Assignment 3 Report

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Dataset Description

The two datasets selected from UCI are IRIS and WINE.

The IRIS is a classic dataset with 4 numeric attribute, ,containing 3 classes of 50 instances each, where each class refers to a type of iris plant.

The WINE are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of 13 constituents found in each of the three types of wines. All attributes are continuous.

Modules of Source Code

there are 4 files in `sourcecode` folder, they are `hac.py`, `kmeans.py`, `experiments.py` and `figure.py`

hac.py

In `hac.py`, there is code which implementing the `Hierarchical Clustering` algorithm. There are two classes in this file. The first one is `Cluster`. It is used to represent a cluster in the algorithm. It stores object members and their indexes in the dataset. And another class is `Hierarchical`. It supplies a `fit` method to process the clustering algotithm. Its code is as follows:

```
        if type(X) != np.ndarray:
            raise Exception('X not a numpy.ndarray')

        clus = [ Cluster((X[i],i)) for i in xrange(X.shape[0])]
        adj_mat = np.matrix(np.zeros((X.shape[0], X.shape[0])))

        #initialize adjacent matrix
        for i in xrange(len(clus)):
            for j in xrange(i, len(clus)):
                dist = linkage(clus[i], clus[j]) if i!=j else float('inf')
                adj_mat[i,j] = adj_mat[j,i] = dist

        #run merge
        while True:
            min_dist = adj_mat.min()
            min_loc = np.where(adj_mat == min_dist)
            x = min_loc[0][0]
            y = min_loc[1][0]
            clus_1 = clus[x]
            clus_2 = clus[y]
            clus_1.merge(clus_2)
            clus.remove(clus_2)
            # delete min_loc[1]-th row and col
            # delete min_loc[1]-th row and col
            adj_mat = np.delete(adj_mat, y, axis=0)
            adj_mat = np.delete(adj_mat, y, axis=1)

            for i in xrange(len(clus)):
                dist = linkage(clus[i], clus_1) if i!= x else float('inf')
                adj_mat[i, x] = dist
                adj_mat[x, i] = dist
            if len(clus) == k:
                break

        #return label
        y_predict = np.array([-1 for i in xrange(X.shape[0])])
        for i, c in enumerate(clus):
            for l in c.mem_idx:
                y_predict[l] = i
        return y_predict
```

After checking the data type of `X`, I initialized the adjacent matrix first. If `i==j`, I give infinity to the position. Although it should be `0`, doing so is convenient for finding minimum distance in adjacent matrix later. Then in the `while` loop, I firstly find the minimum distance using the `min()` function supplied by `numpy`, and using `numpy.where` to find the corresponding clusters. Then, the two clusters are merged into one and the columns and row of one cluster is removed from adjacent matrix. After that, the new distance between the new cluster and other clusters are calculated and the matrix is updated. If the number of leaving clusters is equal to `k`, the loop will end and the method return the result; If not, the loop will go on. Then, I supply three kinds of linkage in this file. They are `Single Linkage`, `Complete Linkage` and `Average Linkage`.

kmeans.py

In this file, I supply the implementation of `K-Means` algorithm. There is only on class named `KMeans` in this file. The code is as follows:

```
class KMeans:

    def fit(self, X, k):
        '''
            KMeans on X, dividing into k clusters

            @X: np.ndarray; shape = [n_samples, n_features]
            @k: int

            #return: np.ndarray, shape = [n_samples,]
        '''
        centers = random.sample(X,k)
        y_predict = np.array([-1 for i in xrange(X.shape[0])])

        while True:
            cls_mean = np.array([ [0. for j in xrange(X.shape[1])] for i in
            cls_count = np.array([0 for i in xrange(k)])
            for i, v in enumerate(X):
                # find the nearest center
                nrst_ctr = 0
                for j, c in enumerate(centers):
                    if np.sum(np.sqrt((v-c)**2)) < np.sum(np.sqrt((v-centers
                        nrst_ctr = j
                # update y_predict, cls_mean and cls_count
                y_predict[i] = nrst_ctr
                cls_mean[nrst_ctr] += v
                cls_count[nrst_ctr] += 1
            for d in xrange(X.shape[1]):
                cls_mean[:, d] /= cls_count

            if np.sum(centers==cls_mean) == cls_mean.shape[0] * cls_mean.sha
                break
            else:
                centers = cls_mean

        return y_predict
```

The only method of KMeans is `fit`. At first, I sample k data points from dataset as initial centers randomly. Then the iteration begins. `cls_mean` is used to store the mean of clusters in this iteration. And `cls_count` records the number of data points in each cluster. After traversing all nodes in dataset, means are calculated by `cls_mean/cls_count`. If all centers are steady, which means `centers==cls_means`, the iteration will be broken, else the loop will go on.

experiments.py

This file supplies the experiments code. First it reads data from json file. Then, for `KMeans`, I set k from 2 to 9 and run the algorithm. Then indexes are calculated. For `Hierarchical Clustering`, k is set from 2 to 9, too. Then with three kinds of linkage, the algorithm are processed. All results are ouputted to json files.

figure.py

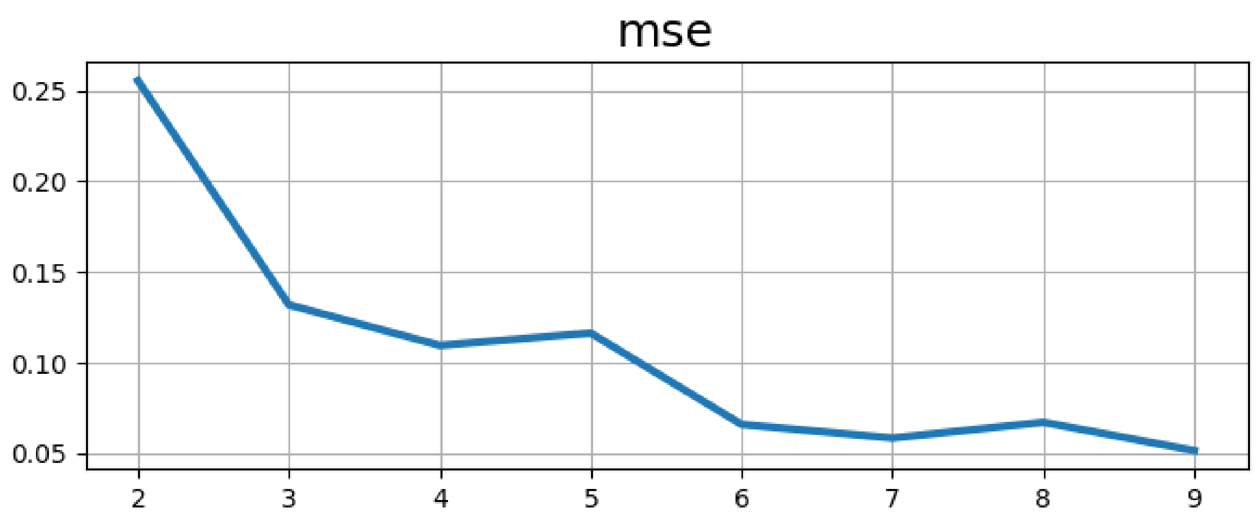
In this file, I draw results plots.

Experiment Results

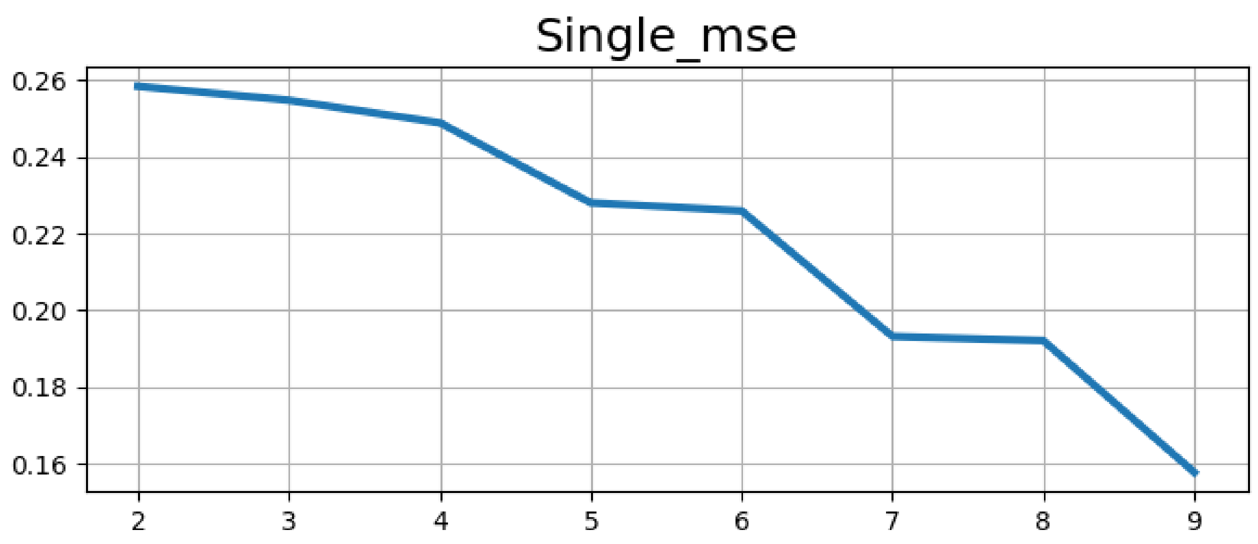
IRIS:

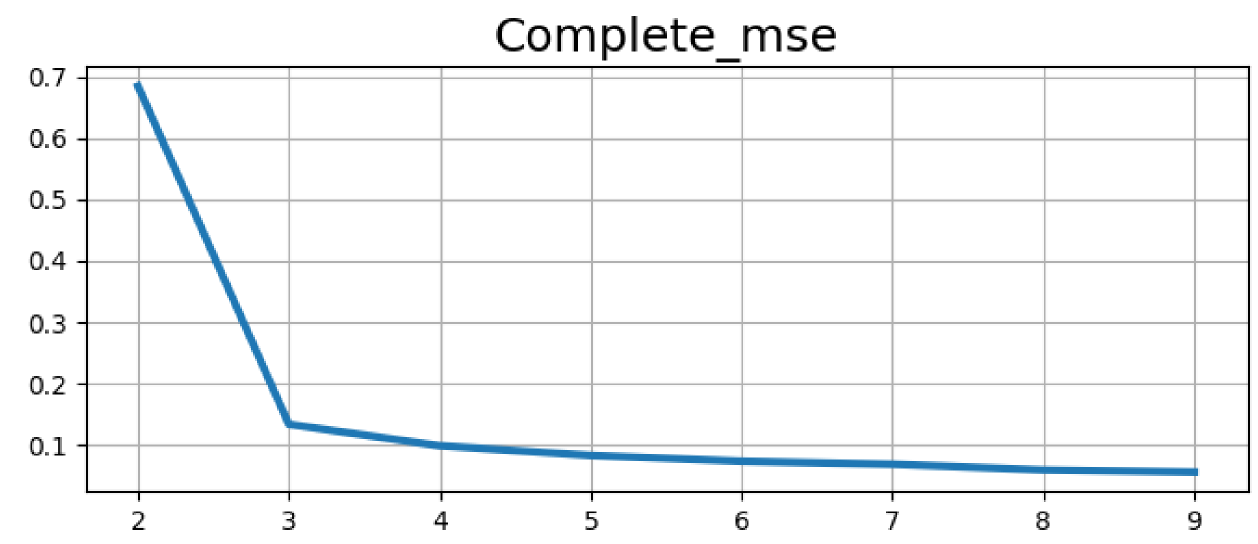
The following figures show the `mse(mean squared error)` of clustering results. The first figre is using `KMeans` and `Hierarchical Clustering` is emploied in the second figure.

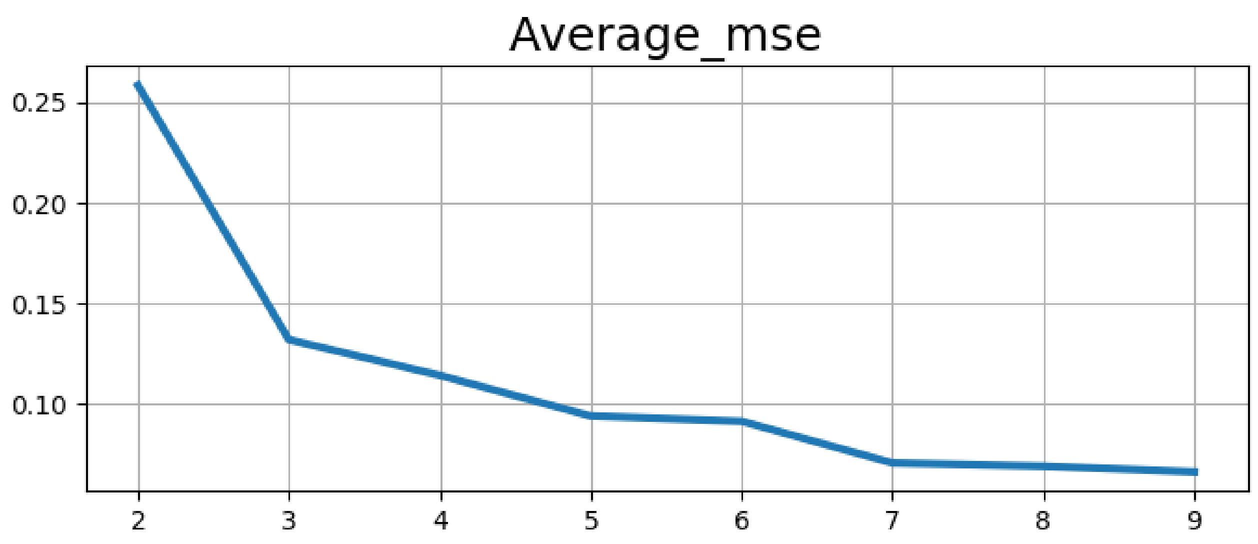
Kmeans



Hierarchical





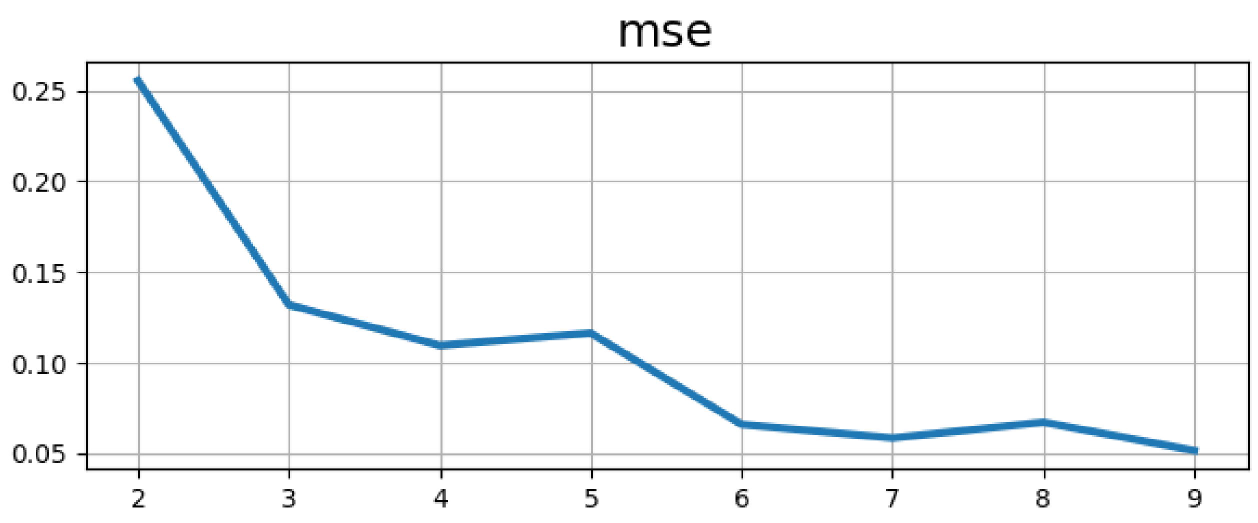


As we know, the `IRIS` dataset is composed by three clusters. `mse` in `KMeans`, `Hierarchical with CompleteLinkage` and `Hierarchical with AverageLinkage` show knee point at k=3. But `Hierarchical with SingleLinkage` does not show the knee point at k=3.

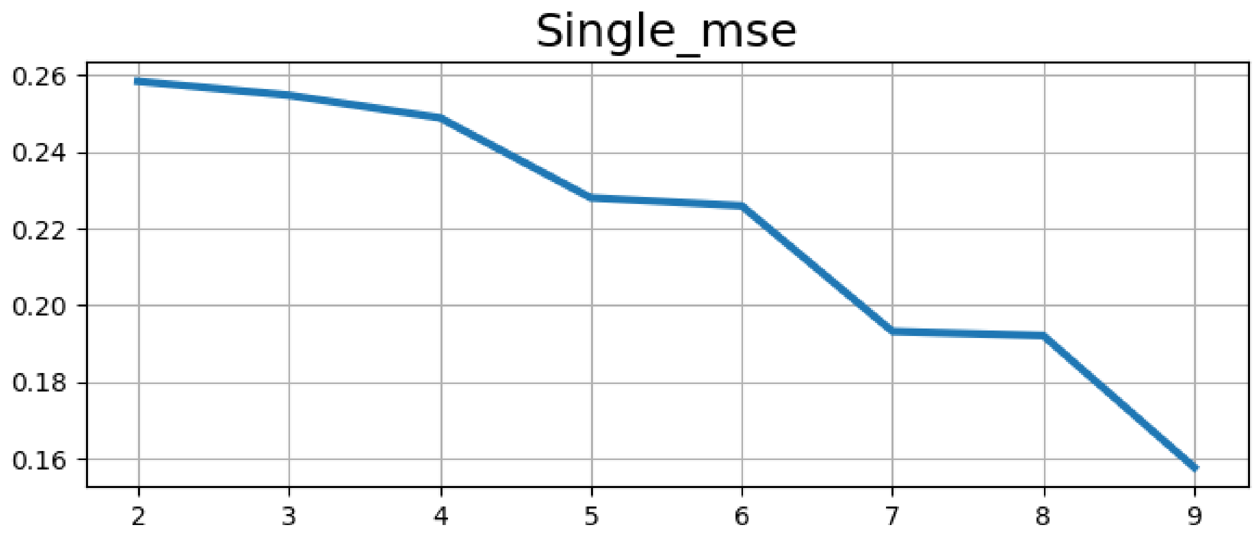
WINE

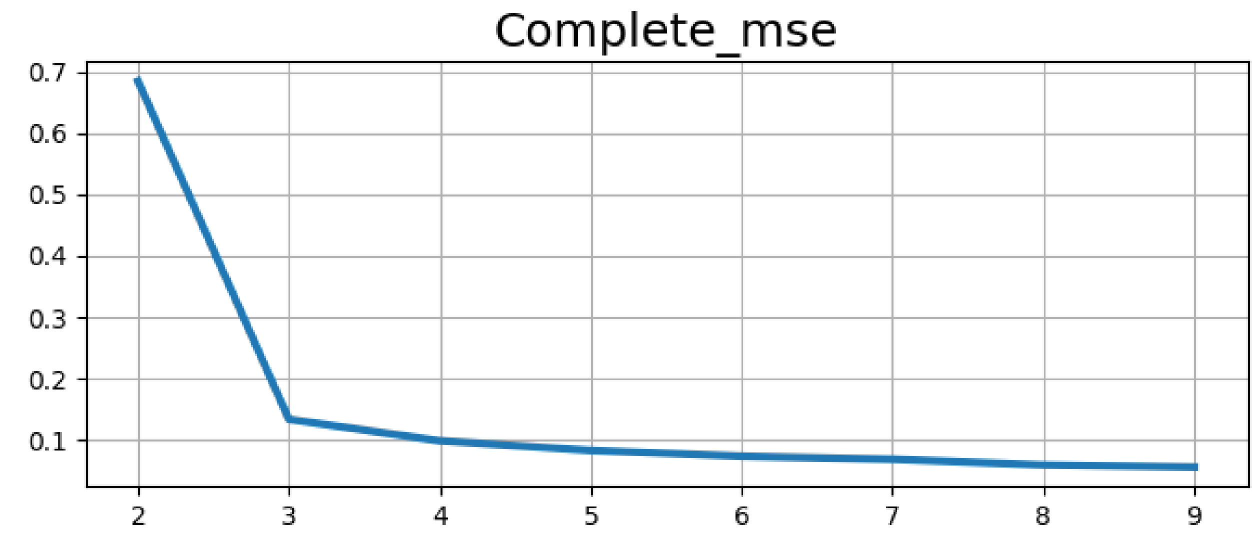
The logic of following two figures is same as those in `IRIS` dataset.

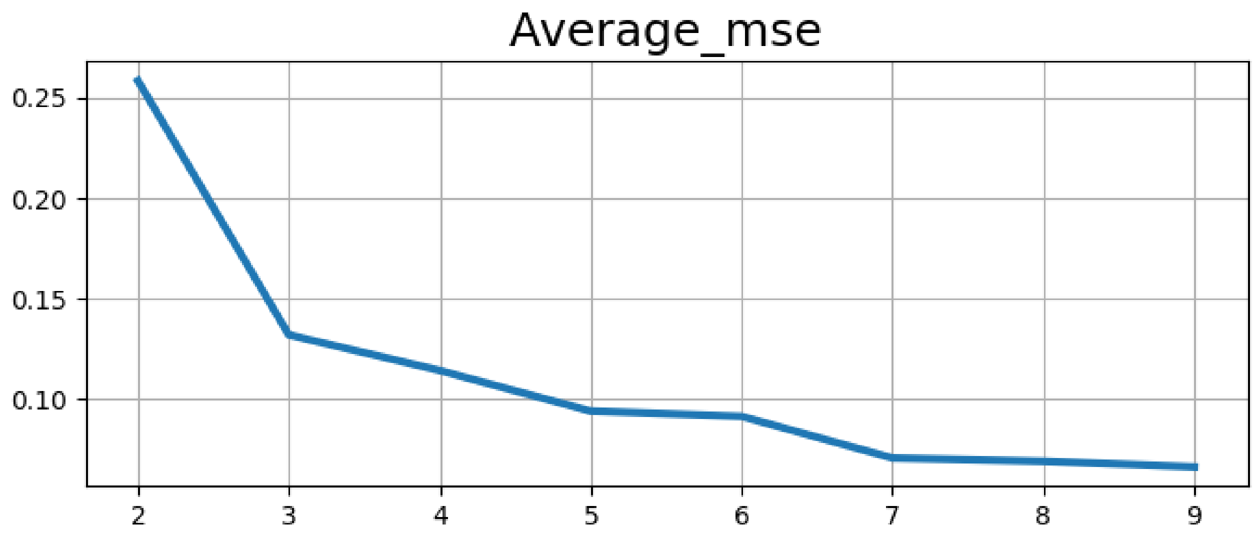
Kmeans



Hierarchical







There are three clusters in the `WINE`, too. We can see `Hierarchical with SingleLinkage` does not show a knee point , either. Knee points appears in all the other plots, and the most obvious knee point shows in `Hierarchical with CompleteLinkage`.

Based on the above results, we can see that both `KMeans` and `Hierarchical` can find the proper distribution of dataset. However, the result of `SingleLinkage` is not good. I think that because it take the minimun distance between clusters, and that may be effected by extreme data points easily.

Improvement

1. In `Hierarchical Clustering`, it takes `O(n^2)` to find the minimum distance in adjacent matrix. However, if heap is used to store the distances, the time cost can be reduced to `O(nlogn)`.
2. In `KMeans` algorithm, the results can be effected easily by dirty data points. We can use `K-Medoids` to replace it. Instead of calculating means of clusters, the point with minimun sum with other points in a same cluster is selected as the center the of cluster. This method is not sensitive to dirty data. However, the time efficiency of this algorithm is worse than `KMeans`