathbf{x}$ is the input to the *logistic unit*.

Each input x_i has an associated weight θ_i. The weights are set to a random value prior to *training*. The *training* process determines these weights.

The product of each input x_i and weight θ_i is summed to produce a weighted sum z.

The output, $h_\theta(x)$, is the the non-linear *activation function*, h, applied to z.

1(b)

Consider the diagram of Question 1(a).

The weighted sum of the inputs, z, is:

$$z = \sum_{j=1}^{n} \theta_j x_j = \theta^T x \tag{1}$$

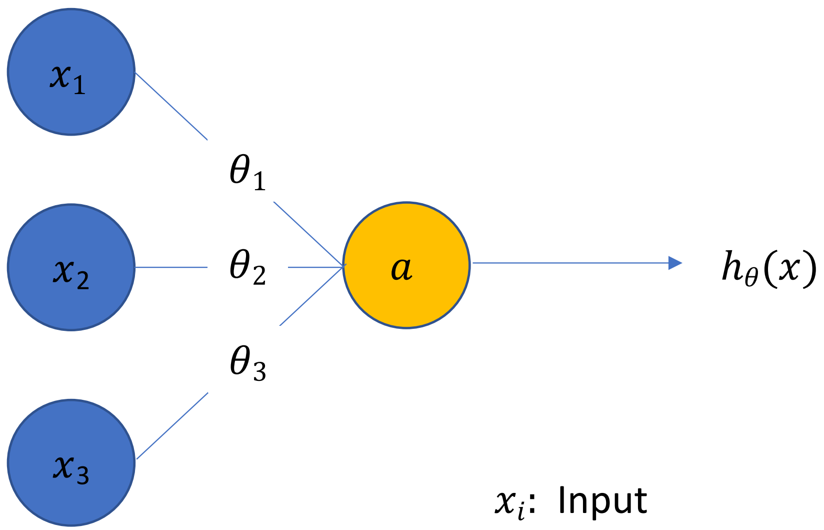
where x_i is the i^{th} element of input vector $\mathbf{x}$ of length n, and θ_i is the associated *weight*.

And, the output from the *logistic unit*, $h_\theta(x)$, is:

$$h_\theta(x) = h(z) \tag{2}$$

where h is a non-linear *activation function*.

Question 1(a) – Basic Logistic Unit



x_i: Input

θ_i: Weight

Weighted Sum: $z = \sum_{j=1}^{n} \theta_j x_j = \theta^T x$

Activation: $a = h(z)$

1(c)

See diagram on following page.

1(d)

Consider the diagram of Question 1(c).

Firstly, consider the data transformation from the input vector $\mathbf{x}$ to the hidden layer. We now need two indices, one for the input vector elements, and one for the *hidden layer* nodes. We will use i for the input vector index, and j for the *hidden layer* nodes.

The weighted sum of the inputs at the j^{th} *hidden layer* node is:

$$z_j = \sum_{i=1}^{n} \theta_{ij} x_i \tag{3}$$

where θ_{ij} is the weight between input element i and *hidden layer* node j, and n is the length of the input vector $\mathbf{x}$.

Secondly, the output from each *hidden layer* node is the non-linear *activation function*, h, applied to each z_j:

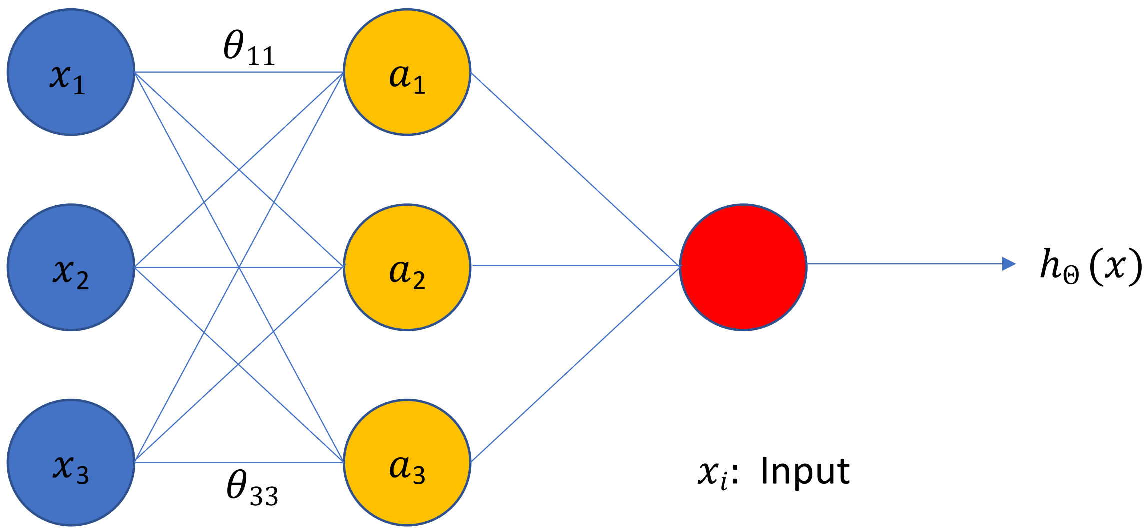
$$h_{\theta j}(x) = h(z_j) \tag{4}$$

And finally, the output from the whole network, $h_{\Theta}(x)$ is the sum of the *hidden layer* outputs:

$$h_{\Theta}(x) = \sum_{j=1}^{m} h_{\theta j}(x) \tag{5}$$

where m is the number of *hidden layer* nodes.

Question 1(c) – Fully Connected, Feed Forward, Artificial Neural Network



x_i: Input

θ_{ij}: Weight, e.g. $\theta_{11}\,\theta_{33}$

Weighted Sums: $z_j = \sum_{i=1}^{n} \theta_{ij} x_i$

Activations: $a_j = h(z_j)$

Input Layer Logistic Units

Hidden Layer Logistic Units

Output Node

1(e)

The cost function typically used to train neural networks for regression problems is *mean square error*:

$$MSE(\Theta) = \frac{1}{m} \sum_i \sum_j (p_j^{(i)} - y_j^{(i)})^2 \tag{6}$$

The cost function typically used to train neural networks for classification problems is *cross-entropy*:

$$C(\Theta) = -\frac{1}{m} \sum_i \sum_j y_j^{(i)} \log(p_j^{(i)}) \tag{7}$$

1(f)

Artificial Neural Networks (ANNs) are described as *shallow* or *deep*, and *wide* or *narrow*. *shallow* or *deep* refers to the number of layers in the network, and *wide* or *narrow* refers to the number of nodes in each layer.

The *credit assignment path*, the CAP, of a neural network is a measure of the number of data transformations that occur as data passes through the network. For *feed-forward* networks the CAP is the number of *hidden layers* plus one.

A *deep* neural network is generally considered to be a network with multiple layers and a CAP > 2.

1(g)

The *universal approximation theorem* states that, with appropriate parameters, single hidden layer feed-forward neural networks are *universal approximators*. This means they can represent any continuous function. However, this requires an exponentially larger number of hidden layer nodes. And, training will not necessarily determine the parameters.

Deep networks provide a powerful representational framework because they have the potential to be *universal approximators*, but with a limited width of hidden nodes. This makes the implementation of *universal approximators* more feasible.

Question 2

2(a)

Gradient Descent algorithms attempt to find the parameters θ which minimise the cost function $C(\theta)$ over the *training set* using an iterative process:

$$\theta^{i+1} = \theta^i - \alpha \nabla_\theta C(\theta) \tag{8}$$

where α is the *learning rate*.

Batch Gradient Descent uses the entire *training set* at each iteration to calculate the gradient partial derivatives, $\nabla_\theta C(\theta)$. This produces accurate values for the partial derivatives, but is potentially slow for large *training sets*.

Stochastic Gradient Descent uses a random sub-set of the *training set* at each iteration to calculate the gradient partial derivatives, $\nabla_\theta C(\theta)$. This is faster than *Batch Gradient Descent*, but can produce erratic values for the partial derivatives.

For *convex* cost functions *Batch Gradient Descent* will always converge to the *local minima* which is also the *global minima*. This is not the case for *non-convex* cost functions, where *local minima* are not necessarily *global minima*. A bad choice of θ^0 may result in *Batch Gradient Descent* getting "stuck" in a *local minima*. Because the gradient partial derivatives of *Stochastic Gradient Descent* are erratic, this provides a mechanism of "jumping out of" a *local minima* and improves the probability of finding the *global minima*.

2(b)

When attempting to find the minimum of a cost function using *Stochastic Gradient Descent*, the iterative process "jumps" around the minimum, and it is difficult to determine when a minimum has been reached. For this reason alternative optimisation algorithms are typically considered for training.

2(c)

Consider the iterative minimisation process:

$$\theta^{i+1} = \theta^i - \alpha \nabla_\theta C(\theta) \tag{9}$$

where α is the *learning rate*.

At each step the process "advances" towards the minimum by the step size $-\alpha \nabla_\theta C(\theta)$, which uses the *current* gradient.

The *Momentum Optimisation* algorithm introduces the idea of including *previous* gradients into the step size. At each step the *current* gradient is summed into a momentum term m, which includes *previous* gradients (remember we use the negative gradient):

$$m^{i+1} = \beta m^i - \alpha \nabla_\theta C(\theta) \tag{10}$$

The β parameter is used to prevent the momentum getting too large, and is set between 0 and 1, typically 0.9.

The momentum m is then used to update θ:

$$\theta^{i+1} = \theta^i + m \tag{11}$$

The result is that we now have an *acceleration* towards the minimum.

This algorithm may result in an overshoot and oscillation before stabilising at the minimum.

2(d)

Consider the momentum update equation of the *Momentum Optimisation* algorithm:

$$m^{i+1} = \beta m^i - \alpha \nabla_\theta C(\theta) \tag{12}$$

This uses the gradient at the current value of θ.

However, the momentum m is pointing in the general direction of the cost function minimum, so it makes sense to use a point further along in this direction, $\theta + \beta m^i$, to calculate the gradient, as this will be already closer to the minimum:

$$m^{i+1} = \beta m^i - \alpha \nabla_\theta C(\theta + \beta m^i) \tag{13}$$

This is called the *Nesterov Accelerated Gradient* algorithm.

θ is updated as per the *Momentum Optimisation* algorithm:

$$\theta^{i+1} = \theta^i + m \tag{14}$$

The *Nesterov Accelerated Gradient* algorithm is an enhancement to the *Momentum Optimisation* algorithm, which can result in a significant increase in speed, and can reduce the overshoot and oscillations previously mentioned.

2(e)

For optimisation problems where the *objective function* has circular contours the negative gradient always points towards the *objective function* minimum. This means that for an iterative process such as *Gradient Descent* the steps are always in the direction of the minimum. This produces swift convergence to the minimum.

For an elongated *objective function*, with steep sides, a narrow valley, and a bend in the valley, the negative gradient will not point towards the *objective function* minimum if the current value of θ is at the opposite end of the valley. Large steps will be taken offset from the minimum direction. This will reduce the convergence rate. And where the negative gradient is the steepest is where the largest offset steps will be taken. This phenomena is observed for *objective functions* with non-circular contours.

The *AdaGrad* algorithm addresses this problem by reducing the learning rate where the negative gradient is steepest. This reduces the step size away from the minima. Where the negative gradient is less steep the *learning rate* is reduced by a lesser amount, preserving the step size towards the minimum.

The *AdaGrad* algorithm uses what is called an *adaptive learning rate*. An advantage of this during *training* is that less tuning of the learning rate α is required, as this is now "self-tuning".

There is a danger though that the *learning rate* will be reduced too much, and the minimisation process comes to a stop before reaching the minimum. This is the reason why *AdaGrad* is not generally used to train deep *neural networks*.

2(f)

2(g)

2(h)

Question 3

3(a)

TODO

3(b)

TODO

3(c)

TODO

3(d)

TODO

3(e)

TODO

3(f)

TODO

Question 4

4(a)

TODO

4(b)

TODO

4(c)

TODO

4(d)

TODO

4(e)

TODO

4(f)

TODO

question_4f

May 7, 2020

[ ]:
```
# Fetch batch function:

def fetch_batch(epoch, batch_index, batch_size):

    return X_batch, y_batch


# Set up computational graph:

import tensorflow as tf
reset_graph ()

n_epochs = 1000
learning_rate = 0.01

X = tf.constant(scaled_housing_data_plus_bias, dtype=tf.float32, name="X")
y = tf.constant(housing_data_target, dtype=tf.float32, name="y")

theta = tf.Variable(tf.random_uniform([n + 1, 1], -1.0, 1.0), name="theta")
y_pred = tf .matmul(X, theta , name="predictions")
error = y_pred - y
mse = tf.reduce_mean(tf.square(error), name="mse")
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
training_op = optimizer.minimize(mse)


# Execute:

init = tf.global_variables_initializer()

with
tf.Session() as sess:
    sess.run(init)
    for epoch in range(n_epochs):
        if epoch % 100 == 0:
            print("Epoch", epoch, "MSE=", mse.eval()) sess.run(training_op)
    best_theta = theta.eval()
```

```python
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```

Listing 1: Question 4f

Question 5

5(a)

TODO

5(b)

TODO

5(c)

TODO

5(d)

TODO

5(e)

TODO

5(f)

TODO