

1 Why Hierarchical Clustering exists (intuition first)

Imagine you don't want the data to just end up in *K fixed buckets*.

Instead, you want to understand:

“Which points are closest first?”

“Which groups merge next?”

“What is the full family tree of the data?”

That **tree of relationships** is exactly what **Hierarchical Clustering** gives you.

It answers:

- Not just *what clusters*,
 - but *how clusters are formed step by step*.
-

2 What is Hierarchical Clustering (conceptual definition)

Hierarchical Clustering builds clusters by **progressively merging or splitting data points**, forming a **tree-like structure** called a **dendrogram**.

There are **two ways to think** about it:

♦ Agglomerative (Bottom-Up) — most common

- Start with **each point as its own cluster**
- Repeatedly **merge the closest clusters**
- Continue until everything becomes **one big cluster**

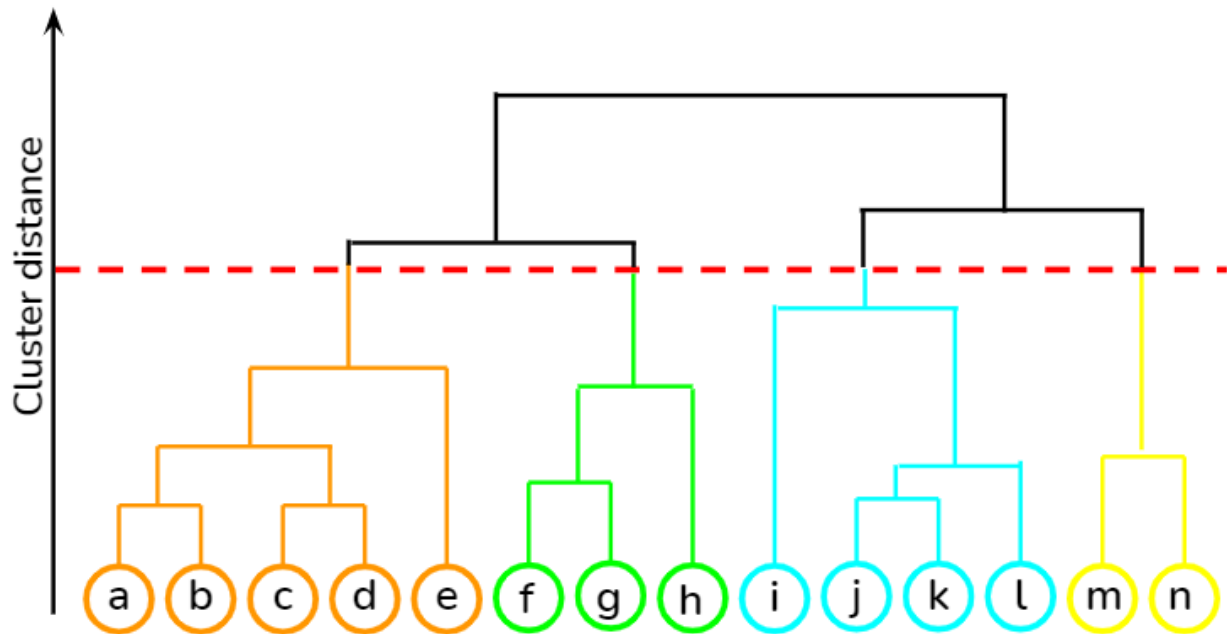
♦ Divisive (Top-Down)

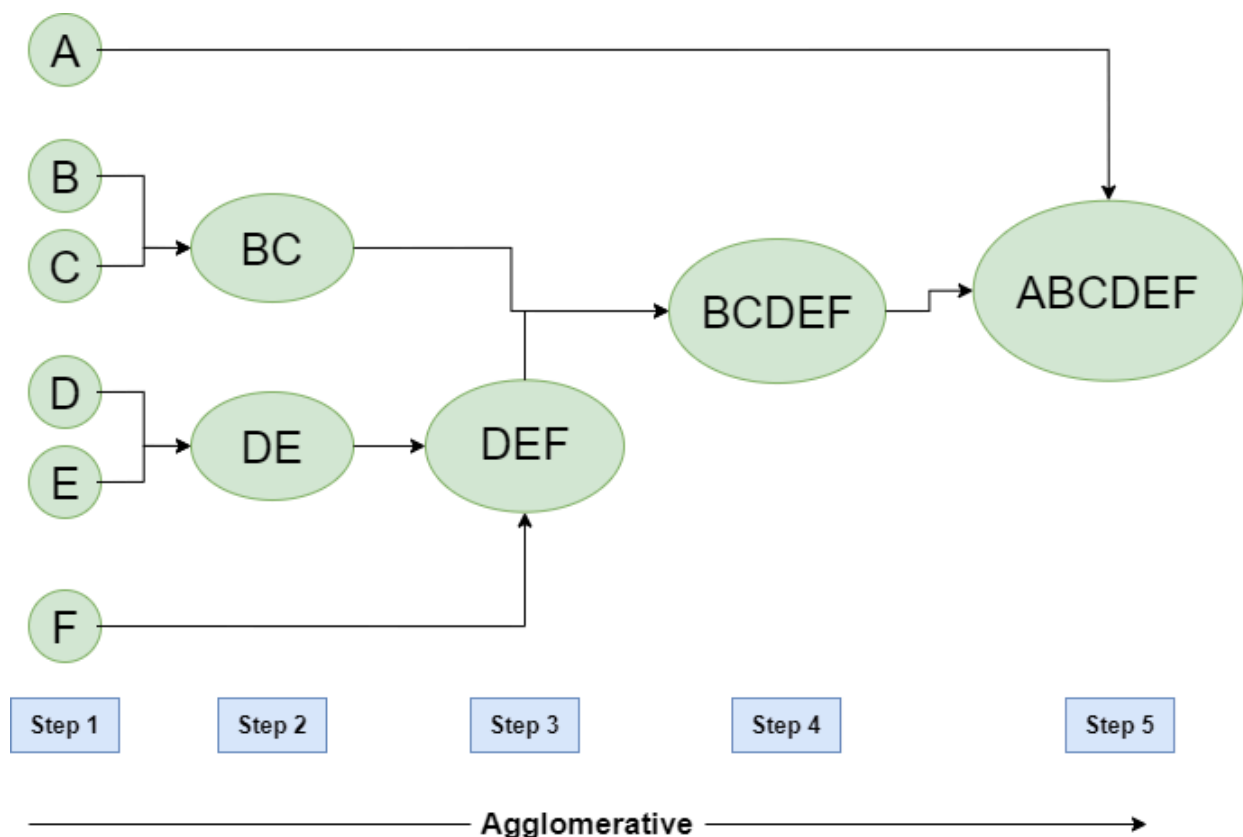
- Start with **all points together**
- Repeatedly **split clusters**

- Less common (computationally expensive)

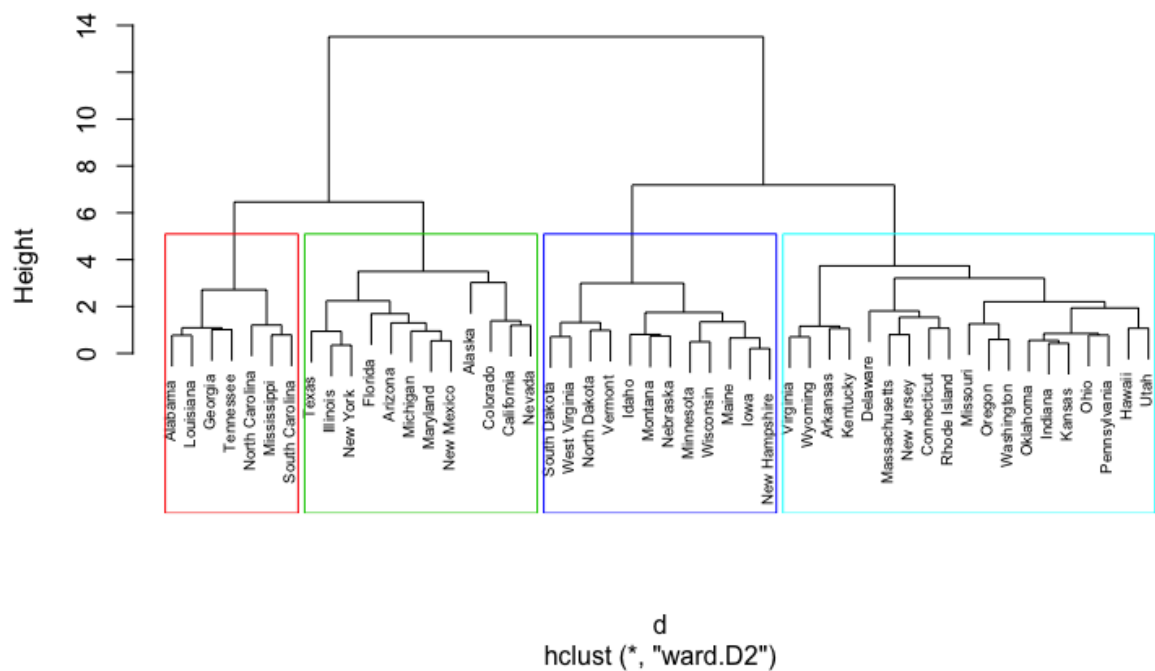
📌 Most textbooks + ML libraries use **Agglomerative**.

3 Visual intuition (very important)





Cluster Dendrogram



Think of the dendrogram like a **family tree**:

- Leaves = individual data points
- Branch height = distance at which clusters merge
- You choose where to **cut the tree** → number of clusters

👉 **Clusters are not fixed** until *you decide the cut*.

4 How Hierarchical Clustering actually works (step-by-step)

Let's say we have points:

A B C D

Step 1: Compute distances

We compute **pairwise distances** between all points.

Step 2: Find closest pair

Suppose:

- A & B are closest → merge them

Now clusters:

{A, B} C D

Step 3: Measure distance between clusters

Here comes a key idea: **How do we define distance between clusters?**

This is called **Linkage**.

5 Linkage methods (core concept)

Linkage defines **how cluster-to-cluster distance is computed**:

Linkage	Idea	Effect
Single	Closest points	Can form chains
Complete	Farthest points	Compact clusters
Average	Mean distance	Balanced
Ward	Minimize variance	Best for spherical data

 This choice **changes the dendrogram shape**.

6 What is K-Means (contrast mindset)

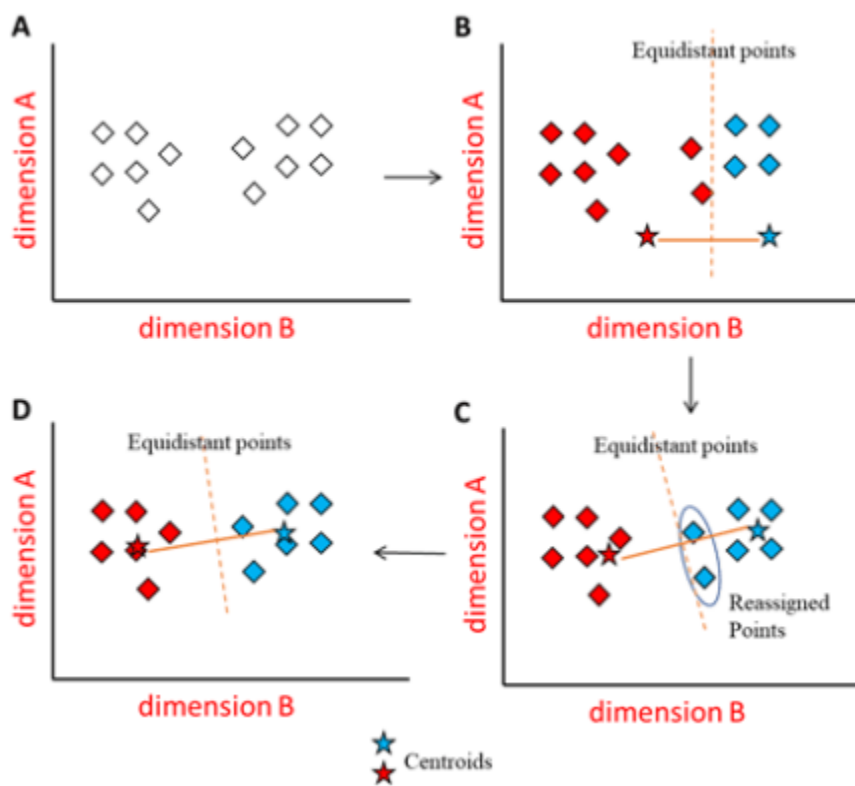
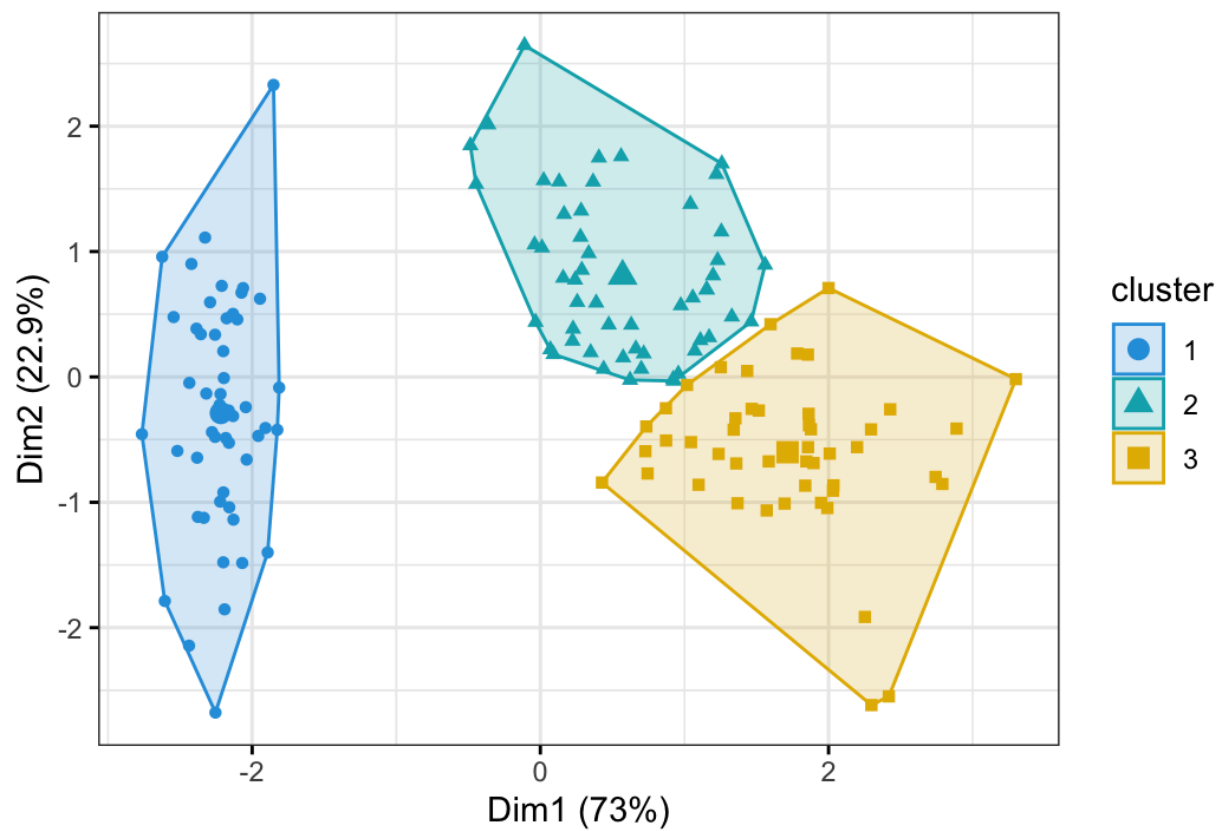
K-Means thinks completely differently:

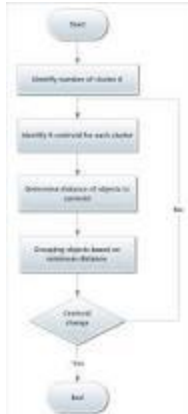
“You tell me K.
I’ll force the data into exactly K clusters.”

It:

- Assumes clusters are **spherical**
- Uses **centroids**
- Optimizes **intra-cluster variance**

Cluster plot





7 Key differences: Hierarchical vs K-Means

🔥 Conceptual comparison (exam & interview gold)

Aspect	Hierarchical	K-Means
Need K beforehand	✗ No	✓ Yes
Output	Tree (dendrogram)	Flat clusters
Cluster shape	Any	Mostly spherical
Sensitive to initialization	✗ No	✓ Yes
Scales to large data	✗ Poor	✓ Good
Interpretability	★★★★★	★★★

📌 Hierarchical = structure discovery

📌 K-Means = fast partitioning

8 Where Cosine Similarity fits in (very important)

- ♦ First: what cosine similarity actually measures

Cosine similarity measures **angle**, not distance.

$$\text{Cosine Similarity} = \frac{\vec{A} \cdot \vec{B}}{\|\vec{A}\| \|\vec{B}\|} = \frac{\|\vec{A}\| \|\vec{B}\| \cos(\theta)}{\|\vec{A}\| \|\vec{B}\|} = \cos(\theta)$$

- Value range: [-1, 1]
- Focuses on **direction**
- Ignores **magnitude**

📌 Think:

“Are these two vectors pointing in the same direction?”

9 Why cosine similarity is powerful in clustering

Cosine similarity is ideal when:

- Magnitude is irrelevant
- Direction matters more

Examples:

- Text documents (TF-IDF vectors)
- User preferences
- Embeddings

Two documents:

$[1, 1, 0, 0]$ and $[10, 10, 0, 0]$

Euclidean distance → large

Cosine similarity → **1 (same direction)**

10 Cosine similarity with Hierarchical vs K-Means

♦ Hierarchical + Cosine

✓ Works **very naturally**

- Just replace distance metric
- Dendrogram reflects semantic similarity

📌 Very common in **NLP clustering**

♦ K-Means + Cosine

⚠ Not natural

- K-Means optimizes Euclidean variance
- Cosine breaks centroid meaning

✓ Workaround:

- Normalize vectors → unit length
- Then Euclidean \approx Cosine

This is called **Spherical K-Means**.

11 Deep example: Text clustering

Documents:

D1: "machine learning ai"

D2: "deep learning ai"

D3: "football match goal"

Vectorized (simplified):

D1 = [1, 1, 1, 0]

D2 = [0, 1, 1, 1]

D3 = [0, 0, 0, 3]

Cosine similarities:

- D1 ↔ D2 → high
- D1 ↔ D3 → low
- D2 ↔ D3 → low

Result:

- Hierarchical + cosine → D1 & D2 merge first
- K-Means (k=2) → {D1,D2}, {D3}

📌 Cosine captures **semantic closeness**, not word count.

12 When to use what (decision rule)

Use Hierarchical Clustering when:

- You want **structure**
- Dataset is **small-medium**
- Interpretability matters
- You don't know K

Use K-Means when:

- Dataset is **large**
- Speed matters

- Clusters are compact
- K is known

Use Cosine Similarity when:

- Direction > magnitude
 - Text, embeddings, user behavior
-

One-line mental models (remember this)

- **Hierarchical**: “Show me the family tree of data”
 - **K-Means**: “Split data into K equal-ish regions”
 - **Cosine**: “Are these pointing the same way?”
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If you want, next we can:

- Dry-run **numerical example step-by-step**
- Compare **Ward vs Complete linkage**
- Show **how elbow method fails for hierarchical**
- Or map this directly to **exam answers (5/10 marks)**

Just tell me the direction 🙌

how it works Hierarchical Clustering ..

Let's strip it down to **how Hierarchical Clustering actually works internally**, step by step — no shortcuts, no hand-waving.

Big picture (one sentence)

Hierarchical Clustering builds clusters by repeatedly merging the closest groups of points, creating a tree (dendrogram) that records every merge.

Step⁰ — What you start with

Assume you have **N data points**.

📌 Initial state:

- Each data point = **its own cluster**
- Total clusters = **N**

Example points (1D for simplicity):

A = 1

B = 2

C = 5

D = 8

Clusters:

{A} {B} {C} {D}

Step¹ — Compute distance matrix (foundation)

Compute **distance between every pair of points**.

Example (Euclidean distance):

	A	B	C	D
A	0	1	4	7
B	1	0	3	6
C	4	3	0	3

D 7 6 3 0

📌 This matrix drives **every** future decision.

Step 2 — Find the closest clusters

Find the **minimum distance** (excluding 0).

👉 Smallest distance = 1 between A and B

So we merge:

$\{A\} + \{B\} \rightarrow \{A, B\}$

Now clusters are:

$\{A, B\}$ $\{C\}$ $\{D\}$

This merge is recorded in the **dendrogram** at height = 1.

Step 3 — Recompute distances (CRITICAL STEP)

Now comes the most important question:

“How far is cluster $\{A, B\}$ from cluster $\{C\}$ or $\{D\}$?”

This depends on **linkage method**.

Step 4 — Linkage decides cluster distance

- ◆ **Single Linkage (minimum distance)**

$\text{dist}(\{A, B\}, C) = \min(\text{dist}(A, C), \text{dist}(B, C))$
 $= \min(4, 3) = 3$

- ◆ **Complete Linkage (maximum distance)**

$$\text{dist}(\{A,B\}, C) = \max(4,3) = 4$$

♦ Average Linkage

$$\text{dist}(\{A,B\}, C) = (4 + 3) / 2 = 3.5$$

📌 Different linkage → different dendrogram.

Step 5 — Merge again

Suppose we use **single linkage**.

Distances now:

$$\{A,B\} \leftrightarrow C = 3$$

$$C \leftrightarrow D = 3$$

Pick one minimum (tie allowed).

Merge:

$$\{C\} + \{D\} \rightarrow \{C,D\}$$

Clusters:

$$\{A,B\} \quad \{C,D\}$$

Record merge at height = 3.

Step 6 — Final merge

Now only two clusters remain.

Compute:

$$\text{dist}(\{A,B\}, \{C,D\})$$

Using single linkage:

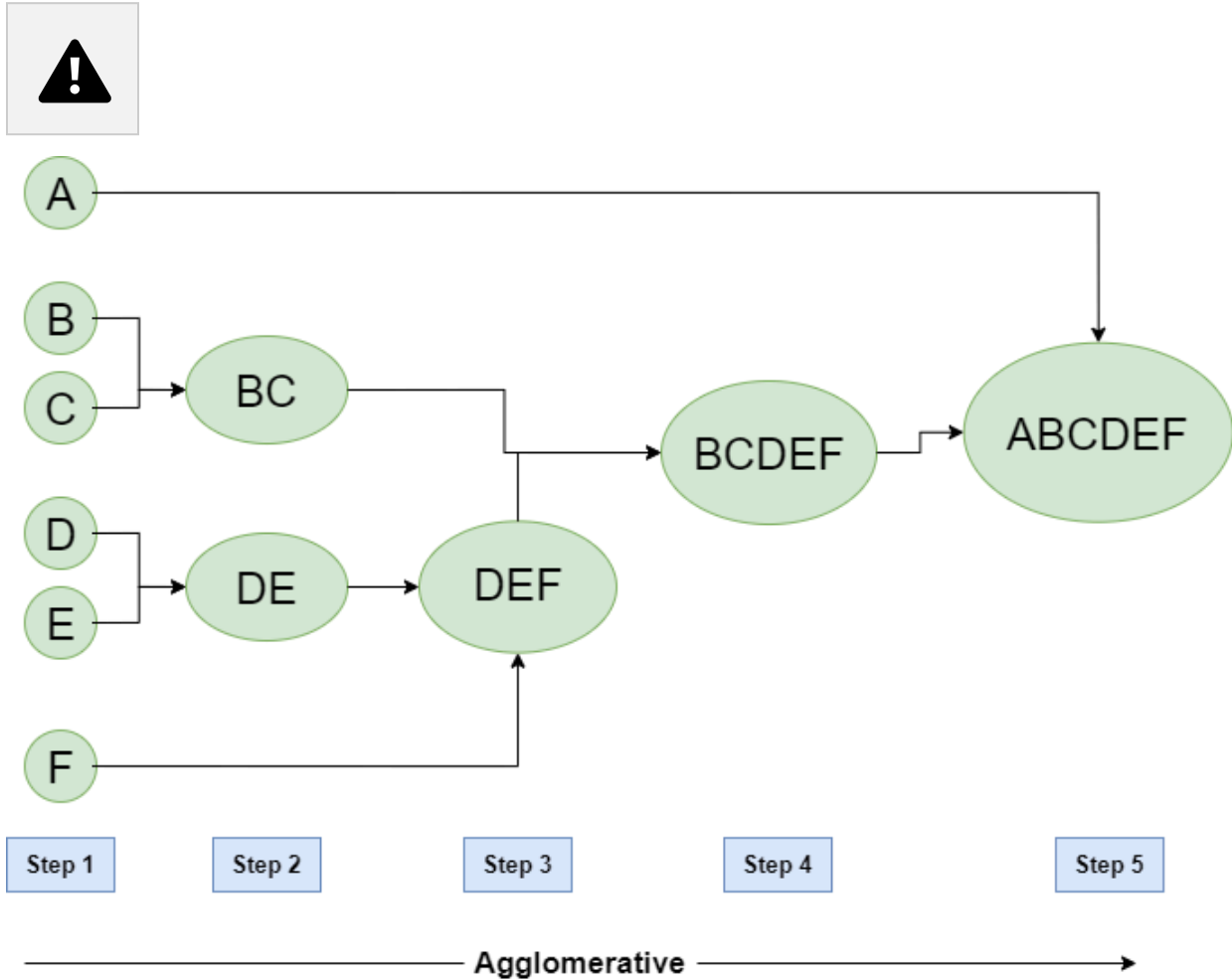
$$\min(A \leftrightarrow C, A \leftrightarrow D, B \leftrightarrow C, B \leftrightarrow D)$$

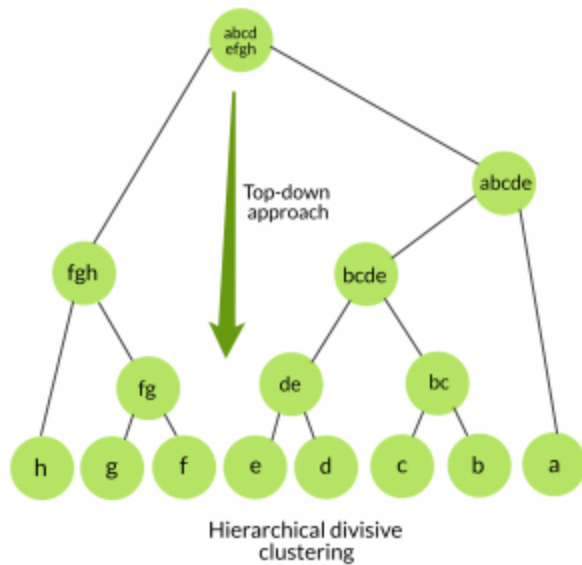
$$= \min(4, 7, 3, 6)$$

$$= 3$$

Merge them → one cluster.

Step 7 — Build the dendrogram (result)





The dendrogram stores:

- Which clusters merged
- At what distance

Nothing is lost. This is why it's powerful.

Step 8 — How clusters are chosen (CUTTING the tree)

Hierarchical clustering **does NOT** output clusters directly.

You decide:

- Draw a horizontal cut at distance = d
- Count how many branches it intersects

That number = **clusters**

📌 This is why:

- You don't need to choose K beforehand

- You can explore multiple clusterings

Step 9 — Why this is fundamentally different from K-Means

Hierarchical	K-Means
Records full history	Forgets history
Tree structure	Flat output
No centroid	Centroid-based
Flexible shape	Spherical bias
Expensive ($O(n^2)$)	Fast ($O(n)$)

Step 10 — Mental animation (remember this)

Think of points as **magnets**:

1. Closest magnets snap together
 2. New bigger magnets form
 3. Repeat until one giant magnet exists
 4. You decide **where to break the chain**
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Final crystal-clear summary

Hierarchical Clustering works by:

1. Treating every point as a cluster

2. Computing all pairwise distances
3. Repeatedly merging the closest clusters
4. Using linkage to define cluster distance
5. Recording merges in a dendrogram
6. Cutting the dendrogram to get clusters