Unsupervised Learning: Clustering

Finding Structure in Unlabeled Data

Nipun Batra

IIT Gandhinagar

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What We'll Learn Today

1. **Why** unsupervised learning? (Motivation)
2. **What** is clustering? (Intuition first!)
3. **How** does K-Means work? (Step-by-step)
4. **When** does it fail? (Limitations)
5. **What** are alternatives? (Hierarchical, DBSCAN)

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5. **What** are alternatives? (Hierarchical, DBSCAN)

Key Points: Key Points

Key Philosophy: We'll build intuition with examples, then add rigor!

Motivation

Supervised vs Unsupervised Learning

Supervised Learning

- Have: Features X + Labels Y
- Goal: Learn $f : X \to Y$
- Example: Spam detection
  - Email text $\to$ Spam/Not Spam

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- Example: Customer segmentation
  - Customer data → Find groups

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Important:

Key Difference: We don't know the "right answer" beforehand!

Why Unsupervised Learning?

Three Main Reasons:

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1. Labels are expensive/impossible to get

- Medical images: Need expert radiologists (costly!)
- Customer behavior: No "true" groupings exist
- Exploratory analysis: Don't know what to look for yet

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   - Find new disease subtypes
   - Identify market segments you didn't know existed
   - Detect anomalies (fraud, network intrusion)

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3. Data preprocessing

- Dimensionality reduction before supervised learning
- Feature extraction
- Data compression

Real-World Applications

Business

- **E-commerce**: Group customers by purchase behavior
- **Marketing**: Segment markets for targeted campaigns
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- **Document clustering**: Organize large text collections
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Science

- **Astronomy**: Classify galaxies
- **Climate**: Identify weather patterns
- **Biology**: Group similar

What is Clustering?

Clustering: The Intuition

Informal Definition:
Group similar objects together, separate dissimilar objects

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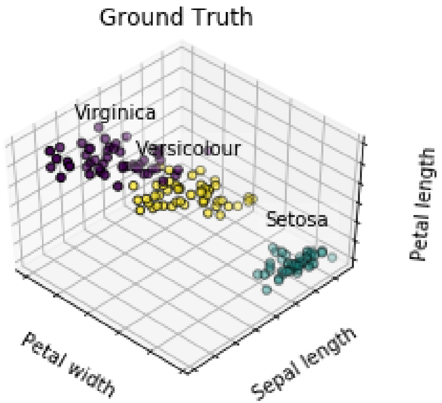
Example: Everyday Example

Organizing your wardrobe:

- **By color**: All red clothes together
- **By type**: All shirts together
- **By season**: All winter clothes together

Same clothes, different clusterings! Choice depends on your

Clustering: Visual Intuition



Iris Dataset: Can you spot the groups?

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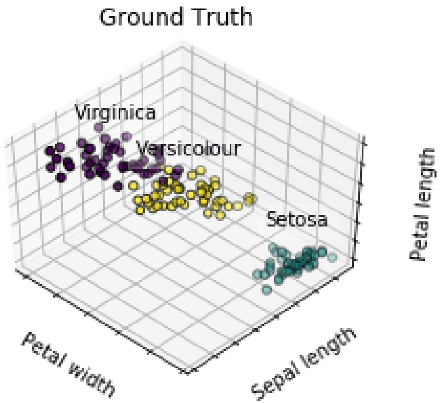

Iris Dataset: Can you spot the groups?

- **Visual**: Easy to see 2-3 distinct groups
- **Question**: How do we make a computer see this?

Formal Problem Statement

Given:

- n data points: $\{x_1, x_2, \ldots, x_n\}$ where $x_i \in \mathbb{R}^d$
- Number of clusters K (sometimes)
- Distance/similarity measure (usually Euclidean)

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- Partition data into K clusters: $C_1, C_2, \ldots, C_K$
- Such that:
  - Points in same cluster are similar (small distances)
  - Points in different clusters are dissimilar (large distances)

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Mathematically:

- $C_1 \cup C_2 \cup \ldots \cup C_K = \{1, 2, \ldots, n\}$ (every point in some cluster)
- $C_i \cap C_j = \emptyset$ for $i \neq j$ (no overlaps)

Types of Clustering Algorithms

Definition (Clustering Algorithm Families)

Different approaches to finding clusters:

1. **Partitioning**: Divide data into K groups
   - K-Means, K-Medoids
   - Need to specify K

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4. **Model-Based**: Assume statistical model
   - Gaussian Mixture Models (GMM)
   - Probabilistic approach

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Today's Focus: K-Means (most popular), then Hierarchical and DBSCAN

K-Means: Intuition First!

K-Means: The Big Idea

Core Intuition:

Each cluster has a center point (centroid).
Assign each point to the nearest centroid.
Update centroids based on assigned points.
Repeat until stable!

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- **K**: Number of clusters
- **Means**: Centroids are computed as means (averages)

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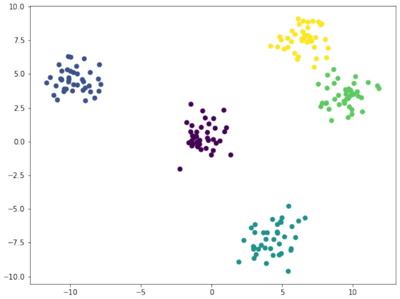
Two-Step Dance:

1. **Assignment**: Points $\rightarrow$ Nearest centroid
2. **Update**: Centroids $\rightarrow$ Mean of assigned points

Repeat until nothing changes!

K-Means: Visual Walkthrough (Step 0)



Raw data: Can you guess $K = 5$?

Start: Pick $K = 5$ centroids randomly (colored points)

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Intuitive Goal:

Make clusters tight - minimize distances within each cluster

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Formal Objective: Minimize Within-Cluster Sum of Squares (WCSS)

$$\text{WCSS} = \sum_{k=1}^{K} \sum_{x_i \in C_k} \|x_i - \mu_k\|^2$$

where:

- $\mu_k = \frac{1}{|C_k|} \sum_{x_i \in C_k} x_i$ is the centroid of cluster k
- $\|x_i - \mu_k\|^2$ is squared distance from point to its centroid

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Important:

In words: Sum of squared distances from each point to its cluster center

Why This Objective Makes Sense

Minimizing WCSS means:

- Points close to their centroid $\rightarrow$ Tight clusters ✓

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Example: Concrete Example

Suppose we have 3 points in cluster C_1: $(0,0),(1,0),(0,1)$

- Centroid: $\mu_1 = (\frac{1}{3}, \frac{1}{3})$
- WCSS for C_1:

$$\|(0,0)-\mu_1\|^2 + \|(1,0)-\mu_1\|^2 + \|(0,1)-\mu_1\|^2 = \frac{2}{3}$$

K-Means Algorithm

K-Means Algorithm: The Recipe

Input:

- Data points $\{x_1, \ldots, x_n\}$
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2. **Repeat** until convergence:
    1) **Assignment Step**:
        - For each point x_i, assign to nearest centroid:

$$C_k^{(t)} = \{i : \|x_i - \mu_k^{(t)}\| \leq \|x_i - \mu_j^{(t)}\| \text{ for all } j\}$$

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   2) **Update Step**:
      - Recompute each centroid as mean of assigned points:
        $$\mu_k^{(t+1)} = \frac{1}{|C_k^{(t)}|} \sum_{i \in C_k^{(t)}} x_i$$

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3. **Convergence**: Stop when assignments don't change (or change is tiny)

K-Means: Assignment Step in Detail

For each point x_i:

1. Compute distance to ALL K centroids:

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Example: Example

Point $x = (2, 3)$, centroids $\mu_1 = (1, 1)$, $\mu_2 = (4, 4)$

- $d_1 = (2 - 1)^2 + (3 - 1)^2 = 5$

K-Means: Update Step in Detail

For each cluster C_k:

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Example: Example

Cluster C_1 has points: $(0,0), (2,0), (0,2)$

$$\mu_1 = \frac{1}{3}[(0,0) + (2,0) + (0,2)] = \left(\frac{2}{3}, \frac{2}{3}\right)$$

K-Means: Worked Example (1/6)

Dataset: 6 points in 2D

Point	**Coordinates**
x_1	$(1, 1)$
x_2	$(2, 1)$
x_3	$(4, 3)$
x_4	$(5, 4)$
x_5	$(1, 3)$
x_6	$(2, 2)$

Goal: Cluster into $K = 2$ groups
Step 0: Initialize centroids randomly

- $\mu_1 = (1, 1)$ (pick x_1)
- $\mu_2 = (5, 4)$ (pick x_4)

K-Means: Worked Example (2/6) - Iteration 1: Assignment

Current centroids: $\mu_1 = (1,1)$, $\mu_2 = (5,4)$

Assign each point to nearest centroid:

Point	$d(\mu_1)$	$d(\mu_2)$	**Nearest**	**Cluster**
$x_1 = (1,1)$	0	$\sqrt{25} = 5$	μ_1	C_1
$x_2 = (2,1)$	1	$\sqrt{18} \approx 4.2$	μ_1	C_1
$x_3 = (4,3)$	$\sqrt{13} \approx 3.6$	$\sqrt{2} \approx 1.4$	μ_2	C_2
$x_4 = (5,4)$	5	0	μ_2	C_2
$x_5 = (1,3)$	2	$\sqrt{17} \approx 4.1$	μ_1	C_1
$x_6 = (2,2)$	$\sqrt{2} \approx 1.4$	$\sqrt{13} \approx 3.6$	μ_1	C_1

Result: $C_1 = \{x_1, x_2, x_5, x_6\}$, $C_2 = \{x_3, x_4\}$

K-Means: Worked Example (3/6) - Iteration 1: Update

Update centroids as means:
Cluster 1: $C_1 = \{(1,1),(2,1),(1,3),(2,2)\}$

$$\mu_1^{\text{new}} = \frac{1}{4}[(1,1)+(2,1)+(1,3)+(2,2)] = \frac{1}{4}(6,7) = (1.5, 1.75)$$

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Cluster 2: $C_2 = \{(4,3),(5,4)\}$

$$\mu_2^{\text{new}} = \frac{1}{2}[(4,3)+(5,4)] = \frac{1}{2}(9,7) = (4.5, 3.5)$$

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Important:

Notice: Centroids moved from $(1,1),(5,4)$ to $(1.5,1.75),(4.5,3.5)$
They shifted toward the "center of mass" of their clusters!

K-Means: Worked Example (4/6) - Iteration 2: Assignment

New centroids: $\mu_1 = (1.5, 1.75)$, $\mu_2 = (4.5, 3.5)$
Reassign points:

Point	$d(\mu_1)$	$d(\mu_2)$	Nearest	Cluster
$x_1 = (1, 1)$	0.9	6.8	μ_1	C_1
$x_2 = (2, 1)$	0.8	7.1	μ_1	C_1
$x_3 = (4, 3)$	3.8	0.4	μ_2	C_2
$x_4 = (5, 4)$	6.8	0.4	μ_2	C_2
$x_5 = (1, 3)$	1.6	3.9	μ_1	C_1
$x_6 = (2, 2)$	0.5	6.6	μ_1	C_1

Result: Same as before! $C_1 = \{x_1, x_2, x_5, x_6\}$, $C_2 = \{x_3, x_4\}$
Convergence: Assignments didn't change $\rightarrow$ STOP!

K-Means: Worked Example (5/6) - Final Clustering

Final clusters:

- **Cluster 1**: $(1, 1), (2, 1), (1, 3), (2, 2)$ with centroid $(1.5, 1.75)$
- **Cluster 2**: $(4, 3), (5, 4)$ with centroid $(4.5, 3.5)$

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WCSS calculation:

$$\begin{aligned}\text{WCSS} &= \sum_{i\in C_1} \|x_i-\mu_1\|^2 + \sum_{i\in C_2} \|x_i-\mu_2\|^2 \\ &= [0.9+0.8+1.6+0.5]+[0.4+0.4] \\ &= 3.8+0.8=4.6\end{aligned}$$

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Key Points: Key Points

Converged in 2 iterations!
Typically converges quickly (5-10 iterations), but worst-case can be slow.

K-Means: Worked Example (6/6) - Visualization

Visual summary:

- **Initial**: Random centroids far from optimal
- **Iteration 1**: Centroids move toward cluster centers
- **Iteration 2**: Centroids stabilize, assignments don't change
- **Final**: Two clear, compact clusters

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Visual summary:

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Example: Key Insight

K-Means is iteratively refining the clustering:

1. Assignment makes WCSS smaller (each point goes to nearest centroid)
2. Update makes WCSS smaller (centroid is optimal for its assigned points)
3. Repeat until can't improve further (local optimum)

K-Means: Mathematical Rigor

Why K-Means Converges: Intuitive Proof

Claim: K-Means always converges

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Claim: K-Means always converges
Intuition: Each step decreases (or keeps same) the objective function WCSS

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Intuition: Each step decreases (or keeps same) the objective function WCSS
Proof sketch:

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   - Cannot increase WCSS (optimal centroid given fixed assignments)
3. **Conclusion**:
   - WCSS decreases or stays same at each step
   - WCSS ≥ 0 (bounded below)
   - Finite number of possible assignments (K^n)
   - Therefore, must converge! ✓

Why Mean Minimizes Sum of Squared Distances

Claim: For points $\{x_1, \ldots, x_m\}$, the mean $\bar{x} = \frac{1}{m}\sum_{i=1}^{m} x_i$ minimizes $\sum_{i=1}^{m} \|x_i - c\|^2$

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Proof: Let $f(c) = \sum_{i=1}^{m} \|x_i - c\|^2$. Taking derivative and setting to zero:

$$\frac{\partial f}{\partial c} = \sum_{i=1}^{m} 2(x_i - c)(-1) = 0$$

$$\sum_{i=1}^{m} (c - x_i) = 0$$

$$mc = \sum_{i=1}^{m} x_i$$

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Key Points: Key Points

This is why we use **means** in K-Means - they're optimal!

K-Means Objective: Equivalent Forms

Form 1: Within-Cluster Sum of Squares

$$\min \sum_{k=1}^{K} \sum_{x_i \in C_k} \|x_i - \mu_k\|^2$$

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Definition (Within-Cluster Variation)

Both forms measure how "tight" clusters are - smaller is better!

K-Means: Complexity Analysis

Time Complexity per iteration:

- **Assignment**: $O(nKd)$
  - For each of n points
  - Compute distance to K centroids
  - Each distance is $O(d)$ (dimensionality)
- **Update**: $O(nd)$
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Practical: Usually converges in < 10 iterations $\rightarrow$ Very fast!

Choosing K: The Elbow Method

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Important:

Trade-off: We want low WCSS but also not too many clusters!

The Elbow Method: Intuition

Idea: Plot WCSS vs K and look for an "elbow"

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Analogy: Hiring employees

- 1$\rightarrow$2 employees: Huge productivity gain
- 2$\rightarrow$3 employees: Still helpful
- 10$\rightarrow$11 employees: Marginal benefit
- 100$\rightarrow$101 employees: Almost no difference

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Key Points: Key Points

Elbow = sweet spot where benefit of adding clusters drops sharply

Elbow Method: Mathematical Formulation

Algorithm:

1. Run K-Means for $K = 1, 2, 3, \ldots, K_{\text{max}}$
2. For each K, compute WCSS(K)
3. Plot WCSS(K) vs K
4. Find "elbow" $=$ maximum curvature point

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Finding elbow programmatically:

- Compute second derivative: $\frac{d^2(\text{WCSS})}{dK^2}$
- Elbow = maximum of second derivative

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Finding elbow programmatically:

- Compute second derivative: $\frac{d^2(\text{WCSS})}{dK^2}$
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Or use heuristic:

$$\text{Elbow} = \arg\max_{K} [\text{WCSS}(K-1) - \text{WCSS}(K)]$$

(biggest drop in WCSS)

Elbow Method: Example

Example WCSS vs K:

K	WCSS
1	1000
2	600 (drop: 400)
3	400 (drop: 200)
4	300 (drop: 100) $\leftarrow$ **Elbow!**
5	250 (drop: 50)
6	220 (drop: 30)

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- Drops slow down after $K = 4$
- Suggests $K = 4$ is optimal

Important:

Note: Elbow method is a heuristic, not a theorem!
Use domain knowledge + elbow method together.

Other Methods to Choose K

Silhouette Score:

- Measures how similar a point is to its own cluster vs other clusters
- Range: $[-1, 1]$, higher is better
- Choose K with highest average silhouette score

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Domain Knowledge:

- Sometimes you know K from context
- Example: Customer segments (budget/mid/premium)
- Example: Image compression (fixed color palette)

When K-Means Fails

K-Means Assumptions

K-Means works well when:

1. Clusters are spherical (same in all directions)

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2. Clusters have similar sizes
3. Clusters have similar densities
4. Data is isotropic (no strong directional patterns)

Important:

Reality: Many real datasets violate these assumptions!
Let's see what happens...

Failure Mode 1: Non-Spherical Clusters

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What happens:

- K-Means uses Euclidean distance
- Creates spherical decision boundaries
- Incorrectly splits elongated clusters

Solution:

- Transform data first (e.g., PCA rotation)
- Use Gaussian Mixture Models (handles ellipsoids)
- Use spectral clustering

Failure Mode 2: Non-Convex Shapes

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Example: Two interleaving crescents (moons)
What happens:

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Solution:

- DBSCAN (handles arbitrary shapes)
- Spectral clustering
- Kernel K-Means (kernel trick!)

Failure Mode 3: Different Cluster Sizes

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Solution:

- Weighted K-Means
- DBSCAN (density-based)
- Hierarchical clustering

Failure Mode 4: Different Densities

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Example: Dense cluster next to sparse cluster
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Solution:

- DBSCAN (explicitly models density)
- HDBSCAN (hierarchical density-based)
- GMM with different covariances

Failure Mode 5: Outliers

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Solutions:

- Pre-process: Remove outliers first
- K-Medoids (uses medians, more robust)
- Trimmed K-Means (ignores worst $\alpha\%$ of points)
- DBSCAN (marks outliers as noise)

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Solution: K-Means++ (discussed next!)

- Smart initialization - spread out initial centroids
- Much more likely to find good solution
- Now default in most libraries

K-Means++

K-Means++: Smarter Initialization

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Key Points: Key Points

How to choose "far apart" centroids?
Use weighted random sampling - points far from existing centroids have higher probability!

K-Means++ Algorithm

Input: Data points $\{x_1, \ldots, x_n\}$, number of clusters K

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(squared distance to nearest already-chosen centroid)

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Then: Run standard K-Means with these initial centroids

K-Means++: Why It Works

Intuition:

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Example: Concrete Example

Suppose we've chosen $\mu_1 = (0, 0)$. Consider two points:

- $x_a = (1, 0)$: $D(x_a) = 1 \rightarrow P(x_a) \propto 1$
- $x_b = (10, 0)$: $D(x_b) = 100 \rightarrow P(x_b) \propto 100$

Point x_b is $100\times$ more likely to be chosen as μ_2!

K-Means++: Theoretical Guarantee

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In English:

- Let $\text{WCSS}_{\text{optimal}} =$ best possible WCSS
- Let $\text{WCSS}_{\text{KM++}} =$ WCSS from K-Means++ (after convergence)
- Then:

$$\mathbb{E}[\text{WCSS}_{\text{KM++}}] \leq O(\log K) \cdot \text{WCSS}_{\text{optimal}}$$

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Key Points: Key Points

K-Means++ is provably better than random initialization
This is why it's now the default in scikit-learn, etc.

K-Means++ vs Standard K-Means

Property	**Random Init**	**K-Means++**
Convergence guarantee	Yes	Yes
Quality guarantee	No	$O(\log K)$-approx
Iterations needed	More	Fewer
Consistency across runs	Poor	Better
Initialization time	$O(1)$	$O(nKd)$
Total time	$O(nKdt)$	$O(nKd(t+K))$

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Practical Advice:

- Always use K-Means++ (default in scikit-learn)
- Initialization cost is negligible compared to iterations
- Better results with fewer iterations

Hierarchical Clustering

Limitations of K-Means

K-Means requires:

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- Running multiple times with different K (elbow method)
- Assumes spherical clusters

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Can we do better?

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- From $K = n$ (each point alone) to $K = 1$ (everything together)
- Visualize as a tree (dendrogram)
- Cut tree at any height to get desired K

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Hierarchical Clustering: Build a tree of nested clusters!

Two Approaches to Hierarchical Clustering

1. Agglomerative (Bottom-Up)

- Start: *n* clusters (each point alone)
- Repeat: Merge two closest clusters
- End: 1 cluster (everything together)
- Most common approach

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Important:

Agglomerative Clustering: Algorithm

Input: Data points $\{x_1, \ldots, x_n\}$
Algorithm:

1. **Initialize**: Start with n clusters, one per point

$$C_i = \{x_i\} \quad \text{for } i = 1, \ldots, n$$

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Key Question: How do we measure distance between clusters (not just points)?

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3. **Average Linkage**:

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

More Linkage Criteria

4. Centroid Linkage:

$$d(C_i, C_j) = \|\mu_i - \mu_j\|$$

where $\mu_i = \frac{1}{|C_i|} \sum_{x \in C_i} x$

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- Can have inversions (not monotonic!)

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$$d(C_i, C_j) = \frac{|C_i||C_j|}{|C_i| + |C_j|} \|\mu_i - \mu_j\|^2$$

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Example: Flexibility

Advantage: Don't need to specify K beforehand!
Run once, then choose K by cutting dendrogram at desired height.

Hierarchical Clustering: Complexity

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Time	$O(nKdt)$	$O(n^2 \log n)$
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ierarchical is much slower for large n (thousands+)

K-Means scales better to large datasets

Hierarchical vs K-Means: When to Use Each?

Property	**K-Means**	**Hierarchical**
Specify K?	Yes	No
Speed (large n)	Fast	Slow
Deterministic?	No	Yes
Cluster shape	Spherical	Flexible
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- Know K (or can use elbow method)

Use Hierarchical when:

- Small-medium dataset ($n < 5000$)
- Want full hierarchy (dendrogram)
- Don't know K beforehand

DBSCAN

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Consider two clusters:

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- Scattered points around core (10 points far away)

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Parameters:

- ε (epsilon): Radius of neighborhood
- MinPts: Minimum number of points in neighborhood to be "dense"

DBSCAN: Key Definitions

1. ε-**neighborhood** of point p:

$$N_\varepsilon(p) = \{q : \|p - q\| \leq \varepsilon\}$$

All points within radius ε of p

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DBSCAN: Visual Example of Point Types

Setup: $\varepsilon = 1$, MinPts $= 4$

[Visual would show: points with circles of radius ε]

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Point Classification:

- **Point A**: Has 5 neighbors $\rightarrow$ Core point
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Cluster = All core points connected + their border points

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Direct density-reachable:

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  1. p is a core point
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Definition (DBSCAN Cluster)

A **cluster** is the maximal set of density-connected points.

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Input: Data points, ε, MinPts
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1. Mark all points as `UNVISITED`

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    4) Else ($p$ is core point):
        – Create new cluster $C$
        – Add $p$ to $C$
        – Expand cluster: recursively add all density-reachable points
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      - Add p to C
      - Expand cluster: recursively add all density-reachable points
3. **Output**: Set of clusters + noise points

DBSCAN: Expand Cluster Procedure

ExpandCluster$(p, N_\varepsilon(p), C)$:

1. Add p to cluster C
2. **For each** point $q \in N_\varepsilon(p)$:
   1) **If** q is `UNVISITED`:
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Result: All density-reachable points from p are in cluster C

DBSCAN: Worked Example (1/4)

Setup: $\varepsilon = 1.5$, MinPts $= 3$
Data: 10 points in 2D

Point	Coords	Point	Coords
A	$(1, 1)$	F	$(2, 2)$
B	$(1, 2)$	G	$(10, 10)$
C	$(2, 1)$	H	$(10, 11)$
D	$(1.5, 1.5)$	I	$(11, 10)$
E	$(2, 3)$	J	$(5, 5)$

Visualize: Three regions - dense cluster left, dense cluster right, one isolated point

DBSCAN: Worked Example (2/4) - Finding Core Points

Check each point's neighborhood:

- **Point A** $(1, 1)$: Neighbors = $\{$A, B, C, D$\}$ (4 points) $\rightarrow$ Core
- **Point B** $(1, 2)$: Neighbors = $\{$A, B, D, E, F$\}$ (5 points) $\rightarrow$ Core
- **Point C** $(2, 1)$: Neighbors = $\{$A, C, D, F$\}$ (4 points) $\rightarrow$ Core
- **Point D** $(1.5, 1.5)$: Neighbors = $\{$A, B, C, D, F$\}$ (5 points) $\rightarrow$ Core
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- **Point G** $(10, 10)$: Neighbors = $\{$G, H, I$\}$ (3 points) $\rightarrow$ Core
- **Point H** $(10, 11)$: Neighbors = $\{$G, H, I$\}$ (3 points) $\rightarrow$ Core
- **Point I** $(11, 10)$: Neighbors = $\{$G, H, I$\}$ (3 points) $\rightarrow$ Core
- **Point J** $(5, 5)$: Neighbors = $\{$J$\}$ (1 point) $\rightarrow$ Noise

DBSCAN: Worked Example (3/4) - Forming Clusters

Start with point A:

- A is core $\rightarrow$ Create **Cluster 1**
- Expand: A can reach B, C, D (all core)
- B can reach E, F (both core)
- Continue expanding: All of {A, B, C, D, E, F} are density-connected
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Continue with unvisited point G:

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2. **No K needed**: Number of clusters determined automatically
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Example Applications:

- Geographic data (cities, disease outbreaks)
- Anomaly detection (fraud, network intrusion)
- Image segmentation (arbitrary region shapes)
- Point cloud processing (3D scanning)

DBSCAN: Disadvantages

1. **Parameter sensitivity**: Results depend heavily on ε and MinPts
2. **Varying density**: Struggles when clusters have different densities
3. **High dimensions**: "Curse of dimensionality" - distances become meaningless
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Solutions:

- HDBSCAN (hierarchical DBSCAN) - handles varying densities

Choosing DBSCAN Parameters

How to choose ε?
K-distance graph method:

1. For each point, compute distance to k-th nearest neighbor (use $k = \text{MinPts}$)
2. Sort these distances
3. Plot sorted k-distances
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- Rule of thumb: $\text{MinPts} \geq d + 1$ where d is dimensionality
- For 2D data: $\text{MinPts} = 3$ or 4
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Comparing Clustering Methods

Clustering Algorithms: Summary Table

Algorithm	**Shape**	K**?**	**Outliers**	**Complexity**
K-Means	Spherical	Yes	Sensitive	$O(nKdt)$
K-Means++	Spherical	Yes	Sensitive	$O(nKd(t+K))$
Hierarchical	Flexible	No	Sensitive	$O(n^2 \log n)$
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Additional Properties:

Algorithm	**Deterministic**	**Scalability**	**High-D OK?**
K-Means	No	Excellent	Yes
K-Means++	No	Excellent	Yes
Hierarchical	Yes	Poor	Moderate
DBSCAN	Yes	Good	No

Decision Tree: Which Algorithm to Use?

Choosing a Clustering Algorithm

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- **Need full hierarchy** $\rightarrow$ Hierarchical
- **Probabilistic model** $\rightarrow$ Gaussian Mixture Models
- **Varying densities** $\rightarrow$ HDBSCAN
- **Very large scale** $\rightarrow$ Mini-Batch K-Means

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General Advice:

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Internal Metrics (no ground truth needed):

- **Silhouette Score**: Measures compactness vs separation
$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$
Range: $[-1, 1]$, higher is better
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External Metrics (if ground truth available):

- **Adjusted Rand Index (ARI)**: Similarity to true labeling

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Solutions:

1. **Dimensionality Reduction first**:
   - PCA: Project to lower dimensions
   - t-SNE: Nonlinear reduction (for visualization)
   - Autoencoders: Neural network-based
2. **Feature Selection**:
   - Remove irrelevant features
   - Use domain knowledge

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- Builds tree of clusters (dendrogram)

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Code and Resources:

Google Colab Notebook

Questions?