Agglomerative Hierarchical Clustering

Agglomerative hierarchical clustering is a technique for grouping a set of data points into a hierarchy of clusters. The algorithm starts by treating each data point as an individual cluster and iteratively merges the closest clusters until a single cluster remains. The linkage function defines the distance between clusters, and there are various linkage methods, such as single linkage, complete linkage, average linkage, and Ward's method.

Mathematical Representation

Let D be the distance matrix, where D_{ij} represents the distance between data points i and j. Initially, each data point is its own cluster, and the clustering process involves merging clusters C_i and C_j with a specified linkage function:

Initialization

- $C_i = \{i\}$ for all i.
- $D_{ij} =$ distance between data points i and j.

Merge

- Find the pair of clusters C_i and C_j with the minimum distance according to the chosen linkage method.
- Merge C_i and C_j into a new cluster $C_{ij} = C_i \cup C_j$.
- Update the distance matrix D to reflect the distances between the new cluster C_{ij} and the remaining clusters.

Repeat

- Repeat the merging step until only a single cluster remains.

Dendrogram

- Construct a dendrogram to visualize the hierarchy of clusters.

Agglomerative Hierarchical Clustering Example

Example Data:

Let's consider a small dataset with three points in a 2D space:

$$X = \{(2,3), (5,8), (1,1)\}$$

Algorithm Steps:

Step 1: Initialization

- Treat each data point as an individual cluster.
- Compute the distance matrix.

	$(2,3)$	$(5,8)$	$(1,1)$
$(2,3)$	0		
$(5,8)$		0	
$(1,1)$			0

Step 2: Merge

- Find the closest clusters and merge them.

In this example, the closest clusters are (2, 3) and (1, 1). Merge them into a new cluster:

New Cluster: $(2,3) \cup (1,1) = \{(2,3), (1,1)\}$

Update the distance matrix:

	$\{(2,3) \cup (1,1)\}$	$(5,8)$
$\{(2,3) \cup (1,1)\}$	0	
$(5,8)$		0

Step 3: Repeat

- Repeat the process until only one cluster remains.

In the next iteration, the closest clusters are $(2,3) \cup (1,1)$ and (5, 8). Merge them into a new cluster:

New Cluster: $\{(2,3),(1,1),(5,8)\}$

Update the distance matrix:

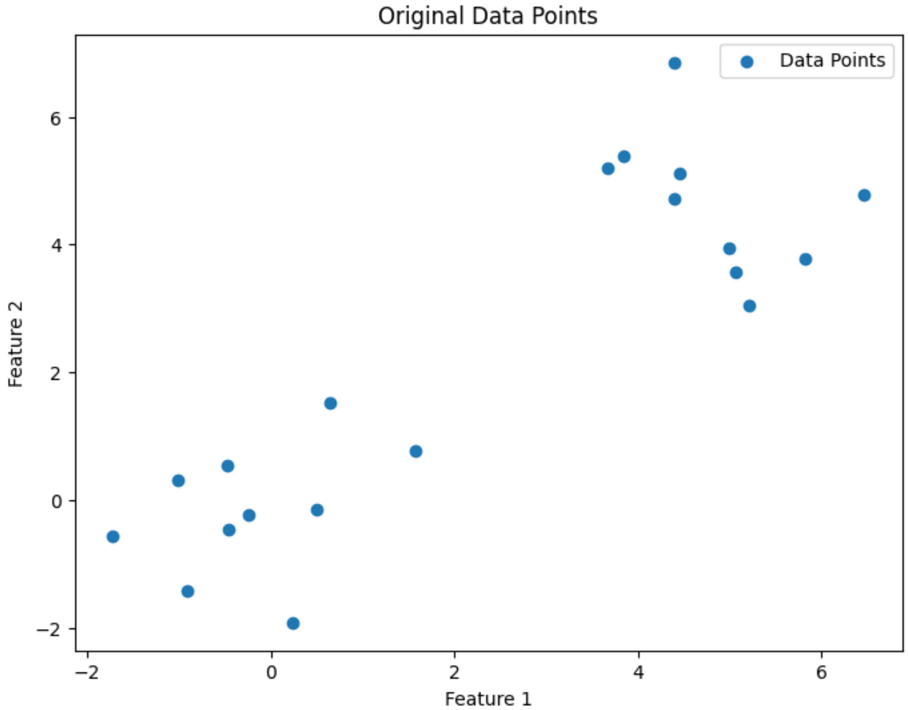
$$\left|\{(2,3),(1,1),(5,8)\}\right|$$

Step 4: Dendrogram

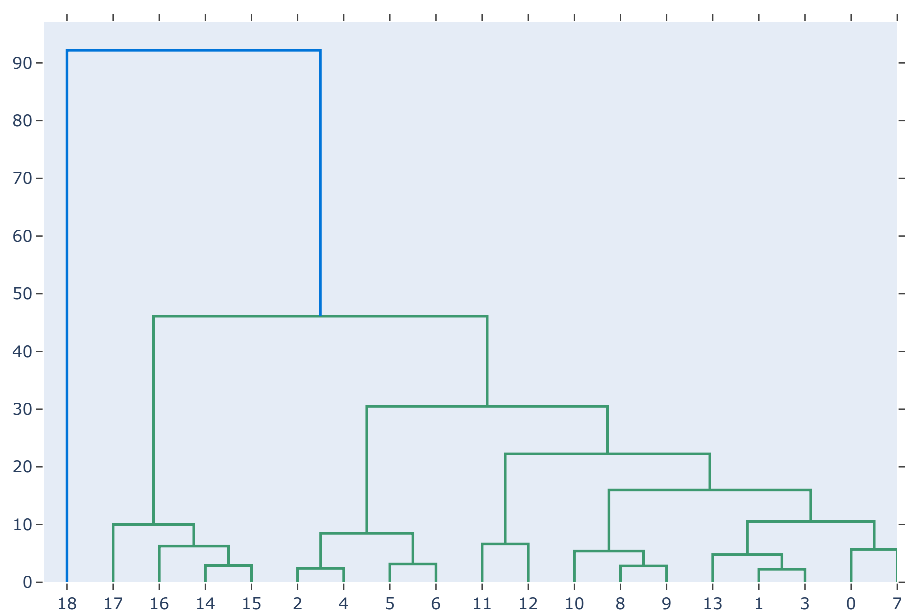
- Construct a dendrogram to visualize the hierarchy of clusters.

The dendrogram shows the merging process and the distances at which clusters were merged.

```
import numpy as np
import plotly.figure_factory as ff
from scipy.cluster.hierarchy import linkage, dendrogram
import matplotlib.pyplot as plt

# Generate a synthetic dataset with two clusters
np.random.seed(42)
cluster1 = np.random.randn(10, 2)
cluster2 = np.random.randn(10, 2) + np.array([5, 5])

X = np.vstack([cluster1, cluster2])

# Plot the original data points
plt.figure(figsize=(8, 6))
plt.scatter(X[:, 0], X[:, 1], label='Data Points')
plt.title('Original Data Points')
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')
plt.legend()
plt.show()

# Calculate pairwise distances
distances = np.linalg.norm(X[:, None] - X, axis=-1)

# Create linkage matrix using Ward's method
Z = linkage(distances, method='ward')

# Create an interactive dendrogram with Plotly
dendrogram = ff.create_dendrogram(Z, orientation='bottom')
dendrogram.update_layout(width=800, height=600)
dendrogram.show()

# # Alternatively, you can also use Matplotlib for visualization
# plt.figure(figsize=(12, 8))
# dendrogram(Z, orientation='top', labels=list(range(1, len(X) + 1)))
# plt.title('Hierarchical Clustering Dendrogram')
# plt.xlabel('Data Points')
# plt.ylabel('Distance')
# plt.show()
```




```
<ipython-input-184-88bbdadf6b0b>:26: ClusterWarning:

scipy.cluster: The symmetric non-negative hollow observation matrix looks suspiciously like an uncondensed distance matrix
```



Advantages

1. **Hierarchy Representation:**
    - Agglomerative Hierarchical Clustering provides a hierarchical structure, allowing users to visualize relationships and similarities among data points at different levels. This facilitates a more nuanced understanding of data structure.

2. **No Fixed Number of Clusters:**
    - Unlike some clustering algorithms, agglomerative hierarchical clustering does not require specifying the number of clusters in advance. This flexibility is beneficial when the optimal number of clusters is unknown.
3. **Flexibility in Linkage Methods:**
    - Users can choose from various linkage methods (e.g., single, complete, average linkage), offering customization based on data characteristics and desired cluster properties.
4. **Interpretability:**
    - The hierarchical structure provides an interpretable representation of relationships between data points, aiding in understanding data structure and making informed decisions.
5. **Incremental Clustering:**
    - Well-suited for incremental clustering, allowing new data points to be added to an existing clustering structure. This adaptability is valuable in scenarios with continuously updated data.
6. **Merge and Split Capability:**
    - Agglomerative clustering supports both merging and splitting of clusters at different hierarchy levels, accommodating various cluster shapes and sizes.
7. **Distance Metric Choice:**
    - Users can choose from a variety of distance metrics based on their data characteristics, making agglomerative hierarchical clustering applicable to different data types.
8. **Noise Handling:**
    - Robust to noise and outliers, as they can be effectively handled during the merging process. This makes it suitable for datasets containing some level of noise.

Limitations:

1. **Computational Complexity:**
    - Agglomerative hierarchical clustering can become computationally expensive, especially for large datasets. The time complexity is O(n^3), making it less efficient for big data scenarios.
2. **Scalability Concerns:**
    - The method may not scale well to large datasets due to its quadratic or cubic time complexity. This can limit its applicability in scenarios with a vast number of data points.
3. **Sensitive to Outliers:**
    - Agglomerative clustering is sensitive to outliers, as they can significantly impact the merging process. Outliers might lead to the formation of suboptimal clusters.
4. **Difficulty in Handling Noise:**
    - While robust to some noise, agglomerative clustering may struggle with high levels of noise, affecting the quality of the resulting clusters.
5. **Subjectivity in Dendrogram Cutting:**
    - Determining the optimal number of clusters involves cutting the dendrogram at a certain height. This process is subjective and may lead to different interpretations and clusterings.
6. **Inability to Undo Merges:**
    - Once clusters are merged, it is not possible to undo the merging process in agglomerative hierarchical clustering. This lack of reversibility can limit its flexibility in certain applications.
7. **Memory Requirements:**
    - The memory requirements can be substantial, especially when dealing with large datasets or deep hierarchies. This may pose challenges for systems with limited memory.
8. **Dependence on Distance Metric:**

- The performance of agglomerative clustering is influenced by the choice of distance metric. Different metrics may lead to different cluster structures, and selecting an appropriate metric is crucial.

9. **Difficulty with Irregular Cluster Shapes:**
    - Agglomerative hierarchical clustering may struggle with datasets containing irregularly shaped clusters, as the method tends to form spherical or convex clusters.
10. **Limited to Euclidean Spaces:**
    - The algorithm is more naturally suited for data in Euclidean spaces, and its performance may degrade when dealing with non-Euclidean or high-dimensional data.