Practical Machine Learning

Guidelines and Submission Instructions:

1. This project is worth 50% of your overall module grade. You should produce **.py file(s)** containing all your code and a project **document** detailing your findings.

2. Upload your report document and your solution python files (**.py files**) as a single .zip file before **23:59 on Sunday Nov 14th**. Please make sure you following the naming scheme specified in the instructions below.

   Please note that Jupyter notebooks are also accepted instead of .py files. However, if you are using Jupyter notebooks then you must still submit the report document separately as specified below.

3. Go to the "Assignment 1" unit on Canvas to upload your file(s).

4. It is your responsibility to make sure you upload the correct files.

5. Please make sure you **fully comment your code**. You should clearly explain the operation of important lines of code.

6. Please note that marks are awarded for code that is efficient with minimum duplication.

7. You should use **NumPy** where possible throughout the assignment. Marks are awarded for the use of NumPy where possible and appropriate. Aside from NumPy you should be using core Python to solve the problems listed below. The use of any high-level toolkit such as Scikit-Learn or high level functions are **not permitted** (except where otherwise stated).

8. Late submissions will be penalized.

   If you submit the assignment after the deadline but within 7 days, 10% will be deducted from your final grade.

   If you submit the assignment more than 7 days after the deadline but within14 days, a 20% penalty will be deducted.

   A grade of 0% will be given to any assignment submitted more than 14 days after the assignment deadline.

9. The data for this assignment can be found in Data.zip in the "Assignment 1" unit on Canvas. Please download and unzip this file. Once the file in unzipped you will see it contains two folders.

   The first is called classification and the second is called clustering. The classification folder contains a training set and a test set. The data in the clustering folder just contains just a single feature dataset. The classification data will be used for Part 1 and the clustering data will be used for Part 2 below.

10. There is a zero-tolerance policy with regards plagiarism. Software is used to detect any plagiarism that may be present in either your submitted document or in your code. CIT policy covering academic honestly and plagiarism can be found here. Any sources used should be clearly cited and referenced. Any plagiarism detected will result in a grade of 0% for the assignment.

11. A discussion forum will be maintained where you can ask assignment related questions. It is very important that you **do not share any code** or refer in any way to the **methodology you are using for solving the problems** outlined below. If you are not fully clear on what is being asked in any part of the questions below you can look for clarification by submitting your question to the discussion forum.

The marks for this assignment will be distributed as follows:

- Part 1: k-NN Algorithm for Classification **(50%)**
- Part 2: KMeans Clustering **(50%)**

Part 1 – Distance Weighted Nearest Neighbour Algorithm for Classification (50 Marks)

You should use the training and test file from the **classification folder** in data.zip for Part 1.

In the classification folder you will find a training and test csv file. There are 20 features in the dataset. There are 8000 instances in the training set and 2000 instances in the test dataset. It is a 4 class classification problem and the target classification value is the final column in each dataset (21th column). There each data contains in total 21 columns, the first 20 correspond to the features and the final corresponds to the target class.

Part 1(A) – Development of Distance Weighted k Nearest Neighbour Algorithm for Classification (25 Marks)

Your objective is to build (from the ground up) a distance weighted k-NN classification algorithm.

As already mentioned, you **should not be using imported functionality** from Scikit Learn (or similar packages) for implementing the kNN (or the evaluation metrics) but should instead implement it in core Python and NumPy.

As part of the code for your k-NN implementation you should include the following:

1. A function called *minkowski_distance*. The primary objective of this function is to calculate the distances between a single query point in feature space and a collection of other data points in feature space (your training instances). The distance formula you should use is the Minkowski distance metric discussed in lectures.

$$d(p,\ q) = \ (\sum_{i=1}^{n} |p_i - \ q_i|^a)^{\frac{1}{a}}$$

   The function *minkowski_distance* should accept as arguments: (i) A single 2D NumPy array containing all the feature data, (ii) A single 1D NumPy array, containing a single query instance and (iii) an integer value specifying the value for the exponent hyper-parameter denoted *a* in the above equation. Please note that the use of 'for loops' in this function will significantly slow down the algorithm. Using NumPy it is possible to implement this function without for loops (Hint: NumPy broadcasting makes this very eary).

   Also, you should not implement the Minkowski distance function using any high-level functions. You should only be using basic NumPy operations such as summation, subtraction etc (you should not be using higher level functions such as numpy.linalg.norm).

The function should return a NumPy array containing the calculated distances from the query point to each of the individual feature instances instances.

2. A function called *predict_class* that will accept the following arguments: (i) A single 2D NumPy array containing all the feature training data, (ii) A single ID NumPy array containing the training class labels (iii) A single 1D NumPy array, containing a single query instance (iv) an integer value specifying the value for the hyper-parameter (denoted *a* in the above equation) and (v) an integer specifying the value of the hyper-parameter *k* (which denotes the number of nearest neighbours). The function should return the predicted class value for the query instance (This function will need to call the *minkowski_distance* function. You may also may find np.argsort useful when coding this function).

3. A function called *calculate_accuracy*, which will take in two NumPy arrays. The first array will contain the true target classification value for all test instances and the second array will contain the predicted class values (predicted by your model) for each test instance. The function should calculate the overall accuracy performance of your model and the accuracy performance for each class.

Include a copy of the above 3 functions in your **report document**. Once you have completed your implementation include the accuracy output achieved by the model for *k=3* and *a=1* into your report document.

Checklist for Part 1(A)

Your **report** should contain the following:

- The accuracy performance values for *k=3* and *a=1*
- Your implementation of the function *minkowski_distance* along with an accompanying written explanation of the code.
- Your implementation of the function *predict_class* along with accompanying written explanation.
- Your implementation of the function *calculate_accuracy* along with accompanying written explanation.

It should be very clear from each of your explanations above that you fully understand the associated code.

Your submitted zip file should contain the full code entitled Part1A.py (If you are using Jupyter notebooks that you name your notebook PartA).

Please note a failure to include the above material in your written report (or a failure to include these functions as named and described above in your code) will incur a significant penalty. Submissions that contain only Jupyter notebooks without an accompanying report containing the above-mentioned elements will not be accepted.

Part 1(B) – Parameters/Techniques Impact Model Performance (25 Marks)

(i) "*By default, a k-NN algorithm will weigh the contribution of each feature equally when using standard Euclidean distance*". In your report clearly explain your understanding of this statement (explain why this is the case and how it could negatively impact the performance of your k-NN model).

Research and present a range of possible methods for tackling this issue in your report. Incorporate one of these methods into your code and assess the impact.

Please take note of the following two points:

• To score well in this section you should expand your research beyond any of the content presented in the lecture notes and support your answer with references where possible. You should clearly explain all techniques presented.

• Incorporate one of these methods in your code and present the results. Please note **it is acceptable to use a high-level toolkit for this section**. **This is only applicable to Part 1 (B) (i).**

(ii) Aside from the above there are a range of other techniques/parameters that you can investigate that could potentially impact the performance of k-NN classification algorithm. Describe the set of techniques/parameters and why they may potentially impact the performance of a kNN.

Select one of these technique/parameters and investigate its impact on the performance of your model.

Checklist for Part 1(B)

Your report should contain the following:

- Your understanding of the statement "*By default, a k-NN algorithm will weigh the contribution of each feature equally when using standard Euclidean distance*" along with potential impact on kNN.
- A detailed account of the research you undertook into a range of possible methods for addressing this problem.
- A detailed description and assessment of the impact of incorporating one of these researched techniques.
- List and describe the techniques/parameters that can potentially impact the performance of a kNN.
- Assessment of one selected technique/parameter on your model performance.

Your submitted zip file should contain the full code entitled Part1B.py (Please note if you are using Jupyter notebooks that you name your notebook Part1B). **I will not accept submissions that contain just Jupyter notebooks without an accompanying report containing the above-mentioned elements.**

Part 2 – Development of KMeans Clustering Algorithm (50 Marks)

You should use the feature dataset from the **clustering folder** in data.zip for Part 2.

In the cluster folder you will find a csv file containing just feature data. There are 6 features in the dataset. There are 800,000 instances.

Part 2(A) – Development of a KMeans Clustering Algorithm (20 Marks)

The objective of this section is to develop a random restart KMeans clustering algorithm using Python and NumPy. As already mentioned, you should only use NumPy and Python in your code (no high-level API such as Scikit Learn).

The KMeans algorithm you develop should reuse the *minkowski_distance* function from Part 1.

Your solution should contain the following functions:

1. A function called *initalize_centroids* that will take in as arguments the feature data and the number of centroids (an integer which we will call k). The function will randomly select k feature instances (k rows of the dataset) and return these as the initial centroids

(the k centroids should be returned as a single array). Please include a short paragraph in your report to explain the code in your own words.

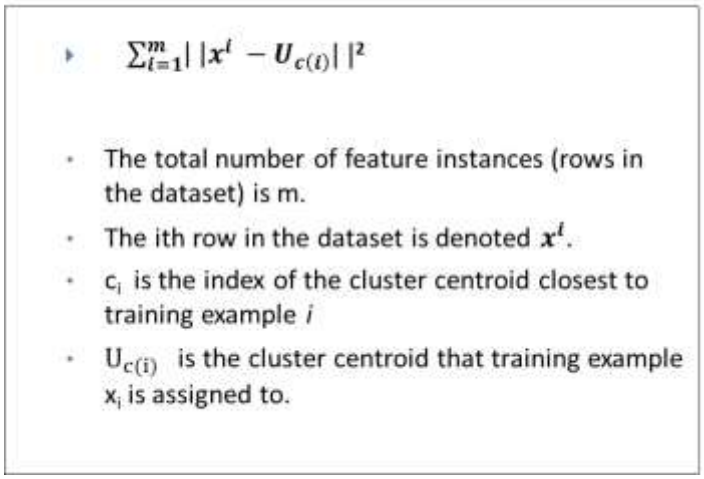
2. A function called *assign_centroids*, which will take in as arguments the feature data and the current array of centroids. This function should calculate the distance between each centroid and all feature data instances (each of the rows in the dataset). It should return the centroid index that is closest to each individual feature instance.

   In other words, if we have 3 centroids and 10 feature instances (10 rows in our data set) then this function calculates the distance between each of the 3 centroids and the 10 rows in the dataset. It will then return an array containing 10 integer index values. The first integer value in the array indicates the index of the centroid to which the first feature instance (first row in dataset) is closest. The second integer value in the array indicates the index of the centroid to which the second feature instance is closest and so on.

   So in the example above, if *assign_centroids* was to return the following array [**2**, **0**, **1**, 1, 2, 0, 0, 1, 1, 0] this would mean that the first feature instance is closest to the 3rd centroid (index 2), the second instance is closest to the 1st centroid (index 0), the third instance is closest to the 2nd centroid (index 1) and so on. Please include a short paragraph in your report explain the code in your own words.

3. A function called *move_centroids*, which will take in as arguments the feature data, an array containing the centroid indices assigned to each feature instance (this is the output of *assign_centroids*) and the current set of centroids. This function will compute the new position of the centroids (by calculating the mean of the datapoints assigned to each specific centroid) and will return an array containing the new centroids. Please include a short paragraph in your report explain the code in your own words.

4. A function called *calculate_cost* which will take in as arguments the feature data, an array containing the centroid indices assigned to each feature instance (this is the output of *assign_centroids*) and the current array of centroids. It should calculate and return the current distortion cost function. The distortion cost function can be calculated below.



Please include a short paragraph in your report explain the code in your own words.

5. A function called *restart_KMeans*, which will take in as arguments the feature data, the number of centroids (an integer), the number of iterations (an integer) and the number of restarts (an integer).

   The number of iterations just specifies the number of iterations of the inner loop of KMeans (consisting of assigning centroids and moving centroids). This can be set to 10 for this problem (for this data your algorithm could converge quickly).

   The number of restarts is the number of times you will restart KMeans from scratch (generate new random centroids and iterate again through the assign centroid and move centroid steps). Again, we will set this value to 10 for our problem.

   The *restart_KMeans* function will use the function described above (1 - 4) to implement a random restart KMeans algorithm and will return the best solution found over the 10 restarts. More specifically it will return:
   - The array of centroid IDs that produced the best distortion cost function value (this defines the cluster to which each feature instance belongs).
   - The corresponding best distortion cost function value

As usual marks will be given for an efficient implementation that minimizes duplication and uses NumPy where possible.

Once you have fully implemented the above code, you should use it to produce an elbow plot and describe what you consider to be the most appropriate number of centroids (clusters) for this dataset. Clearly explain your interpretation of the plot and how you selected the appropriate number of clusters (centroids).

Checklist for Part 2(A)

Your **report** should contain the following:
- Your implementation of the function *generate_centroids* along with accompanying written explanation.
- Your implementation of the function *assign_centroids* along with accompanying written explanation.
- Your implementation of the function *move_centroids* along with accompanying written explanation.
- Your implementation of the function *calculate_cost* along with accompanying written explanation.
- Your implementation of the function *restart_KMeans*
- A picture of the elbow plot you produced and your written interpretation of the elbow plot and your justification for the selection of the appropriate number of clusters (centroids)

Your submitted zip file should contain the full code entitled Part2A.py (Please note if you are using Jupyter notebooks that you name your notebook Part2A). **Submissions that contain just Jupyter notebooks without an accompanying report containing the above-mentioned elements will not be accepted.**

Part 2(B) – Researching Alternatives to KMeans (30 Marks)

When dealing with large amount of data, the KMeans algorithm can be quite slow. The number of necessary distance calculations is ($n*c*a$) where n is the number of feature instances (rows in our dataset), c is the number of centroids and a is the number of iterations (of course this does not consider the issue of random restarts).

A number of alternative strategies have been proposed in literature to improve the performance of the KMeans category of clustering algorithm. A commonly used alternative to KMeans, which is particularly useful when dealing with large amounts of data is called Mini-Batch KMeans. You can find details of the implantation in Section 2 of this paper.

You should research Mini-Batch KMeans and include a max one-page description of its operation in your report document. To grade well in this section, you should demonstrate that you clearly understand the operation of this algorithm. Implement the mini-batch variant by modifying your existing implementation of KMeans from Part 2 (A) and compare and it's performance with the standard KMeans algorithm from Part 2 (A).

Checklist for Part 2(B)

Your **report** should contain the following:

- An explanation of each of the modifications you made to your original KMeans code in order to implement the minibatch variant. The explanation should contain the snippets of code you modified and a clear accompanying written explanation.
- A written summary of the performance of the standard KMeans algorithm and the minibatch variant.

Your submitted zip file should contain the full code entitled Part2B.py (Please note if you are using Jupyter notebooks that you name your notebook Part2B).

Please note a failure to include the above material in your written report (or a failure to include these functions as named and described above in your code) will incur a penalty. I will not accept submissions that contain just Jupyter notebooks without an accompanying report containing the above-mentioned elements.