Advanced Data Analysis

DATA 71200

Class 12: Unsupervised Learning (Clustering)

Clustering

- **Algorithms that assign data points to groups (especially for unlabeled data)**
  - In the absence of labels, evaluation is challenging
    - Often performed through visualization
- **Useful for**
  - Exploratory data analysis
  - Pre-processing data

k-Means

- ***k*** **- number of clusters specified**
- **Finds cluster centers through an iterative process**
  - Assign data points to cluster with nearest cluster center
    - Initialized randomly for the first iteration
  - Update the cluster center with the assigned data points
  - Repeat until no updates are needed
- **Boundaries are determined by placement of cluster centers**

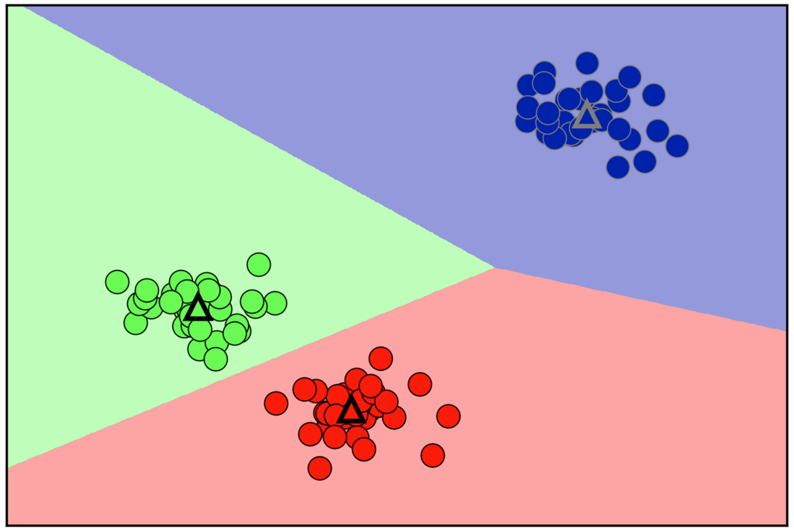

Figure 3-24. Cluster centers and cluster boundaries found by the k-means algorithm

Muller, Andreas C. and Sarah Guido. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

k-Means

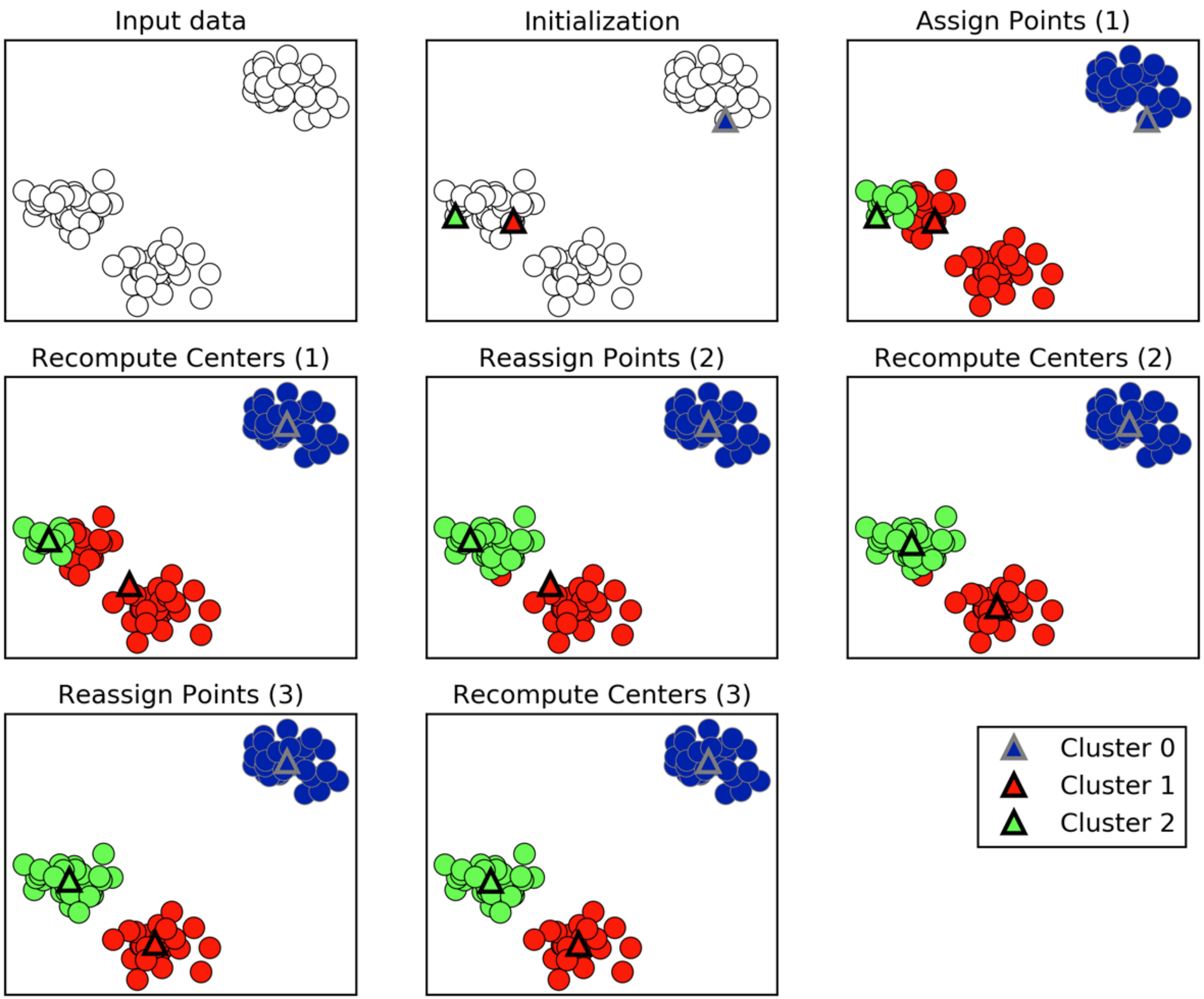

Figure 3-23. Input data and three steps of the k-means algorithm

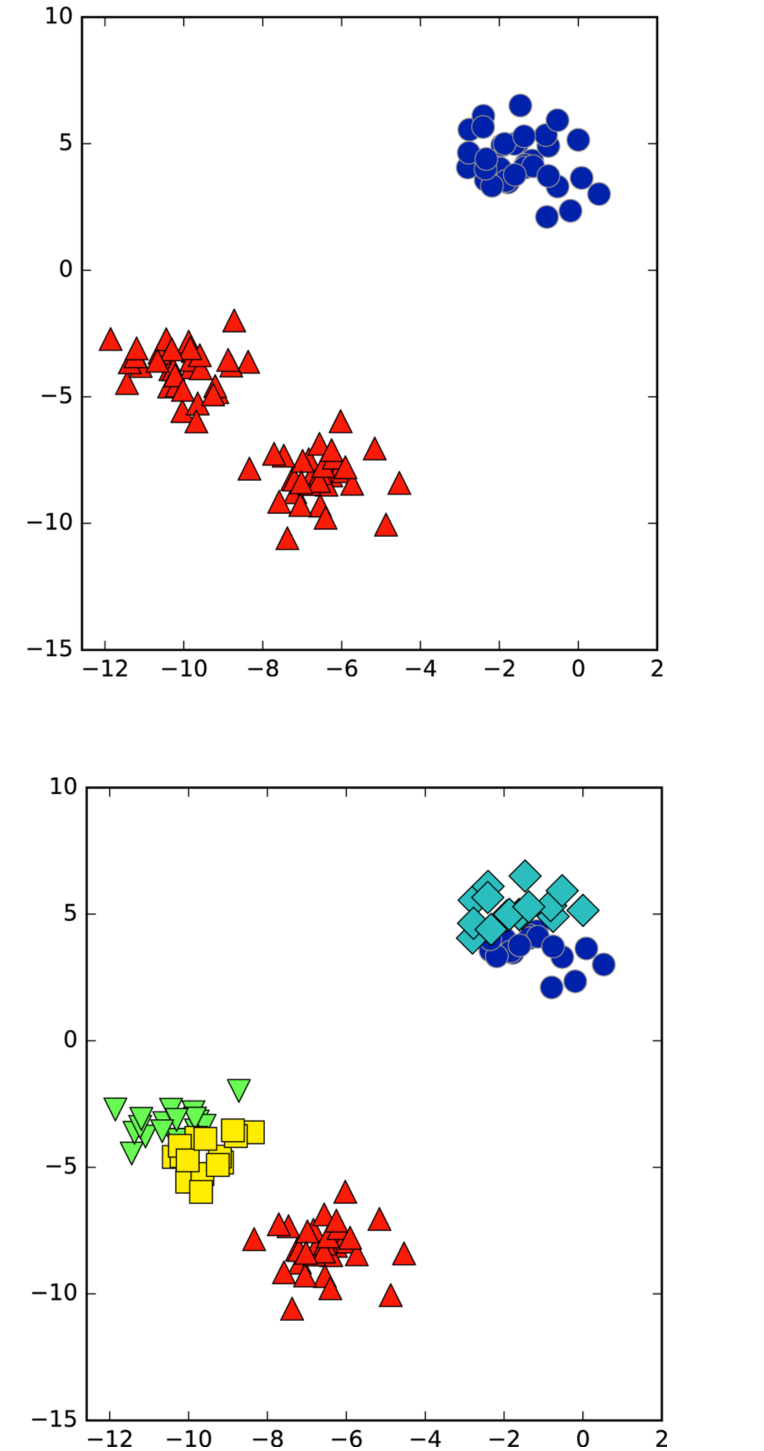

Figure 3-26. Cluster assignments found by k-means using two clusters (top) and five clusters (bottom)

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k-Means

- **Assumes the classes have the same width/diameter**
- **This causes issues with non-spherical clusters or clusters with complex shapes**

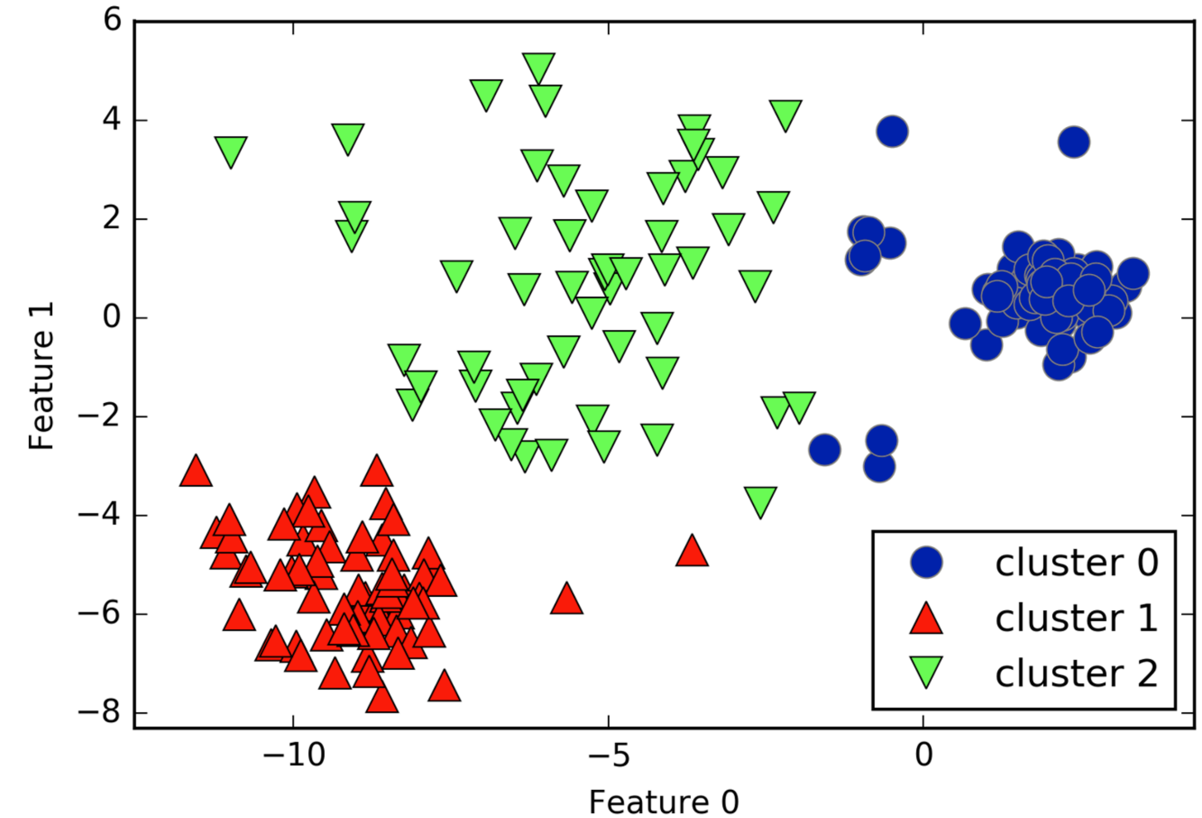

Figure 3-27. Cluster assignments found by k-means when clusters have different densities

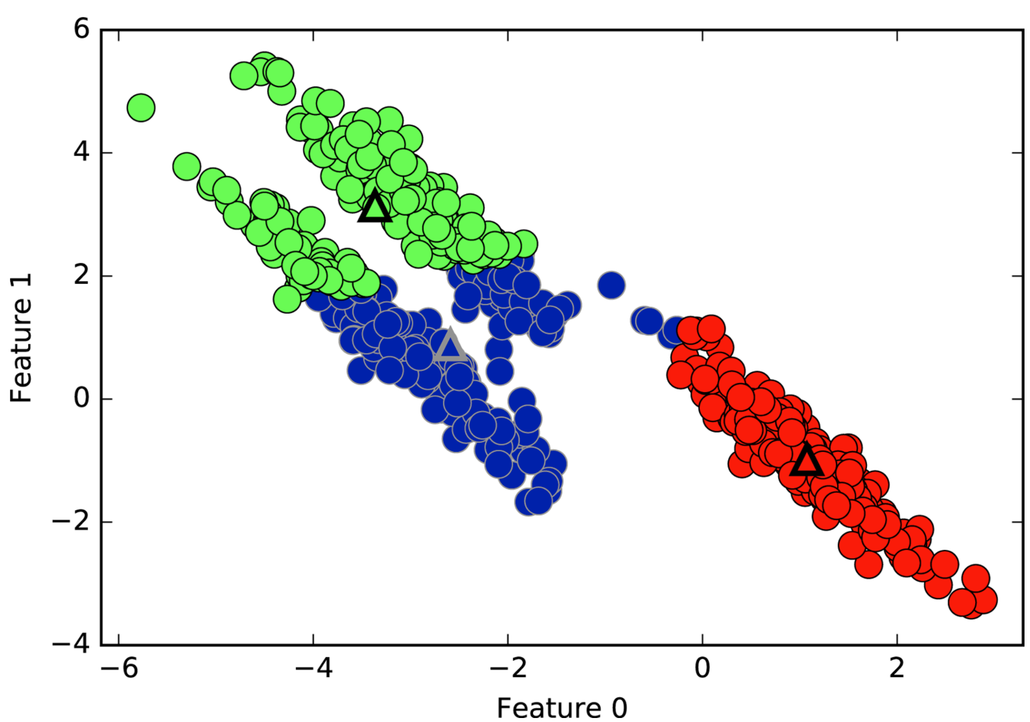

Figure 3-28. k-means fails to identify nonspherical clusters

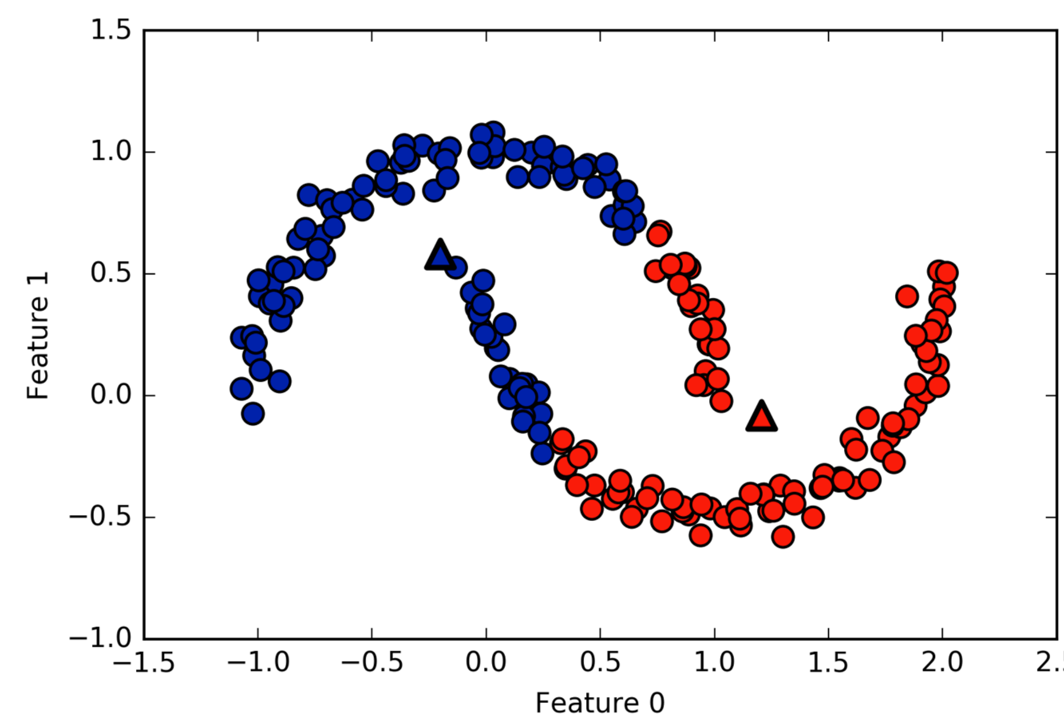

Figure 3-29. k-means fails to identify clusters with complex shapes

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k-Means

- **The constant-width limitation can be partially overcome with a larger number of clusters**

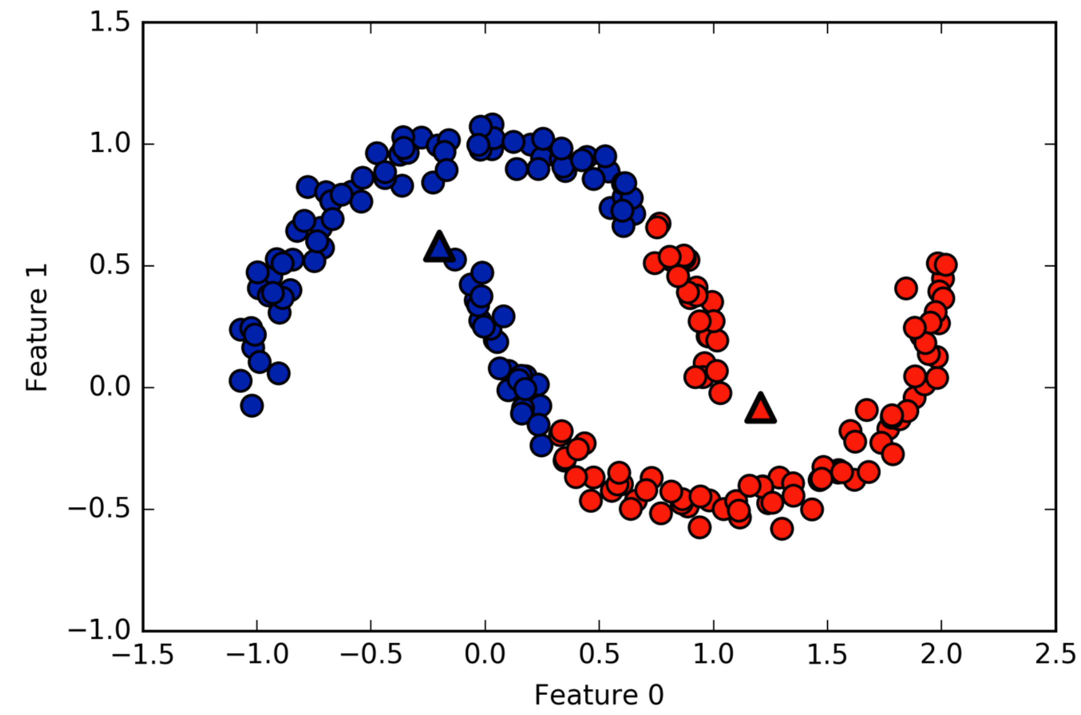

Figure 3-29. k-means fails to identify clusters with complex shapes

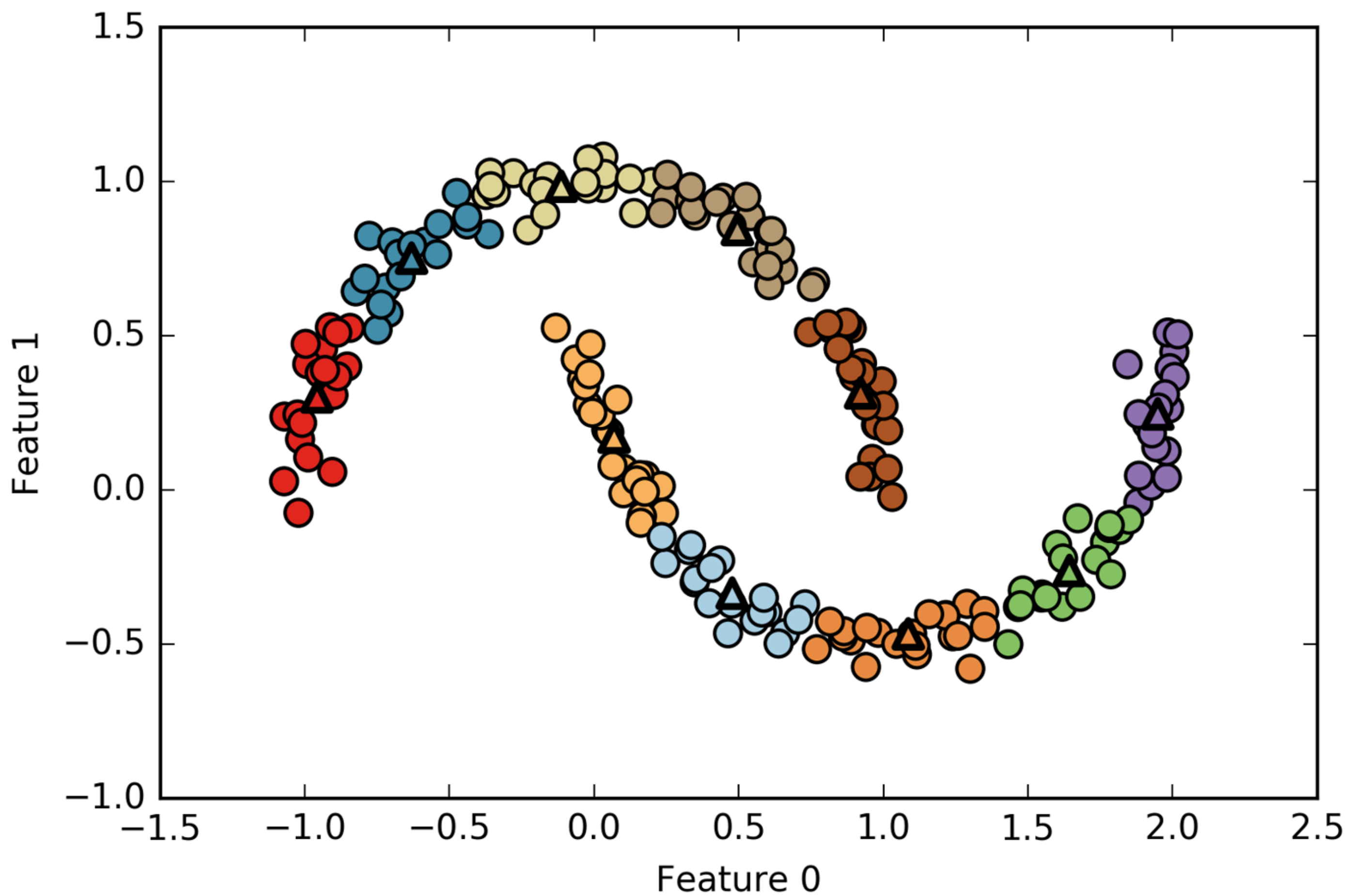

Figure 3-32. Using many k-means clusters to cover the variation in a complex dataset

Muller, Andreas C. and Sarah Guido. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

k-Means

- **Best Practices**
  - Can run in batches on very large datasets
- **Strengths**
  - Easy to understand
  - Runs relatively quickly
- **Weaknesses**
  - Based on random initialization
  - Need to specify the number of clusters
  - Clusters have consistent widths and shapes

Agglomerative Clustering

- Starts by creating a cluster for each point
- Then amalgamates nearest clusters based on linkage criteria until the stopping criteria is reached

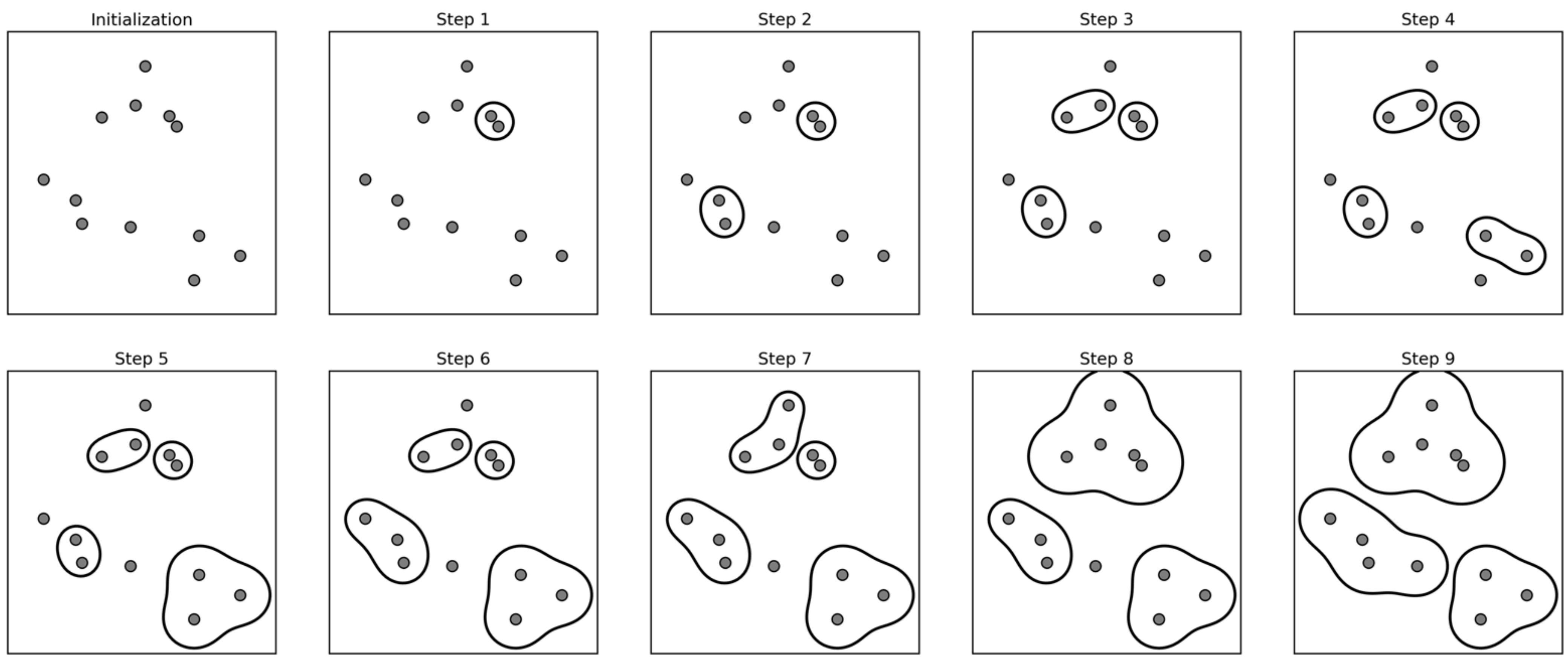

Figure 3-33. Agglomerative clustering iteratively joins the two closest clusters

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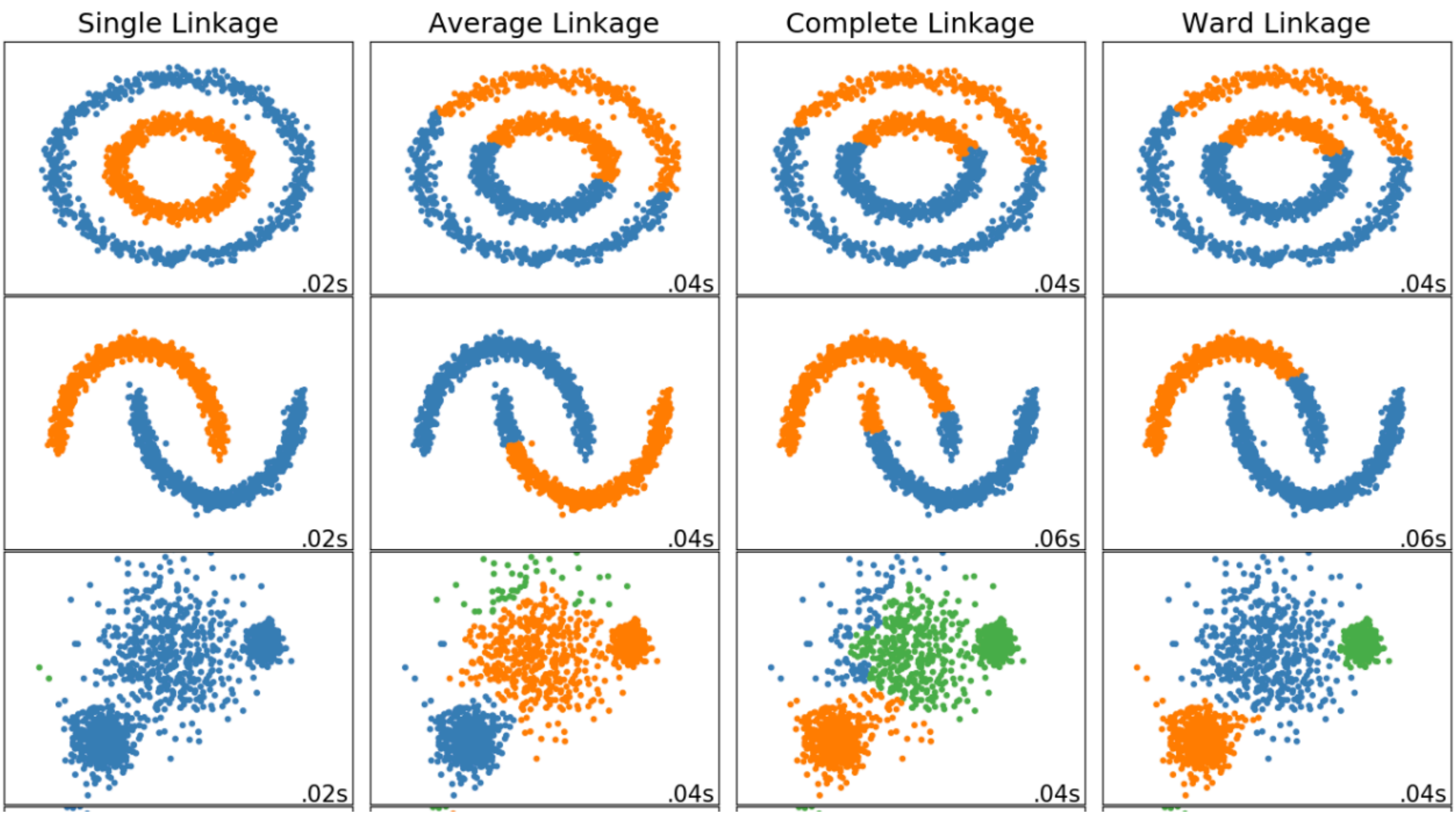
Agglomerative Clustering



uses the **minimum** of the distances between all observations of the two sets

uses the **average** of the distances of each observation of the two sets

uses the **maximum** distances between all observations of the two sets

minimizes the **variance** of the clusters being merged

https://towardsdatascience.com/machine-learning-algorithms-part-12-hierarchical-agglomerative-clustering-example-in-python-1e18e0075019
https://scikit-learn.org/stable/modules/generated/sklearn.cluster.AgglomerativeClustering.html

Agglomerative Clustering

- Looking at all possible clusters simultaneously provides information about the hierarchical relationship of the clusters
- Dendrograms allow for visualization of multidimensional datasets, also providing information about cluster distance

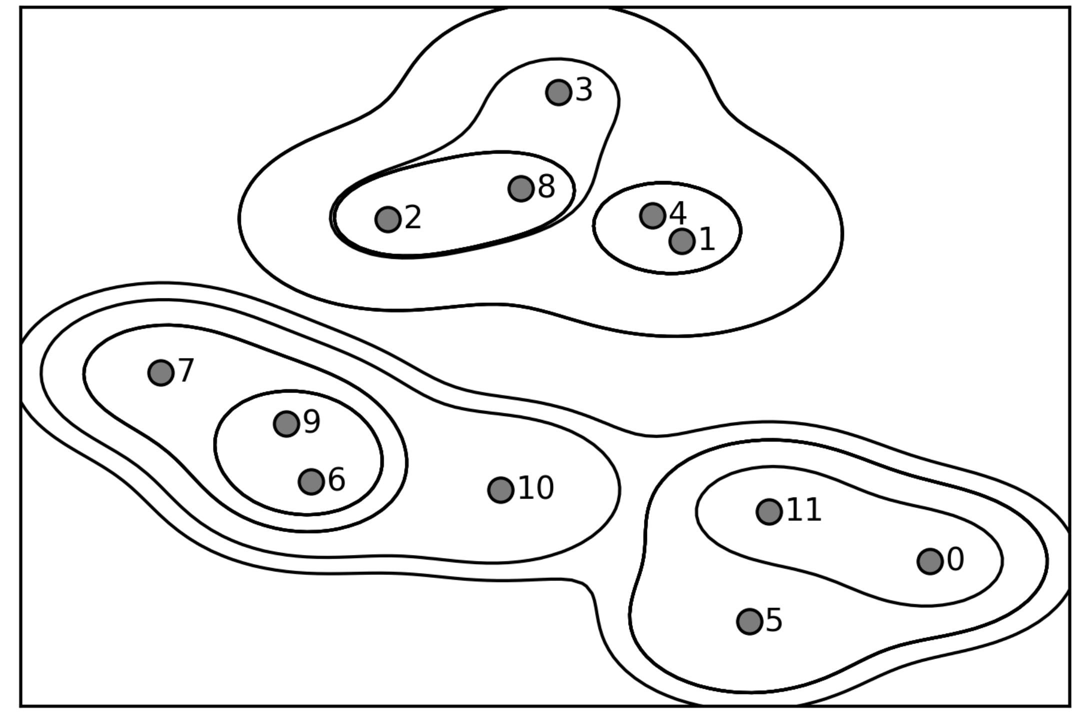


Figure 3-35. Hierarchical cluster assignment (shown as lines) generated with agglomerative clustering, with numbered data points (cf. Figure 3-36)

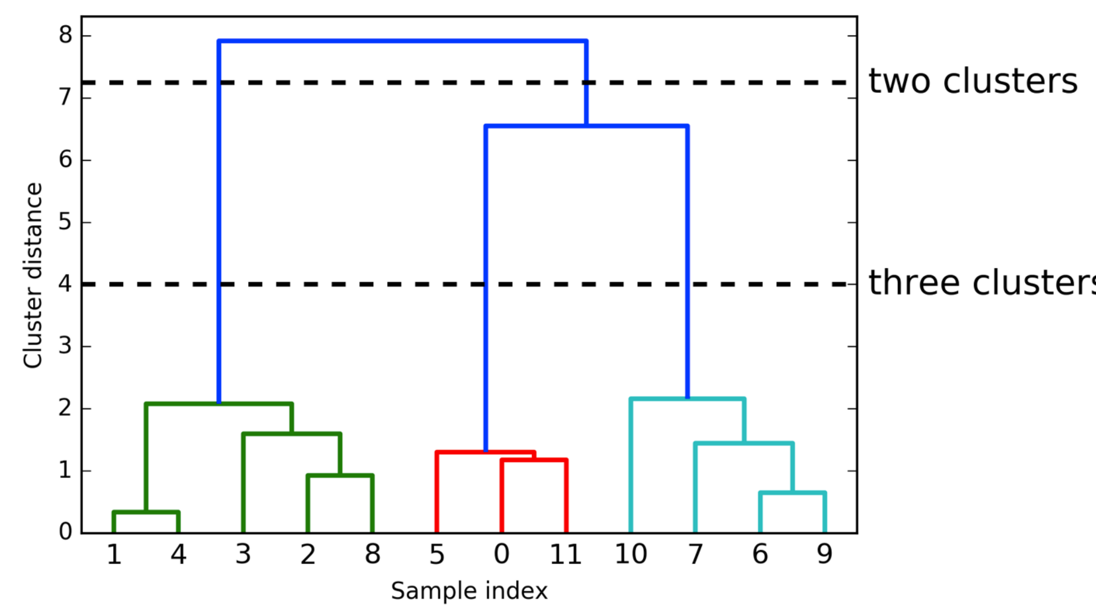


Figure 3-36. Dendrogram of the clustering shown in Figure 3-35 with lines indicating splits into two and three clusters

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Agglomerative Clustering

- **Parameters**
  - Linkage criteria: ward, average, complete
  - Stopping criteria: number of clusters
- **Strengths**
  - Easy to understand/visualize
- **Weaknesses**
  - Not able to make prediction on new data
  - In scikit-learn you need to specify the number of clusters

DBSCAN

- **Density-based spatial clustering of applications with noise**
- **Do not need to specify the number of clusters**
- **Attempts to distinguish between densely and sparsely populated areas of the data space**
  - Core points - cluster centers
  - Boundary points - within a cluster
  - Noise

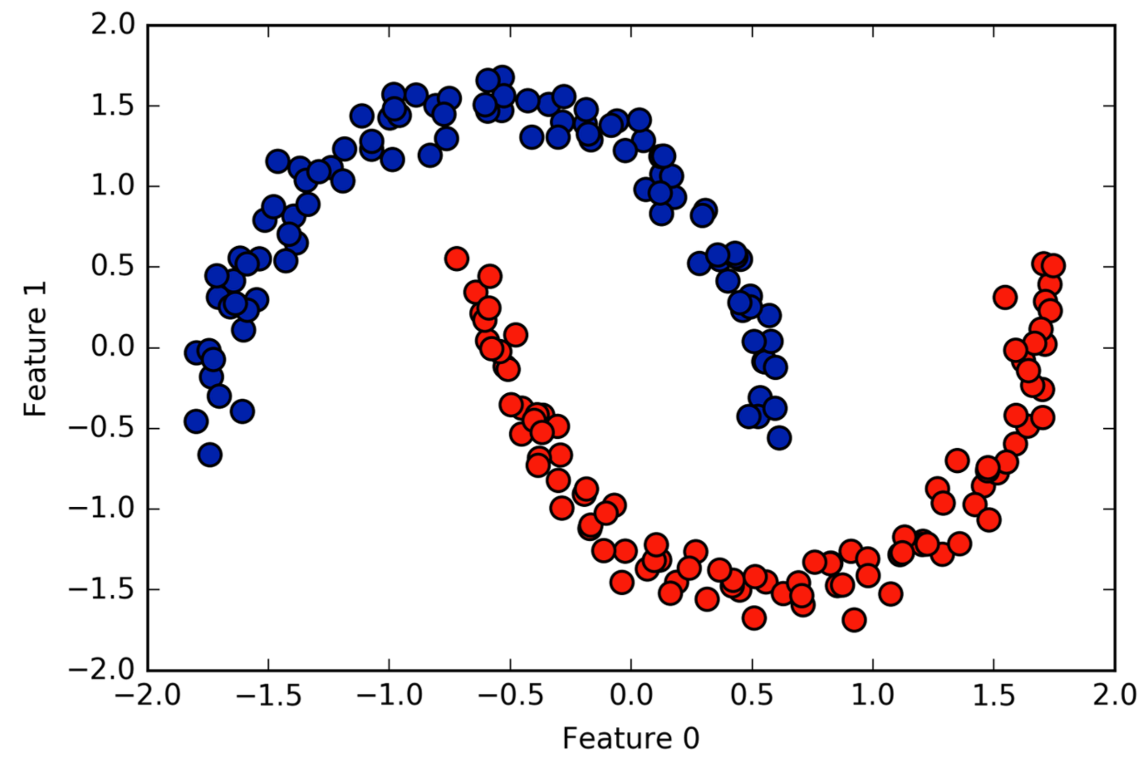

Figure 3-38. Cluster assignment found by DBSCAN using the default value of eps=0.5

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DBSCAN

- Procedure (repeated until clusterable data has been addressed)
    - Select a data point and check how many other data points are within the specified distance
    - If there are as many as the specified minimum number, data point is considered a core sample
        - Data points within the minimum distance are boundary points
    - If there are multiple core samples within the specified distance, they are merged into a single cluster and their neighbors are also visited
- If points aren't clustered, they are classified as noise

DBSCAN

- **Increasing eps results in more points per cluster**
- **Increasing min_samples results in more being classified as noise**

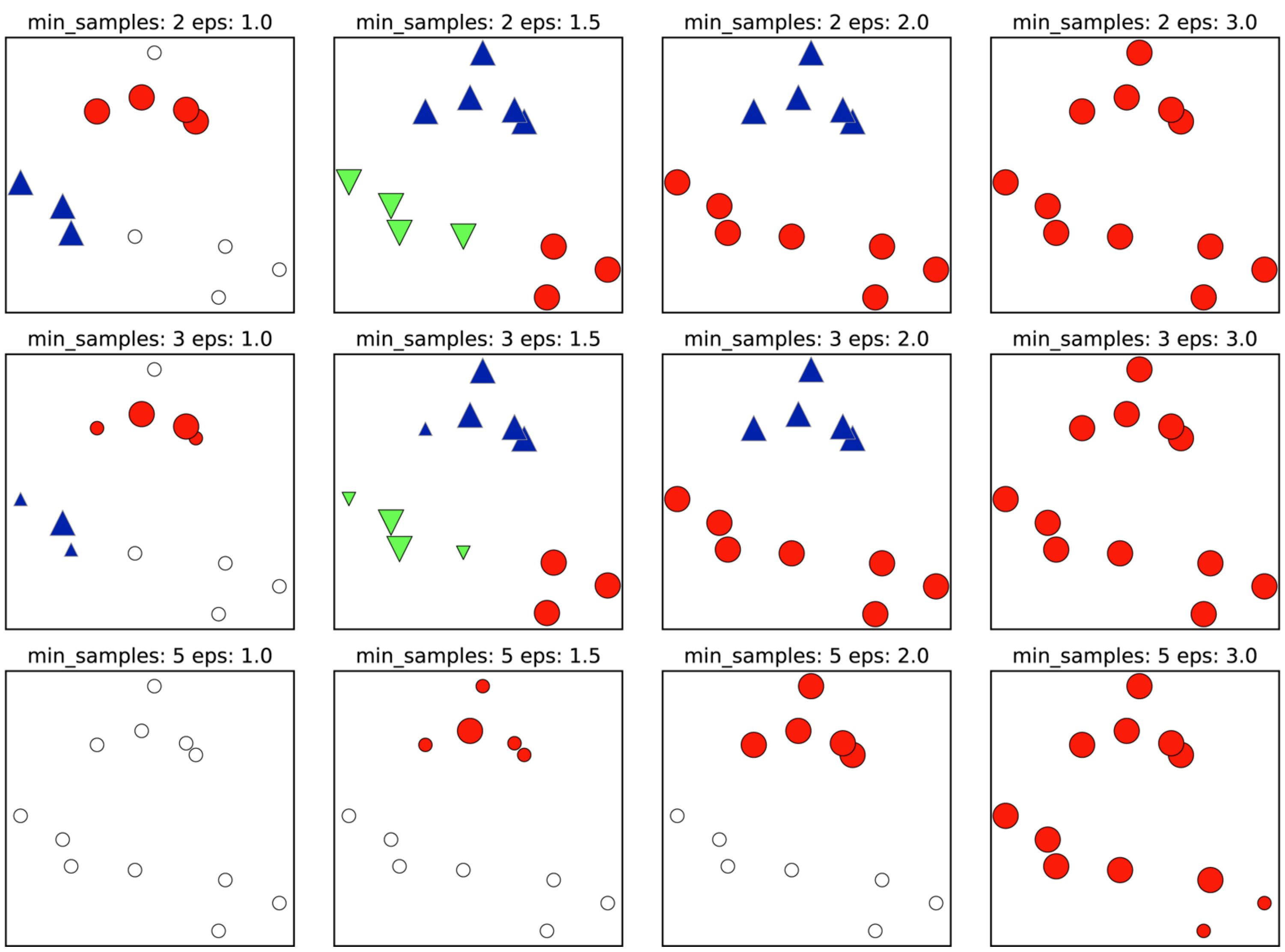

Figure 3-37. Cluster assignments found by DBSCAN with varying settings for the min_samples and eps parameters

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DBSCAN

- **Best Practices**
  - Scaling data can improve clustering results with DBSCAN
- **Parameters**
  - eps - determines distance the algorithm looks for data points
  - min_samples - determines the minimum number of data points within eps distance necessary to form a cluster
- **Strengths**
  - Able to cluster complex shapes
- **Weaknesses**
  - Cluster assignment depends on order the points are visited
  - Results sensitive to the settings of min_samples and eps

Evaluating Clustering

With Ground Truth: Adjusted Rand Index (ARI)

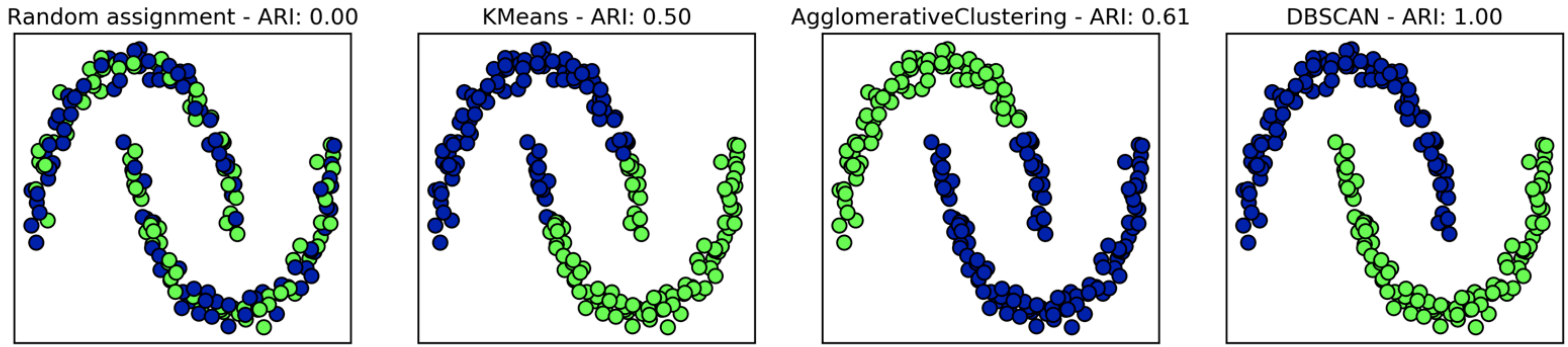

Figure 3-39. Comparing random assignment, k-means, agglomerative clustering, and DBSCAN on the two_moons dataset using the supervised ARI score

With No Ground Truth: Silhouette Coefficient

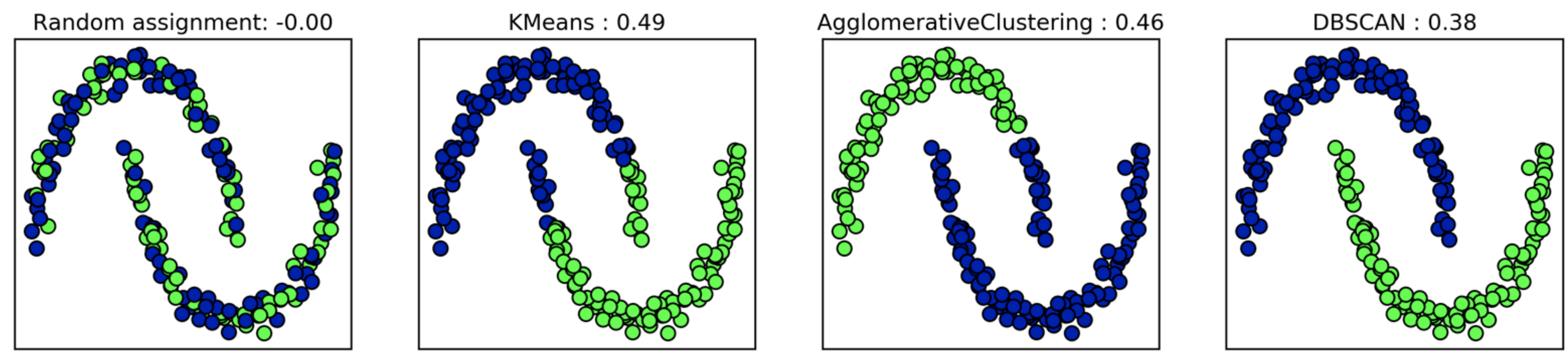

Figure 3-40. Comparing random assignment, k-means, agglomerative clustering, and DBSCAN on the two_moons dataset using the unsupervised silhouette score—the more intuitive result of DBSCAN has a lower silhouette score than the assignments found by k-means

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