Unsupervised Learning (Detailed)

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The need for Unsupervised Learning

- Aids the search of patterns in data.
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Places where you will see unsupervised learning

- It can be used to segment the market based on customer preferences.
- A data science team reduces the number of dimensions in a large dataset to simplify modeling and reduce file size.
- Anomaly detection in network traffic or fraud detection
- Document clustering and topic modeling
- Image segmentation in computer vision
- Gene expression analysis in bioinformatics

Real-World Examples of Unsupervised Learning

- **E-commerce**: Grouping customers by purchasing behavior for personalized recommendations
- **Social Networks**: Detecting communities and user groups
- **Healthcare**: Identifying disease subtypes from patient data
- **Astronomy**: Classifying galaxies and celestial objects
- **Climate Science**: Identifying weather patterns and climate zones
- **Manufacturing**: Quality control by detecting anomalous products

Clustering

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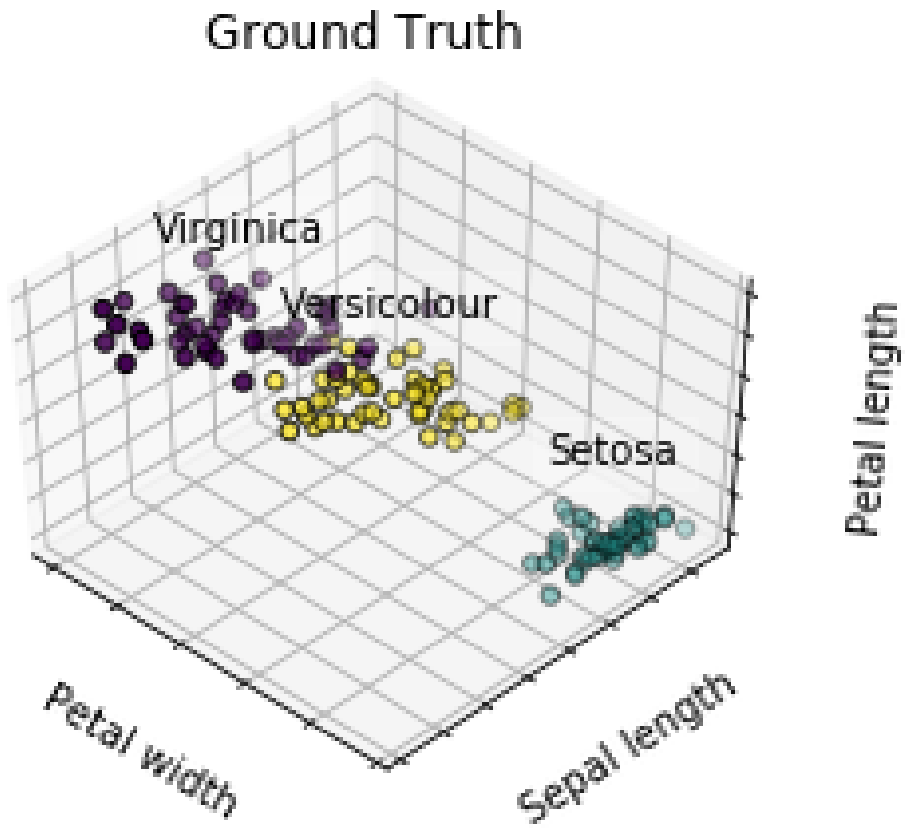
REQUIREMENTS: A predefined notion of similarity/dissimilarity. **Examples:**
Market Segmentation: Customers with similar preferences in the same groups. This would aid in targeted marketing.

Clustering



Iris Data Set with ground truth

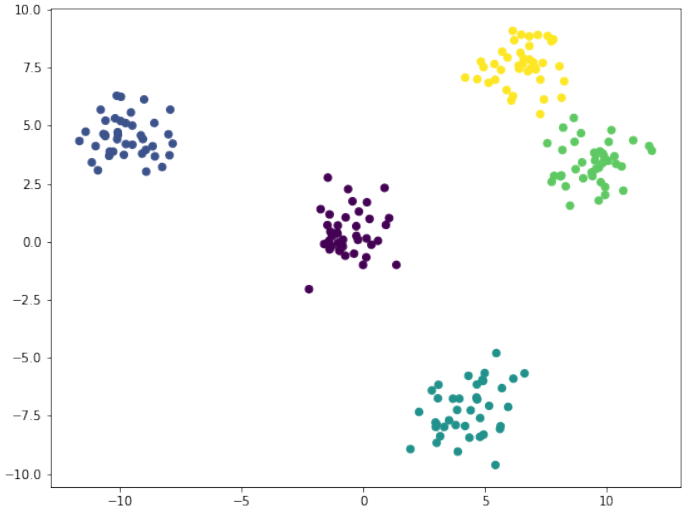
Types of Clustering Algorithms

- **Partitioning Methods**: K-Means, K-Medoids
- **Hierarchical Methods**: Agglomerative, Divisive
- **Density-Based Methods**: DBSCAN, OPTICS
- **Model-Based Methods**: Gaussian Mixture Models
- **Grid-Based Methods**: STING, CLIQUE

K-Means Clustering

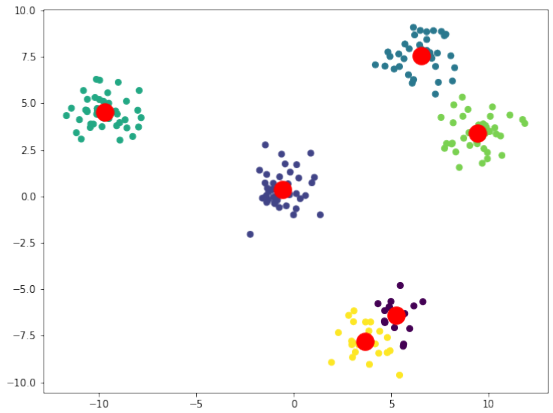
K-Means Clustering

- N points in a R^d space.
- C_i: set of points in the i^{th} cluster.
- $C_1 \cup C_2 \cup \ldots C_k = \{1, \ldots, n\}$
- $C_i \cap C_j = \{\phi\}$ for $i \neq j$

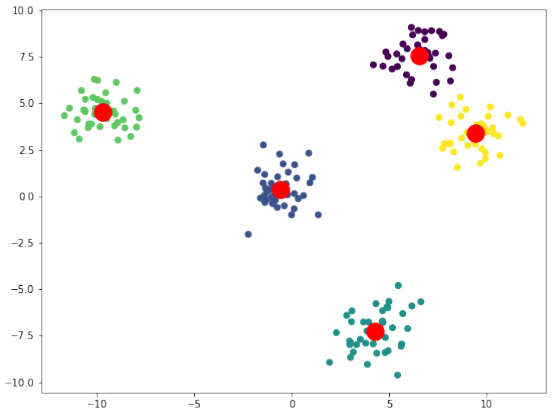


Dataset with 5 clusters

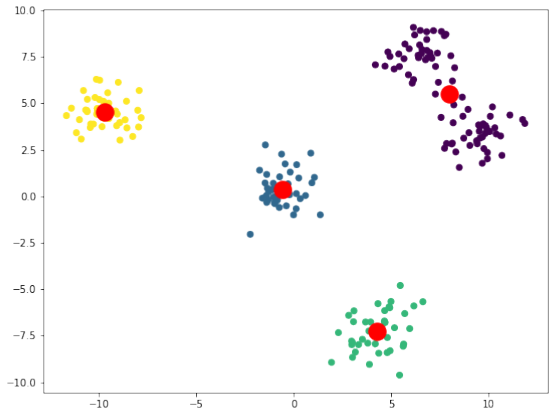
K-Means Clustering



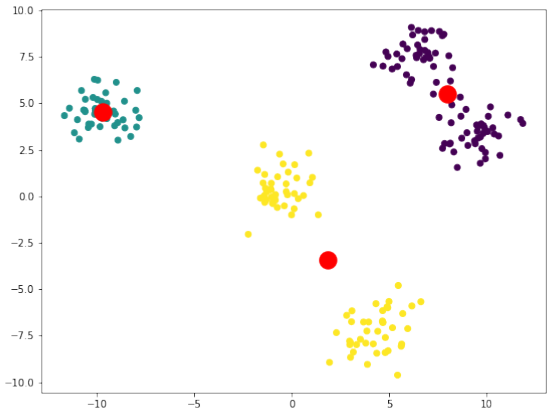
K=6



K=5



K=4



K=3

K-Means Intuition

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$$WCV\left(C_i\right) = \frac{1}{|C_i|} \texttt{ (Distance between all points)}$$

$$WCV\left(C_i\right) = \frac{1}{|C_i|} \sum_{a \in C_i} \sum_{b \in C_i} ||x_a - x_b||_2^2$$

where $|C_i|$ is the number of points in C_i

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1. Randomly assign a cluster number i to every point (where $i \in \{1, \ldots k\}$)
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Working of K-Means Algorithm

K-Means Convergence: Intuitive Proof (1/3)

Key Idea: The objective function (total within-cluster variance) decreases at each step and is bounded below.

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Objective Function:

$$J = \sum_{i=1}^{k} \sum_{x \in C_i} ||x - \mu_i||^2$$

where μ_i is the centroid of cluster C_i

K-Means Convergence: Intuitive Proof (2/3)

Step 1: Update Centroids

- Fix cluster assignments, optimize centroids
- For each cluster C_i, the centroid that minimizes $\sum_{x \in C_i} ||x - \mu_i||^2$ is $\mu_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$
- This is the mean of the points in the cluster
- This step cannot increase J (optimal choice given fixed assignments)

K-Means Convergence: Intuitive Proof (3/3)

Step 2: Update Assignments

- Fix centroids, reassign each point to nearest centroid
- For each point x, assign to $\arg\min_i ||x - \mu_i||^2$
- This step cannot increase J (each point moves to minimize its contribution)

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Conclusion:

- J decreases (or stays same) at each iteration
- $J \geq 0$ (bounded below)
- Finite number of possible assignments
- Therefore, algorithm must converge!

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Note: Converges to a **local minimum**, not necessarily global

Why does K-Means work?

$$\text{Let, } \mu_i \in R^d = \text{Centroid for } i^{th} \text{ cluster}$$

$$= \frac{1}{|C_i|} \sum_{a \in C_i} x_a$$

Why does K-Means work?

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This shows that K-Means gives the **local minima**.

K-Means: Time and Space Complexity

Time Complexity:

- Per iteration: $O(nkd)$ where
  - n = number of points
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  - d = number of dimensions
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- Store data points and centroids

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Practical Note: Usually converges quickly, but worst-case can be exponential

K-Means Failure Modes

K-Means Failure Mode 1: Non-Spherical Clusters

- K-Means assumes spherical (isotropic) clusters
- Fails with elongated, elliptical, or irregular shapes
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Example: Two elongated, parallel clusters will be incorrectly split

K-Means Failure Mode 2: Different Cluster Sizes

- K-Means tends to create equal-sized clusters
- Struggles when true clusters have vastly different sizes
- Large clusters may be split, small clusters may be merged

K-Means Failure Mode 3: Different Densities

- Assumes similar density across all clusters
- Fails when clusters have different densities
- Dense clusters may be over-segmented
- Sparse clusters may absorb nearby points incorrectly

K-Means Failure Mode 4: Non-Convex Shapes

- K-Means creates convex decision boundaries
- Cannot handle non-convex shapes (e.g., crescents, rings)
- Example: Two interleaving half-moon shapes

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Solution: Use kernel K-Means or other methods (DBSCAN, spectral clustering)

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- Random initialization can lead to poor local minima
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Solution: K-Means++ initialization (discussed next!)

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Solutions:

- Pre-process to remove outliers
- Use K-Medoids (more robust)
- Use trimmed K-Means

K-Means Failure Mode 7: Choosing K

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Methods to choose K:

- Elbow method (plot inertia vs k)
- Silhouette analysis
- Gap statistic
- Domain knowledge

K-Means++

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Key Idea:

- First centroid: chosen uniformly at random
- Subsequent centroids: chosen with probability proportional to squared distance from nearest existing centroid
- Spreads out initial centroids

K-Means++ Algorithm

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2. For $i = 2, 3, \ldots, k$:
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3. Proceed with standard K-Means algorithm

K-Means++: Why Does It Work?

Intuition:

- Points far from existing centroids are more likely to be chosen
- Ensures good coverage of the data space
- Reduces chance of multiple centroids in same cluster

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Theoretical Guarantee:

- K-Means++ initialization is $O(\log k)$-competitive with optimal clustering
- Expected objective value is at most $O(\log k)$ times optimal
- Much better than random initialization (no guarantees)

K-Means++ Example (1/3)

Step 1: Choose first centroid randomly

- Say we pick point A
- $\mu_1 = A$

K-Means++ Example (2/3)

Step 2: Choose second centroid

- Compute $D(x)^2$ for all points (distance to A)
- Point B very far from A has high $D(B)^2$
- Point C close to A has low $D(C)^2$
- Probability of choosing B as μ_2 is much higher than C

K-Means++ Example (3/3)

Step 3: Choose third centroid (if $k = 3$)

- Now compute $D(x)^2 =$ min distance to μ_1 or μ_2
- Points far from both A and B have higher probability
- Likely to choose point from third cluster region

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Result: Initial centroids spread across data, one per true cluster (ideally)

K-Means++ vs Standard K-Means

Advantages of K-Means++:

- Better convergence to global optimum
- Fewer iterations typically needed
- More consistent results across runs
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Practical Note: K-Means++ is now the default in most libraries (scikit-learn, etc.)

Hierarchical Clustering

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Gives a clustering of all the clusters

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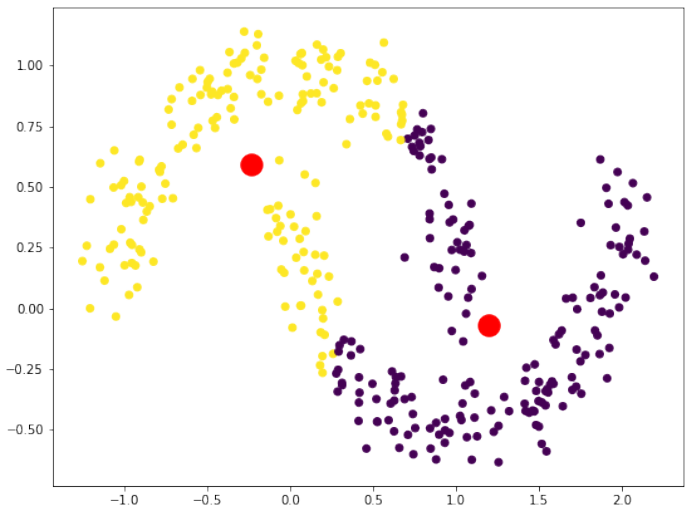
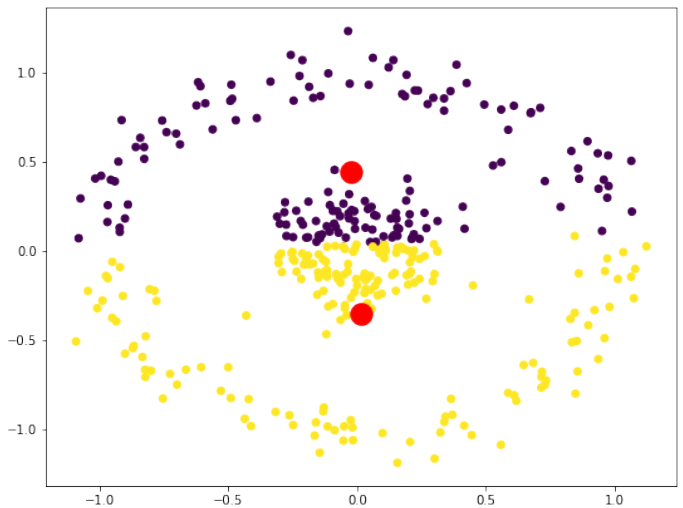


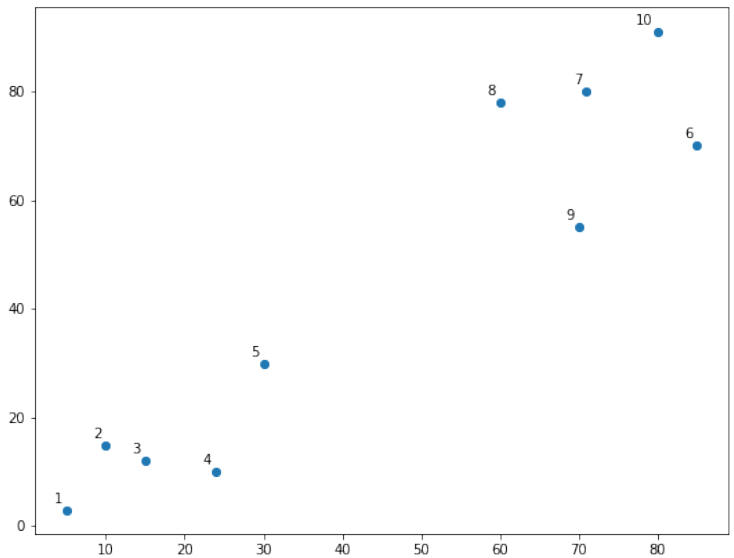


Examples where K-Means fails

Algorithm for Hierarchical Clustering

Agglomerative (Bottom-Up):

1. Start with each point in its own cluster (n clusters)



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Algorithm for Hierarchical Clustering

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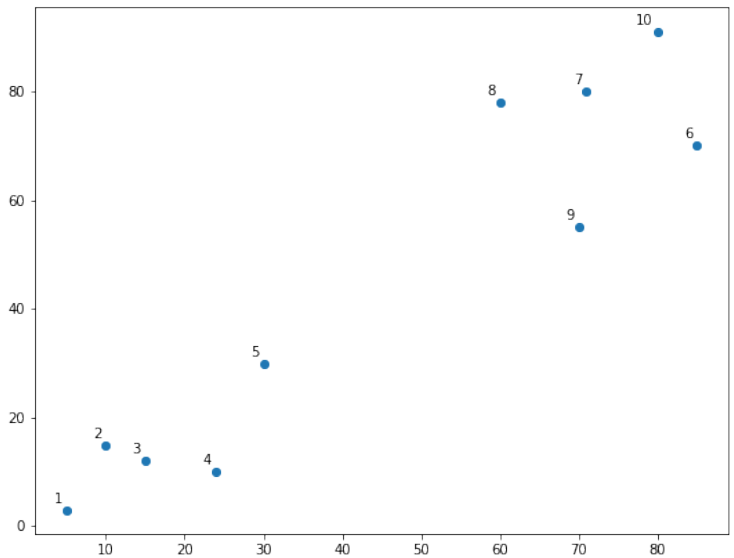

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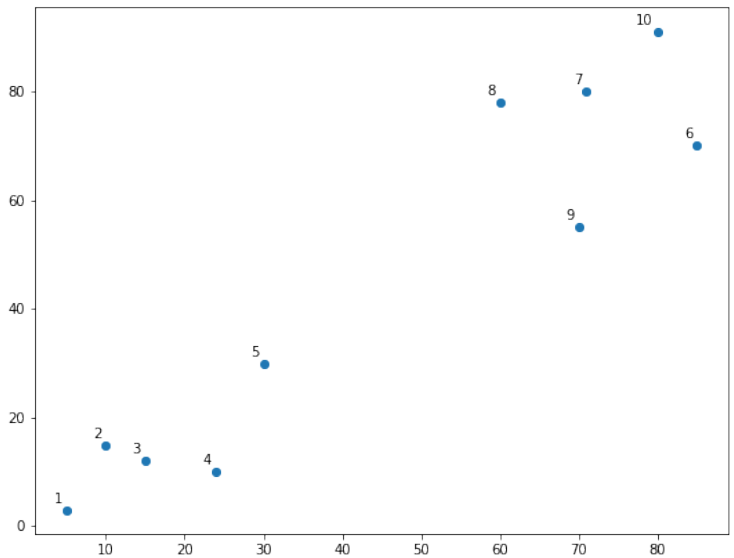

Example Dataset

Algorithm for Hierarchical Clustering

Agglomerative (Bottom-Up):

1. Start with each point in its own cluster (n clusters)
2. Repeat until all points are in a single cluster:
   1) Identify the 2 closest clusters
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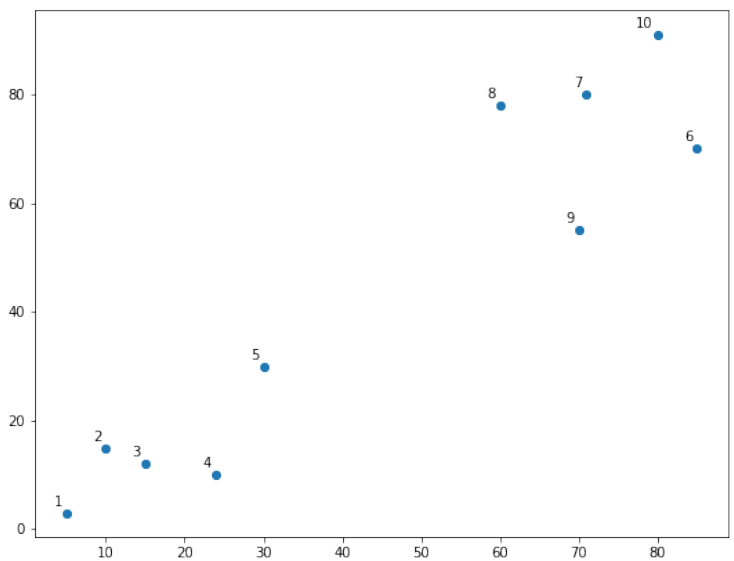

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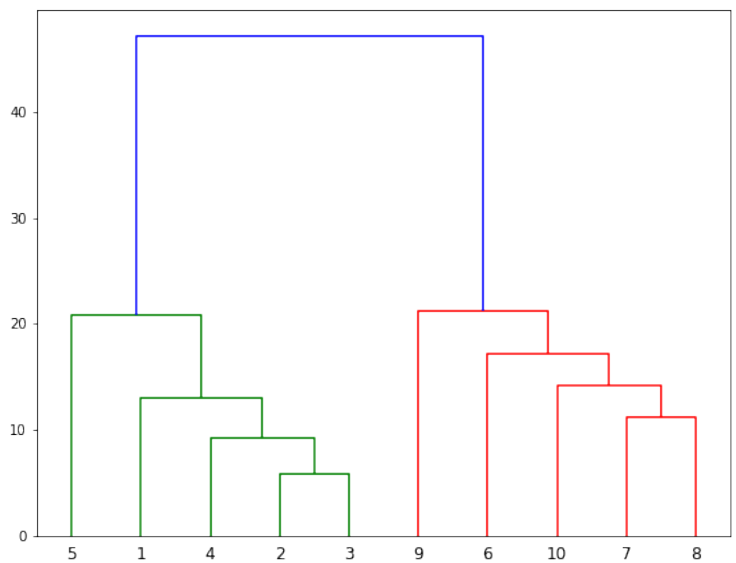

Final Clustering

Joining Clusters/Linkages

Complete
Max inter-cluster similarity

Single
Min inter-cluster similarity

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Dissimilarity between cluster centroids

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Average Linkage: Average distance between all pairs of points

- $d(C_i, C_j) = \frac{1}{|C_i||C_j|} \sum_{x \in C_i} \sum_{y \in C_j} d(x, y)$

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Ward's Method: Minimizes within-cluster variance when merging

Density-Based Clustering

Density-Based Clustering: Motivation

Problem with K-Means and Hierarchical:

- Assume clusters are convex and isotropic
- Struggle with arbitrary shapes
- Sensitive to noise and outliers

Density-Based Clustering: Motivation

Problem with K-Means and Hierarchical:

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Density-Based Idea:

- Clusters are dense regions separated by sparse regions
- Can find arbitrarily shaped clusters
- Can identify noise/outliers

DBSCAN: Density-Based Spatial Clustering

Key Concepts:

- ϵ-**neighborhood**: Points within distance ϵ of a point p
- **Core point**: Has at least `MinPts` points in its ϵ-neighborhood
- **Border point**: Not a core point, but in ϵ-neighborhood of core point
- **Noise point**: Neither core nor border

DBSCAN Algorithm

Parameters: ϵ (radius), `MinPts` (minimum points)

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Algorithm:

1. Mark all points as unvisited
2. For each unvisited point p:
   1) Mark p as visited
   2) Find all points in ϵ-neighborhood of p
   3) If $|\text{neighborhood}| \geq$ `MinPts`:
      - Create new cluster
      - Add p and expand cluster (recursively add neighbors)
   4) Else: mark p as noise (may be changed later)

DBSCAN: Advantages

- Can find arbitrarily shaped clusters
- Robust to outliers (marks them as noise)
- No need to specify number of clusters
- Only two parameters: ϵ and `MinPts`
- Deterministic (same result each run)

DBSCAN: Disadvantages

- Sensitive to parameter choice (ϵ, `MinPts`)
- Struggles with varying density clusters
- Not suitable for high-dimensional data (curse of dimensionality)
- Cannot cluster datasets with large differences in densities
- Time complexity: $O(n^2)$ (can be $O(n \log n)$ with spatial index)

DBSCAN Example

Dataset: Points in 2D with two clusters and noise

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Parameters: $\epsilon = 0.5$, $\texttt{MinPts} = 4$
Result:

- Dense regions become clusters
- Sparse points between clusters marked as noise
- Can handle non-convex shapes (e.g., crescents, rings)

Choosing DBSCAN Parameters

ϵ **(radius)**:

- Plot k-nearest neighbor distance graph
- Look for "elbow" where distance increases sharply
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`MinPts`:

- Rule of thumb: $\texttt{MinPts} \geq d + 1$ where d is dimensionality
- Larger values: more robust to noise, but may merge clusters
- Smaller values: more sensitive, may create many small clusters

Density-Based Methods: Variants

OPTICS (Ordering Points To Identify Clustering Structure):

- Extension of DBSCAN
- Produces reachability plot showing cluster structure
- Can extract clusters at different densities

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HDBSCAN (Hierarchical DBSCAN):

- Builds hierarchy of clusters
- Automatically selects stable clusters
- More robust parameter selection

Comparing Clustering Methods

Method	**Shape**	**Outliers**	**K?**	**Speed**
K-Means	Spherical	Sensitive	Yes	Fast
K-Means++	Spherical	Sensitive	Yes	Fast
Hierarchical	Any	Sensitive	No	Slow
DBSCAN	Arbitrary	Robust	No	Medium

Comparing Clustering Methods

Method	Shape	Outliers	K?	Speed
K-Means	Spherical	Sensitive	Yes	Fast
K-Means++	Spherical	Sensitive	Yes	Fast
Hierarchical	Any	Sensitive	No	Slow
DBSCAN	Arbitrary	Robust	No	Medium

Choosing a Method:

- Known k, spherical clusters: K-Means++
- Arbitrary shapes, noise: DBSCAN
- Hierarchy needed: Hierarchical
- Large data: K-Means++ or Mini-Batch K-Means

More Code

Google Colab Link