Assignment-1

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CS9030 Assignment-1				

0.0.9 Problem Statement

Implement the following algorithms on the Iris dataset using Python/R language.

- **K-means algorithm:** This has to be done ourselves without using libraries. Also provide visualization of the output as a Cluster plot.
- **DBSCAN** algorithm (density-based clustering): This can be done using Python/R packages. Also provide visualization of the output as a Cluster plot.
- Agglomerative Hierarchical clustering algorithm: This can be done using Python/R packages. For output, only a dendrogram (as a tree structure) is sufficient (suitable package available).

1 Implementing K-Means Algorithm without any external packages/libraries

As per the requirements of the given assignment problems, no external packages will be used to implement kmeans algorithm. Only simple Python lists and classes will be used to store and manipulate the data.

1.0.1 My Approach

- There will be a Datapoint class whose attribute dims will store the coordinates of the datapoint in a list. There will be essential class methods like adding two Datapoints, finding squared euclidean distance between two, etc. while will be useful in our later operations.
- After loading data, we will have a list data of Datapoint objects from iris.data file.
- Random k Datapoints will be selected as centroids and stored in centroids list which is nothing but a list of Datapoint objects.
- The squared euclidean distances will be calculated on the go and eventually the Datapoint will be assigned a cluster with the help of cluster tags, i.e., the assignment will be stored in a separate list called Cluster Tags.
- The cluster tag is a list where the indices will correspond to the indices of Datapoint in data list and the values will correspond to the indices of a particular centroid in centroids list.
- Eventually, the centroids will be updated by performing addition and division by some scalar quantity on Datapoints and we will check whether they match with the old ones.
- If they match, the algorithm stops. Else the iterations continue.
- Then we will find the optimal value of k by elbow method by running kmeans from k = 2 to k = 10 and finding the WCSS and plotting it on a graph.
- After that, we will run kmeans with optimal value of k, record the centroids and cluster assignments.
- Then we shall produce the output both in text form and nice 3D scatter plot.

1.1 Step 1: Creating a Datapoint class

- Since every datapoint can have multiple features (coordinates or dimensions), we will create a dedicated Datapoint class for the data points for easy handling of data.
- The attribute of Datapoint class, dims, is a list of coordinates(or features) of a single data point.
- Other class methods are created to calculate the squared euclidian distance between two points, adding two points, dividing the point by some scalar quantity as these operations are often required in K-Means Algorithm.

```
[89]: from typing import List

class Datapoint:
    def __init__(self, dims: List[float]):
        self.dims = dims

def __repr__(self):
        return f"Pt{self.dims}"

def dis(self, other):
        dis = 0.0
        for i in range(len(self.dims)):
            dis += (self.dims[i] - other.dims[i])**2 # squared euclidean_u

distance
    return dis
```

```
def __add__(self, other):
        Will be used during updation of centroids in finding the average of all_{\sqcup}
\hookrightarrow points
        11 11 11
       new_dims = []
       for i in range(len(self.dims)):
            new_dims.append(self.dims[i] + other.dims[i])
       return Datapoint(new_dims)
   def __truediv__(self, scalar: int):
        Will be used during updation of centroids in finding the average of all_{\sqcup}
\hookrightarrow points
       new_dims = []
       for i in range(len(self.dims)):
            new_dims.append(self.dims[i] / scalar)
       return Datapoint(new_dims)
   def __eq__(self, other):
       return self.dims == other.dims
```

1.2 Step 2: Loading the dataset

- We will load our data from a csv file where each row is an individual data point
- So eventually, we will have a list of Datapoint objects

[Pt[5.1, 3.5, 1.4, 0.2], Pt[4.9, 3.0, 1.4, 0.2], Pt[4.7, 3.2, 1.3, 0.2], Pt[4.6, 3.1, 1.5, 0.2], Pt[5.0, 3.6, 1.4, 0.2], Pt[5.4, 3.9, 1.7, 0.4], Pt[4.6, 3.4, 1.4, 0.3]]

As you can see, we have now successfully loaded our data in data list.

1.3 Step 3: Implementing K-Means Algorithm

```
[91]: def kmeans(data: List[Datapoint], k: int):
          import random
          # Randomly initialize the centroids
          centroids: List[Datapoint] = random.sample(data, k)
          # This list will contains the assignment(tags) of every Datapoint to which
       ⇔cluster it belongs
          # the cluster number will be nothing but the index of the centroid(of that \Box
       →cluster) in the centroids list
          cluster_tags = [None] *len(data)
          # iteration begins and will continue until we get equal centroids
          while True:
              for i in range(len(data)):
                  pt = data[i]
                  min_dis = float('inf')
                   #calculating distance of pt with every centroid and eventually \Box
       \hookrightarrow finding the closest one
                  for j in range(len(centroids)):
                       dis = pt.dis(centroids[j])
                       if dis < min_dis:</pre>
                           min_dis = dis
                           cluster_tags[i] = j
              # updating the centroids after assigning cluster tag to each Datapoint
              # creating a new list of centroids with all datapoints having dims_
       \rightarrow initially 0
              new_centroids: List[Datapoint] = [Datapoint([0]*len(data[0].dims)) for __
              counts = [0]*k # to store count of Datapoints in each cluster
              for i in range(len(data)):
                  tag = cluster_tags[i]
                  new_centroids[tag] = new_centroids[tag] + data[i] # adding the_
       →datapoints together to eventually find the average
                  counts[tag] += 1
              for i in range(len(new_centroids)):
                   if counts[i] > 0:
                       new_centroids[i] = new_centroids[i] / counts[i]
              if new_centroids == centroids:
                  break
              else:
                  centroids = new_centroids
```

```
return centroids, cluster_tags, counts
```

1.4 Step 4: Finding optimal value of k

- We shall first calculate the within cluster sum of squares for clusters for every k
- Then we will plot the wcss for every k from 2 to 10
- We shall plot the data using the matplotlib package
- Then we shall find the optimal value of k

```
[95]: import matplotlib.pyplot as plt
      def elbow_method(data: List[Datapoint], max_k: int):
          wcss_list = []
          for k in range(2, max_k+1):
              centroids, cluster_tags, _ = kmeans(data, k)
              WCSS = wcss(data, centroids, cluster_tags)
              wcss_list.append(WCSS)
              print(f"For k = \{k\}, WCSS = \{WCSS: .2f\}")
          # Plotting the elbow graph
          plt.figure(figsize=(10, 6))
          plt.plot(range(2, max_k + 1), wcss_list, marker='o')
          plt.title('WCSS PLot to find Optimal k')
          plt.xlabel('Number of clusters (k)')
          plt.ylabel('WCSS')
          plt.xticks(range(2, max_k + 1))
          plt.grid()
          plt.show()
      elbow_method(data, 10)
```

```
For k = 2, WCSS = 152.37

For k = 3, WCSS = 78.94

For k = 4, WCSS = 71.34

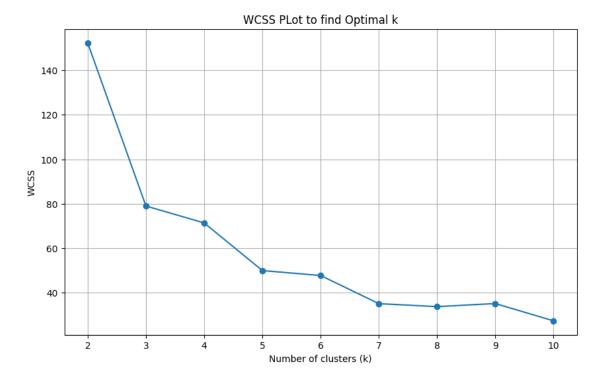
For k = 5, WCSS = 49.88

For k = 6, WCSS = 47.66

For k = 7, WCSS = 34.99

For k = 8, WCSS = 33.65

For k = 9, WCSS = 35.05
```



As we see, the highest decrease in WCSS occurs when we move from k = 2 to k = 3. And then WCSS decreases at a very low rate. So k=3 is the optimal value by the elbow method.

Seeing the crude output of K-Means Algorithm for optimal value k=3

```
[97]: data = load_data("iris/iris.data")
    k = 3
    centroids, cluster_tags, counts = kmeans(data, k)
    for i in range(len(centroids)):
        print(f"The centroid of cluster {i} is {centroids[i]}")
        print(f"Number of datapoints = {counts[i]}")
```

The centroid of cluster 0 is Pt[5.0059999999999, 3.418000000000006, 1.464, 0.243999999999]

Number of datapoints = 50

The centroid of cluster 1 is Pt[5.88360655737705, 2.740983606557377,

4.388524590163935, 1.4344262295081966]

Number of datapoints = 61

The centroid of cluster 2 is Pt[6.853846153846153, 3.0769230769230766,

5.715384615384615, 2.053846153846153]

Number of datapoints = 39

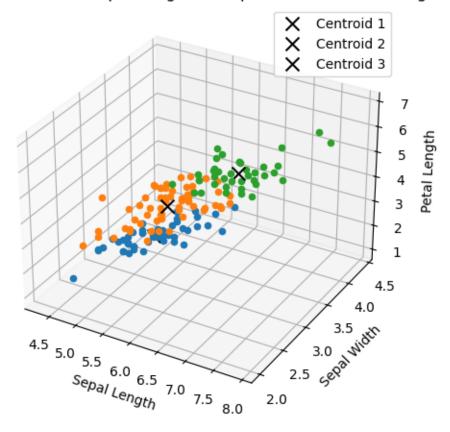
1.5 Step 5: Visualization of Clusters

- As we can see, we are printing the output in a very crude way.
- Let us visualise the cluster data as a 3D scatter plot.
- Since there are 4 attributes, we can pick 3 attributes out of 4 in 4C3 ways, i.e., 4 ways. So there will be 4 scatter plots.

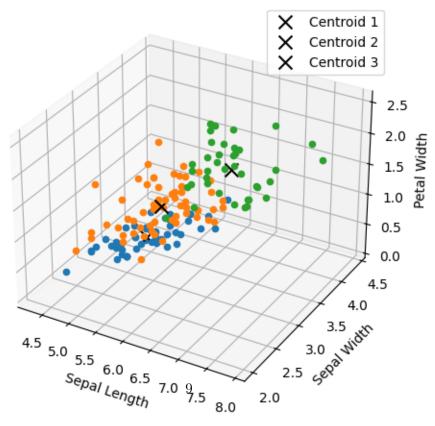
```
[104]: from mpl_toolkits.mplot3d import Axes3D
       import matplotlib.pyplot as plt
      def visualize(data: List[Datapoint], centroids: List[Datapoint], cluster_tags:
       →List[int]):
           # Feature combinations with their indexes
           feature combinations = \lceil
               (0, 1, 2), # Sepal Length, Sepal Width, Petal Length
               (0, 1, 3), # Sepal Length, Sepal Width, Petal Width
               (0, 2, 3), # and so on ...
               (1, 2, 3)
           ]
           feature_names = ['Sepal Length', 'Sepal Width', 'Petal Length', 'Petal_
        -Width'
           # First figure: 2 subplots
           fig1 = plt.figure(figsize=(8, 12))
          for index, (x_idx, y_idx, z_idx) in enumerate(feature_combinations[:2]): #_U
        \rightarrow First 2 combinations
               ax = fig1.add_subplot(2, 1, index + 1, projection='3d') # 2 row, 1
        \hookrightarrow columns
               # Scatter plot for data points
               for i in range(len(data)):
                   ax.scatter(data[i].dims[x_idx], data[i].dims[y_idx], data[i].
        \rightarrowdims[z_idx],
                              c=f'C{cluster_tags[i]}', marker='o')
               # Scatter plot for centroids
               for i in range(len(centroids)):
                   ax.scatter(centroids[i].dims[x_idx], centroids[i].dims[y_idx],__
       c='k', marker='x', s=100, label=f'Centroid {i+1}')
               xlabel, ylabel, zlabel = feature_names[x_idx], feature_names[y_idx],__
        \rightarrow feature_names[z_idx]
               ax.set_xlabel(xlabel)
               ax.set_ylabel(ylabel)
               ax.set_zlabel(zlabel)
```

```
ax.set_title(f'3D Visualization: {xlabel} vs {ylabel} vs {zlabel}')
        ax.legend()
    plt.show()
    # Second figure: 2 subplots
    fig2 = plt.figure(figsize=(8, 12))
    for index, (x_idx, y_idx, z_idx) in enumerate(feature_combinations[2:]): #_U
\hookrightarrow Last 2 combinations
        ax = fig2.add\_subplot(2, 1, index + 1, projection='3d') # 2 row, 1_{\square}
\rightarrow columns
        for i in range(len(data)):
            ax.scatter(data[i].dims[x_idx], data[i].dims[y_idx], data[i].
\rightarrowdims[z_idx],
                       c=f'C{cluster_tags[i]}', marker='o')
        for i in range(len(centroids)):
            ax.scatter(centroids[i].dims[x_idx], centroids[i].dims[y_idx],__
c='k', marker='x', s=100, label=f'Centroid {i+1}')
        xlabel, ylabel, zlabel = feature_names[x_idx], feature_names[y_idx],_u
→feature_names[z_idx]
        ax.set_xlabel(xlabel)
        ax.set_ylabel(ylabel)
        ax.set_zlabel(zlabel)
        ax.set_title(f'3D Visualization: {xlabel} vs {ylabel} vs {zlabel}')
        ax.legend()
    plt.show()
visualize(data, centroids, cluster_tags)
```

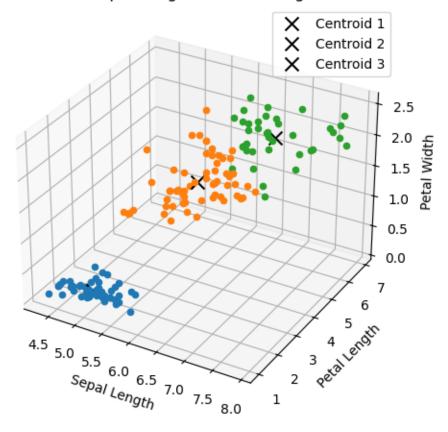
3D Visualization: Sepal Length vs Sepal Width vs Petal Length



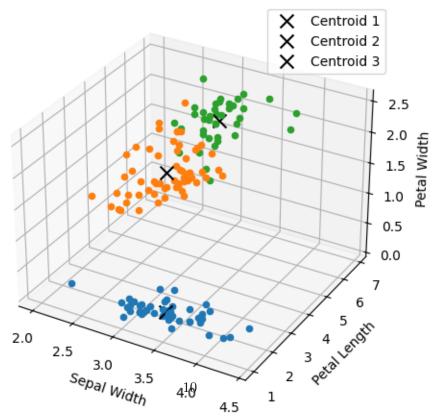
3D Visualization: Sepal Length vs Sepal Width vs Petal Width



3D Visualization: Sepal Length vs Petal Length vs Petal Width



3D Visualization: Sepal Width vs Petal Length vs Petal Width



You can see the four different scatter plots based on different combinations chosen among the four attributes.

2 DBSCAN Clustering Algorithm

2.1 Step 1: Importing all the necessary packages

```
[1]: import numpy as np
  import pandas as pd
  from sklearn.preprocessing import StandardScaler
  from sklearn.cluster import DBSCAN
  from sklearn.neighbors import NearestNeighbors
  import seaborn as sns
  import matplotlib.pyplot as plt
```

2.2 Step 2: Loading the dataset from csv file

```
[2]: iris_df = pd.read_csv('iris/iris.data')
iris_df.head()
```

```
[2]: 5.1 3.5 1.4 0.2 Iris-setosa 0 4.9 3.0 1.4 0.2 Iris-setosa 1 4.7 3.2 1.3 0.2 Iris-setosa 2 4.6 3.1 1.5 0.2 Iris-setosa 3 5.0 3.6 1.4 0.2 Iris-setosa 4 5.4 3.9 1.7 0.4 Iris-setosa
```

2.3 Step 3: Data Preprocessing

As we can see, we need to add column headers to define the feature names and remove the species columns from our dataset.

```
[3]: columns = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width',

→'species']

iris_df = pd.read_csv('iris/iris.data', header=None, names=columns)

iris_df
```

```
[3]:
           sepal_length
                          sepal_width petal_length
                                                        petal_width
                                                                              species
                     5.1
                                   3.5
                                                   1.4
                                                                 0.2
                                                                          Iris-setosa
     1
                     4.9
                                   3.0
                                                   1.4
                                                                 0.2
                                                                          Iris-setosa
     2
                     4.7
                                   3.2
                                                   1.3
                                                                 0.2
                                                                          Iris-setosa
     3
                     4.6
                                   3.1
                                                   1.5
                                                                 0.2
                                                                          Iris-setosa
                                                                 0.2
     4
                     5.0
                                   3.6
                                                   1.4
                                                                          Iris-setosa
                     . . .
                                   . . .
                                                   . . .
                                                   5.2
     145
                     6.7
                                   3.0
                                                                 2.3 Iris-virginica
```

146	6.3	2.5	5.0	1.9	Iris-virginica
147	6.5	3.0	5.2	2.0	Iris-virginica
148	6.2	3.4	5.4	2.3	Iris-virginica
149	5.9	3.0	5.1	1.8	Iris-virginica

[150 rows x 5 columns]

Now we will remove the unnecessary column species

```
[4]: X = iris_df.drop(columns=['species'], errors='ignore')
```

We will now standardize our data.

```
[5]: scaler = StandardScaler()
    X_scaled = scaler.fit_transform(X)
    # displaying the scaled data
    pd.DataFrame(X_scaled, columns=X.columns)
```

[5]:		sepal_length	sepal_width	petal_length	petal_width
	0	-0.900681	1.032057	-1.341272	-1.312977
	1	-1.143017	-0.124958	-1.341272	-1.312977
	2	-1.385353	0.337848	-1.398138	-1.312977
	3	-1.506521	0.106445	-1.284407	-1.312977
	4	-1.021849	1.263460	-1.341272	-1.312977
	145	1.038005	-0.124958	0.819624	1.447956
	146	0.553333	-1.281972	0.705893	0.922064
	147	0.795669	-0.124958	0.819624	1.053537
	148	0.432165	0.800654	0.933356	1.447956
	149	0.068662	-0.124958	0.762759	0.790591

[150 rows x 4 columns]

As you can see, each feature is scaled so that its mean is 0 and its standard deviation is 1.

2.4 Step 4: Find Optimal value of ε (epsilon)

```
[6]: neigh = NearestNeighbors(n_neighbors=4)
nbrs = neigh.fit(X_scaled)
distances, indices = nbrs.kneighbors(X_scaled)
```

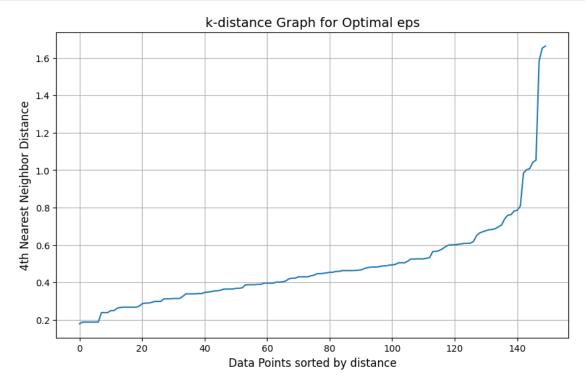
Sort distances for plotting

```
[7]: distances = np.sort(distances[:, 3])
```

Plotting k-distance graph

```
[8]: plt.figure(figsize=(10, 6))
plt.plot(distances)
plt.xlabel('Data Points sorted by distance', fontsize=12)
```

```
plt.ylabel('4th Nearest Neighbor Distance', fontsize=12)
plt.title('k-distance Graph for Optimal eps', fontsize=14)
plt.grid(True)
plt.show()
```



As we can see, at 0.8, there is a sharp increase. Hence choosing epsilon=0.8 as the optimal value.

2.5 Step 4: Apply DBSCAN with the Optimal Epsilon

Taking Epsilon=0.8 and min pts=5

```
[12]:
            sepal_length sepal_width petal_length petal_width
                                                                     0.2
       0
                       5.1
                                      3.5
                                                      1.4
                                                                                  0
                                                                     0.2
       1
                       4.9
                                      3.0
                                                      1.4
                                                                                  0
       2
                       4.7
                                      3.2
                                                      1.3
                                                                     0.2
                                                                                  0
       3
                                                      1.5
                                                                     0.2
                                                                                  0
                       4.6
                                      3.1
       4
                       5.0
                                      3.6
                                                      1.4
                                                                     0.2
                                                                                  0
       . .
                       . . .
                                      . . .
                                                      . . .
                                                                     . . .
       145
                       6.7
                                      3.0
                                                      5.2
                                                                     2.3
                                                                                  1
       146
                                                      5.0
                       6.3
                                      2.5
                                                                     1.9
                                                                                  1
       147
                       6.5
                                      3.0
                                                      5.2
                                                                     2.0
                                                                                  1
       148
                       6.2
                                      3.4
                                                      5.4
                                                                     2.3
                                                                                  1
       149
                       5.9
                                      3.0
                                                      5.1
                                                                     1.8
                                                                                  1
```

[150 rows x 5 columns]

- A new column called cluster has been added which contains the cluster labels (0, 1, 2, ...)
- Points labeled as -1 are **noise points** or outliers.

2.6 Step 5: Visualizing the Clusters in 2D

Since there are four features in the Iris dataset, we can create pairplots for each combination of features.

```
[10]: iris_df['pred_label'] = iris_df['cluster'].apply(lambda x: 'Noise' if x == -1_⊔ 
→else f'Cluster {x}')

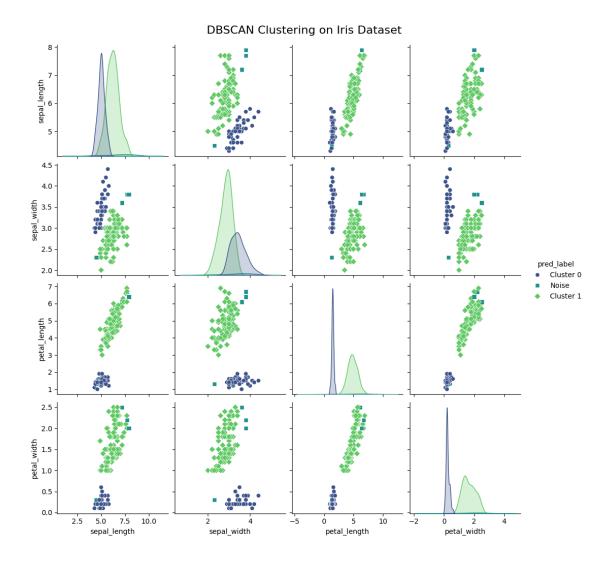
pairplot_data = iris_df[['sepal_length', 'sepal_width', 'petal_length', 
→'petal_width', 'pred_label']]

# Plot the pairplot for all features, color-coded by predicted label

sns.pairplot(pairplot_data, hue='pred_label', diag_kind="kde", 
→palette="viridis", markers=["o", "s", "D"])

plt.suptitle('DBSCAN Clustering on Iris Dataset', y=1.02, fontsize=16)

plt.show()
```



2.7 Step 6: Evaluating the clusters

We can check: - How many points were assigned to each cluster. - How many points were classified as noise (label -1). - The total number of valid clusters.

```
[11]: cluster_counts = iris_df['pred_label'].value_counts()
    print("Cluster Counts:")
    print(cluster_counts.to_string(index=True))

# Count valid clusters (excluding noise)
    n_clusters = len(set(dbscan_labels)) - (1 if -1 in dbscan_labels else 0)

#Count noise points
    n_noise = list(dbscan_labels).count(-1)
```

```
print(f"Number of clusters (excluding noise): {n_clusters}")
print(f"Number of noise points: {n_noise}")

Cluster Counts:
pred_label
Cluster 1 97
Cluster 0 49
Noise 4
Number of clusters (excluding noise): 2
Number of noise points: 4
```

3 Agglomerative Hierarchical Clustering Algorithm

3.1 Step 1: Importing all the necessary packages

```
[6]: import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler
from sklearn.cluster import AgglomerativeClustering
from scipy.cluster.hierarchy import dendrogram, linkage
```

3.2 Step 2: Loading the dataset from csv file

```
[7]: iris_df = pd.read_csv('iris/iris.data')
iris_df.head()
```

```
[7]: 5.1 3.5 1.4 0.2 Iris-setosa 0 4.9 3.0 1.4 0.2 Iris-setosa 1 4.7 3.2 1.3 0.2 Iris-setosa 2 4.6 3.1 1.5 0.2 Iris-setosa 3 5.0 3.6 1.4 0.2 Iris-setosa 4 5.4 3.9 1.7 0.4 Iris-setosa
```

3.3 Step 3: Data Preprocessing

As we can see, we need to add column headers to define the feature names and remove the species columns from our dataset.

```
[8]: columns = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width', 

→'species']

iris_df = pd.read_csv('iris/iris.data', header=None, names=columns)

iris_df
```

```
[8]:
           sepal_length sepal_width petal_length petal_width
                                                                             species
     0
                    5.1
                                  3.5
                                                  1.4
                                                                0.2
                                                                         Iris-setosa
     1
                    4.9
                                  3.0
                                                  1.4
                                                                0.2
                                                                         Iris-setosa
     2
                    4.7
                                  3.2
                                                  1.3
                                                                0.2
                                                                         Iris-setosa
     3
                    4.6
                                                  1.5
                                                                0.2
                                  3.1
                                                                         Iris-setosa
     4
                    5.0
                                  3.6
                                                  1.4
                                                                0.2
                                                                         Iris-setosa
     . .
                     . . .
                                   . . .
                                                  . . .
                                                                . . .
     145
                    6.7
                                  3.0
                                                  5.2
                                                                2.3
                                                                     Iris-virginica
     146
                    6.3
                                  2.5
                                                  5.0
                                                                     Iris-virginica
                                                                1.9
     147
                    6.5
                                  3.0
                                                  5.2
                                                                2.0
                                                                     Iris-virginica
     148
                    6.2
                                  3.4
                                                  5.4
                                                                     Iris-virginica
                                                                2.3
     149
                    5.9
                                  3.0
                                                  5.1
                                                                     Iris-virginica
                                                                1.8
```

[150 rows x 5 columns]

Now we will remove the unnecessary column species

```
[9]: X = iris_df.drop(columns=['species'], errors='ignore')
```

We will now standardize our data.

```
[10]: scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)
# displaying the scaled data
pd.DataFrame(X_scaled, columns=X.columns)
```

[10]:		sepal_length	sepal_width	petal_length	petal_width
	0	-0.900681	1.032057	-1.341272	-1.312977
	1	-1.143017	-0.124958	-1.341272	-1.312977
	2	-1.385353	0.337848	-1.398138	-1.312977
	3	-1.506521	0.106445	-1.284407	-1.312977
	4	-1.021849	1.263460	-1.341272	-1.312977
	145	1.038005	-0.124958	0.819624	1.447956
	146	0.553333	-1.281972	0.705893	0.922064
	147	0.795669	-0.124958	0.819624	1.053537
	148	0.432165	0.800654	0.933356	1.447956
	149	0.068662	-0.124958	0.762759	0.790591

[150 rows x 4 columns]

As you can see, each feature is scaled so that its mean is 0 and its standard deviation is 1.

3.4 Step 4: Perform Agglomerative Hierarchical Clustering

We will perform AHC using different linkage methods: single, complete, average, and ward.

```
[15]: linkage_methods = ['single', 'complete', 'average', 'ward']
```

```
# dictionary to hold the cluster labels for each method
clusters = {}

for method in linkage_methods:
    ahc = AgglomerativeClustering(n_clusters=3,linkage=method)
    clusters[method] = ahc.fit_predict(X_scaled)

#number of clusters formed for each method
for method, labels in clusters.items():
    n_clusters = len(set(labels)) - (1 if -1 in labels else 0)
    print(f"Number of clusters using {method} linkage: {n_clusters}")
```

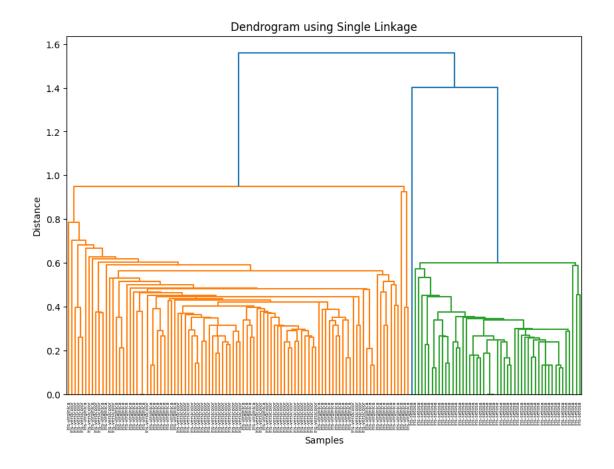
```
Number of clusters using single linkage: 3
Number of clusters using complete linkage: 3
Number of clusters using average linkage: 3
Number of clusters using ward linkage: 3
```

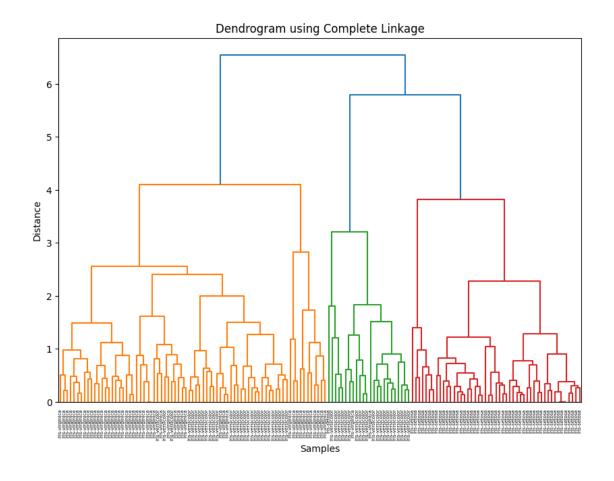
3.5 Step 5: Visualize Dendrograms

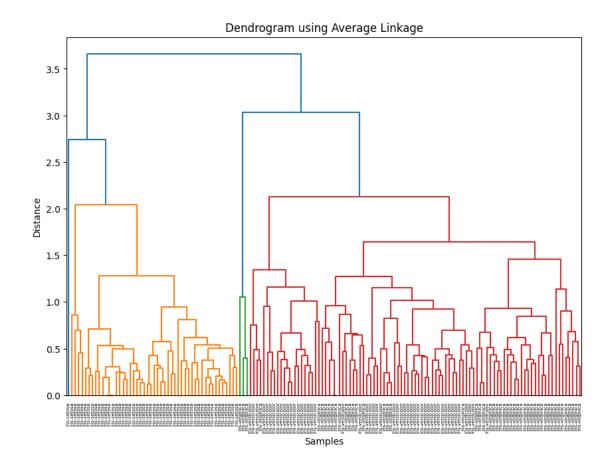
```
[16]: def plot_dendrogram(method):
    # Create linkage matrix
    Z = linkage(X_scaled, method=method)

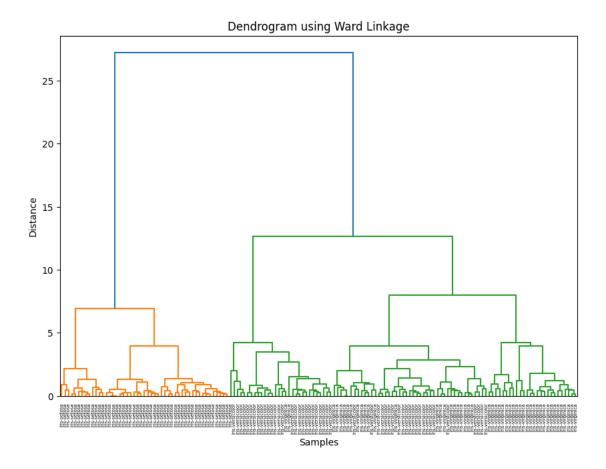
# Create a dendrogram
    plt.figure(figsize=(10, 7))
    dendrogram(Z, labels=iris_df['species'].values)
    plt.title(f'Dendrogram using {method.capitalize()} Linkage')
    plt.xlabel('Samples')
    plt.ylabel('Distance')
    plt.show()

#dendrograms for each linkage method
for method in linkage_methods:
    plot_dendrogram(method)
```









3.6 Step 6: Evaluating the Results

49

24

1

```
[19]: for method in linkage_methods:
          iris_df[f'cluster_{method}'] = clusters[method]
          print(f"\nCluster assignments using {method.capitalize()} linkage:")
          print(iris_df[f'cluster_{method}'].value_counts().to_string(index=True))
     Cluster assignments using Single linkage:
     cluster_single
          100
     0
     2
           49
     1
            1
     Cluster assignments using Complete linkage:
     cluster_complete
          77
     0
```

```
Cluster assignments using Average linkage: cluster_average
```

- 1 97
- 0 50
- 2 3

Cluster assignments using Ward linkage:

cluster_ward

- 0 71
- 1 49
- 2 30