Homework 4
CS540 Sp23

Assignment Goals

- Process fun real-world data
- Implement hierarchical clustering
- Visualize the clustering process

You are to perform hierarchical clustering on publicly available Pokemon stats. Each Pokemon is defined by a row in the data set. Because there are various ways to characterize how strong a Pokemon is, we summarize the stats into a shorter feature vector. For this assignment, you must represent a Pokemon's quality by 6 numbers:

Attack, Sp. Atk, Speed, Defense, Sp. Def, and HP

After each Pokemon is represented as a 6-dimensional feature vector ($x_1, \ldots, x_6$), you need to cluster the first n Pokemon with hierarchical agglomerative clustering (HAC). Your function should work similarly to scipy.cluster.hierarchy.linkage() with method='complete'.

Program Overview

The data in CSV format can be found in the file Pokemon.csv. Note, there is no starter code for this assignment. If you feel stuck, refer to the starter code from past assignments. You will have to write a few python functions for this assignment. Here is a high level description of each for reference:

1. load_data(filepath) — takes in a string with a path to a CSV file, and returns the data points as a list of dicts. Section 0.1
2. calc_features(row) — takes in one row dict from the data loaded from the previous function then calculates the corresponding feature vector for that Pokemon as specified above, and returns it as a numpy array of shape (6,). The dtype of this array should be int64. Section 0.2
3. hac(features) — performs complete linkage hierarchical agglomerative clustering on the Pokemon with the ($x_1, \ldots, x_6$) feature representation, and returns a numpy array representing the clustering. Section 0.3
4. imshow_hac(Z, names) — visualizes the hierarchical agglomerative clustering on the Pokemon's feature representation. Section 0.4

You may implement other helper functions as necessary, but these are the functions we are testing. In particular, your final python file is just a suite of functions, you should not have code that runs outside of the functions. To test your code, you may want a "main" method to put it all together. Make sure, you either delete any testing code running outside functions or wrap it in a if __name__=="__main__":. This is discussed more in Section 0.5.

Program Details

0.1 load_data(filepath)

Summary. [20pts]

- Input: string, the path to a file to be read.
- Output: list, where each element is a dict representing one row of the file read.

Details.

1. Read in the file specified in the argument, filepath. Note, the DictReader from Python's csv module is useful but, depending on your python version, this might return OrderedDicts instead of normal dicts. Make sure you convert to dict as appropriate if you choose to use this function.
2. Return a list of dictionaries, where each row in the dataset is a dictionary with the column headers as keys and the row elements as values.

You may assume the file exists and is a properly formatted CSV.

0.2 calc_features(row)

Summary. [20pts]

- Input: dict representing one Pokemon.
- Output: numpy array of shape (6,) and dtype int64. The first element is x_1 and so on with the sixth element being x_6.

Details. This function takes as input the dict representing one Pokemon, and computes the feature representation $(x_1, \ldots, x_6)$. Specifically,

1. x_1 = Attack
2. x_2 = Sp. Attack
3. x_3 = Speed
4. x_4 = Defense
5. x_5 = Sp. Def
6. x_6 = HP

Note, these stats in the dict may not be int. Make sure to convert each relevant stat to int when computing each x_i. Return a numpy array having each x_i in order: $x_1, \ldots, x_6$. The shape of this array should be (6,). The dtype of this array should be int64. Remember, this function works for only one Pokemon at a time, not all of the ones that you loaded in load_data simultaneously. Make sure you are outputting the exact data structures with appropriate types as specified or you risk a major reduction in points.

0.3 hac(features)

Summary. [50pts]

- Input: list of numpy arrays of shape (6,), where each array is an $(x_1, \ldots, x_6)$ feature representation as computed in Section 0.2. The total number of feature vectors, i.e. the length of the input list, is n. Note, we test your code on different n's as stated in Section 0.5).

- Output: numpy array of shape $(n-1) \times 4$. For any i, $Z[i, 0]$ and $Z[i, 1]$ represent the indices of the two clusters that were merged in the ith iteration of the clustering algorithm. Then, $Z[i, 2] = d(Z[i, 0], Z[i, 1])$ is the complete linkage distance between the two clusters that were merged in the ith iteration (this will be a real value, not integer like the other quantities). Lastly, $Z[i, 3]$ is the size of the new cluster formed by the merge, i.e. the total number of Pokemon in this cluster. Note, the original Pokemon are considered clusters indexed by $0, \ldots, n-1$, and the cluster constructed in the ith iteration ($i \geq 1$) of the algorithm has cluster index $(n-1) + i$. Also, there is a tie-breaking rule specified below that must be followed.

Details. For this function, we would like you to mimic the behavior of SciPy's HAC function, linkage(). You may not use this function in your implementation, but we strongly recommend using it to verify your results! This is how you can test your code.

Distance. Using complete linkage, perform the hierarchical agglomerative clustering algorithm as detailed in lecture. Use the standard Euclidean distance function for calculating the distance between two points. You may implement your own distance function or use numpy.linalg.norm(). Other distance functions might not work as expected so check it works on the CSL machines first! You are liable for any reductions in points you might get for using a package distance function.

Outline. Here is one possible path you could follow to implement hac()

1. Number each of your starting data points from 0 to $n-1$. These are their original cluster numbers.

2. Create an $(n - 1) \times 4$ array or list. Iterate through this array/list row by row. For each row,

   (a) Determine which two clusters you should merge and put their numbers into the first and second elements of the row, *Z*[*i,* 0] and *Z*[*i,* 1]. The first element listed, *Z*[*i,* 0] should be the smaller of the two cluster indexes.

   (b) The complete-linkage distance between the two clusters goes into the third element of the row, *Z*[*i,* 2]

   (c) The total number of Pokemon in the cluster goes into the fourth element, *Z*[*i,* 3]

   If you merge a cluster containing more than one Pokemon, its index (for the first or second element of the row) is given by *n* + the row index in which the cluster was created.

3. Before returning the data structure, convert it into a NumPy array if it isn't one already.

For this method to run efficiently when n is large you should maintain a distance matrix throughout the process to avoid having to recalculate the distances between points or clusters. You should be able to run hac efficiently on all 800 Pokemon. To create the distance matrix we will leverage the following:

Suppose we have a set of n vectors x1, x2, ..., xn in d-dimensional space. The square distance between two vectors x_i and x_j can be represented as:

$$\left|\left|x_i + x_j\right|\right|^2 = \left|\left|x_i\right|\right|^2 + \left|\left|x_j\right|\right|^2 - 2(x_i \bullet x_j)$$

To simplify the computation, we can use the Gramian matrix G which is defined as the matrix whose entries are the dot products of all pairs of vectors x_i and x_j . The diagonal elements of G form a vector g, which represents the squares of the lengths of the vectors. By combining these terms, we can write the square distance matrix D^2 as the sum of a vector of ones and the transpose of the vector g minus twice the Gramian matrix G. In other words, D^2 is obtained by adding the outer product of the vector g and the transpose of a vector of ones, and subtracting twice the Gramian matrix G.To get the distance matrix we need to take the square root of D^2, do not forget this step.

$$D^2 = \left(\left|\left|x1_i\right|\right|_2^2 |1|\right) + \left(\left|\left|x2_i\right|\right|_2^2 |1|\right) - 2 * X1@X2.T$$

For our problem you will need to start by converting your feature input into a numpy array of shape (n,6) lets call it X. We will have three components:

comp1 = $\left(\left|\left|x1_i\right|\right|_2^2 |1|\right)$, comp2 = $\left(\left|\left|x2_i\right|\right|_2^2 |1|\right)$, comp3 = $-2 * X1@X2.T$

Comp1 and comp2 are created by taking the sum of X^2. Comp1 should have shape (n,1) and comp2 should have shape (n,). Comp3 just has the original X as X1 and X2.

For example, if you have a NumPy array called distance_matrix then distance_matrix[3,4] is equal to the euclidean distance between the Pokemon at index 3 and 4 in the features input. You can compare your output with scipy.spatial.distance_matrix, please note we are using Euclidean distance for this assignment.

Tie Breaking. When choosing the next two clusters to merge, we pick the pair having the smallest complete-linkage distance. In the case that multiple pairs have the same distance, we need additional criteria to pick between them. We do this with a tie-breaking rule on indices as follows: Suppose $(i_1, j_1), \ldots, (i_h, j_h)$ are pairs of cluster indices with equal distance, i.e., $d(i_1, j_1) = \cdots = d(i_h, j_h)$, and assume that $i_t < j_t$ for all t (so each pair is sorted). We tie-break by picking the pair with the smallest first index, i. If there are multiple pairs having first index i, we need to further distinguish between them. Say these pairs are $(i, t_1), (i, t_2), \ldots$ and so on. To tie-break between these pairs, we pick the pair with the smallest second index, i.e., the smallest t value in these pairs. Be aware that this tie-breaking strategy may not produce identical results to linkage().

0.4 imshow_hac(Z, names)

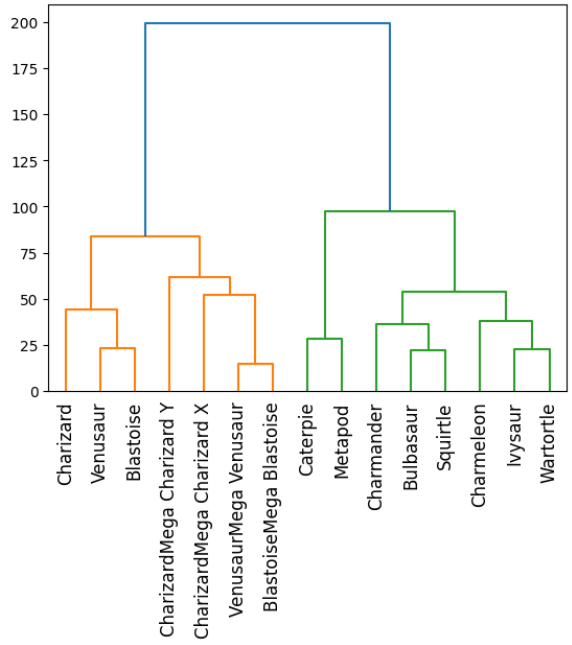
Summary. [10pts]

- Input: numpy array *Z* output from hac, and list of string names corresponding to Pokemon names with size n by 1.
- Output: None, simply plt.show() a graph that visualizes the hierarchical clustering. You should use dendrogram in the scipy module with labels set to names and leaf_rotation = ??.

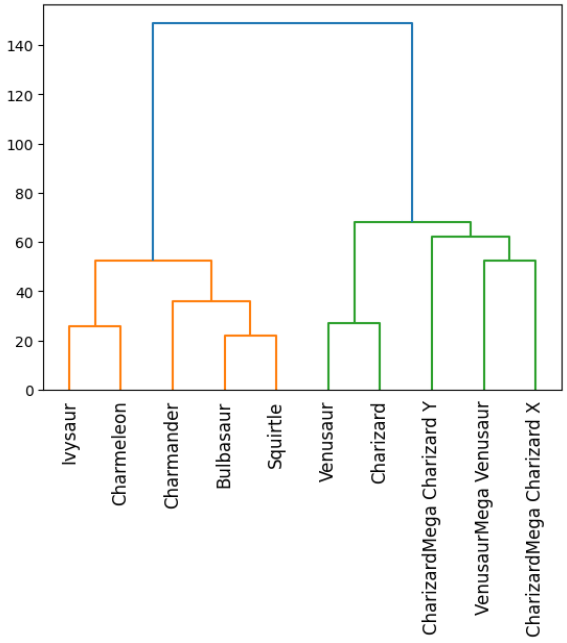
Details. Your plot will likely cut off the x labels. For the graph to look like the below examples you will need to create a subplot before the dendrogram and call tight_layout() on the figure before plt.show().

Here are some examples of successful visualizations for different sized lists of Pokemon

N = 15



N = 10



0.5 Testing

To test your code, try running the following lines in a main method or in a jupyter notebook for various choices of n:

```
features_and_names = [(calc_features(row), row['Name']) for row in load_data('Pokemon.csv')[:n]]

Z = hac([row[0] for row in features_and_names])

names = [row[1] for row in features_and_names]

imshow_hac(Z,names)
```

For the hac function we will test on both small and large values of *n* up to 800, the entire Pokeman set. We will test on n <= 30 for imshow_hac. You can then compare your clustering to what linkage() would give you (remember, set method = 'complete'), and look at the different clustering visualizations.

Submission Details

- Please submit your files in a zip file named hw4_<netid>.zip
- Inside your zip file, there should be only one file named: hw4.py
- All code should be contained in functions or under a if __name__=="__main__":
- Be sure to remove all debugging output before submission.