

## 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*.
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## 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:

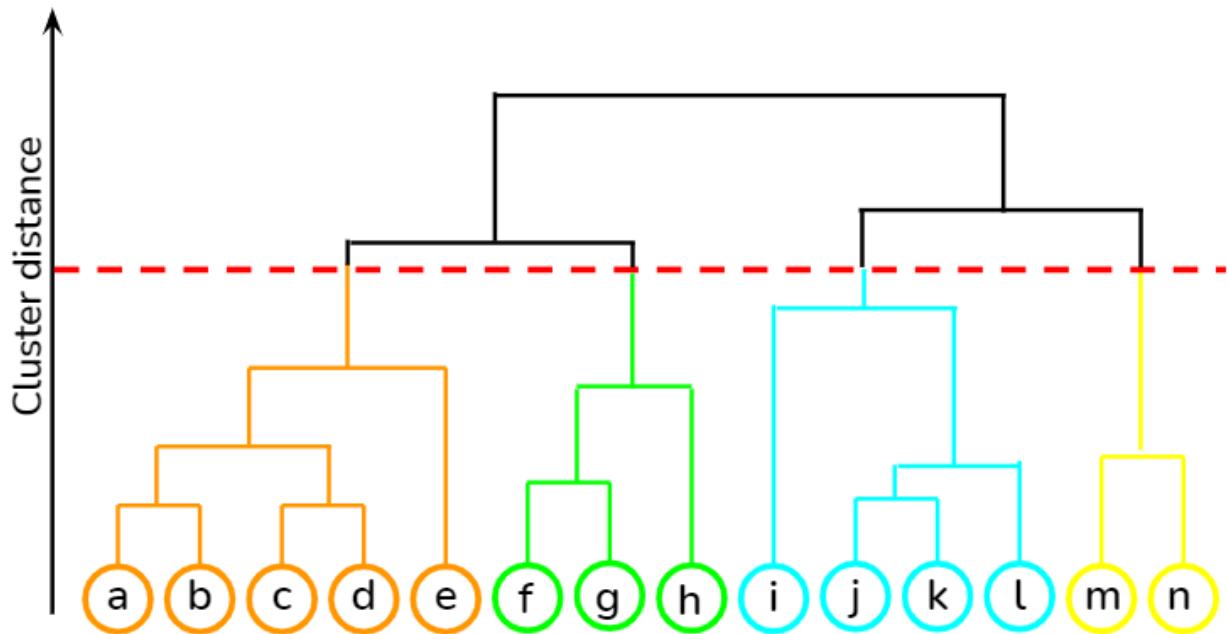
- ◆ **Agglomerative (Bottom-Up) — most common**
  - Start with **each point as its own cluster**
  - Repeatedly **merge the closest clusters**
  - Continue until everything becomes **one big cluster**
- ◆ **Divisive (Top-Down)**
  - Start with **all points together**
  - Repeatedly **split clusters**

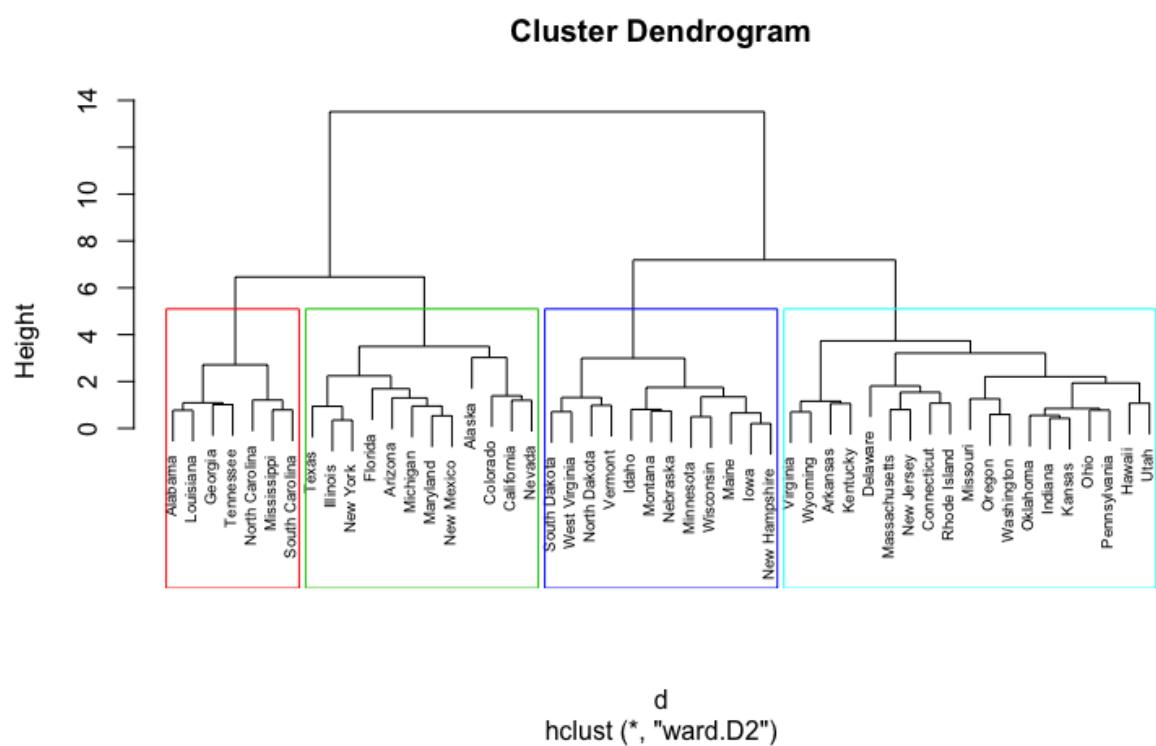
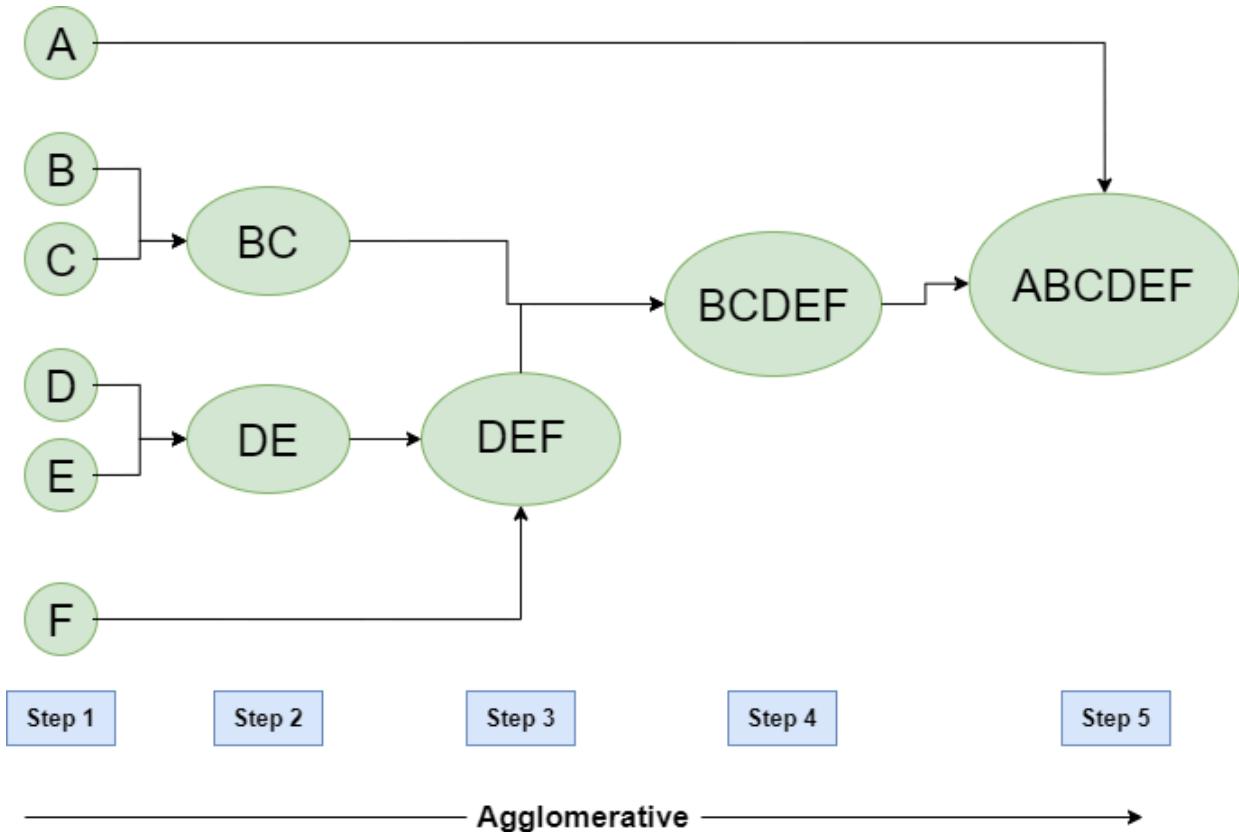
- Less common (computationally expensive)

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

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### ③ Visual intuition (very important)





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.**

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## 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**.

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## 5 Linkage methods (core concept)

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

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

💡 This choice **changes the dendrogram shape**.

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## 6 What is K-Means (contrast mindset)

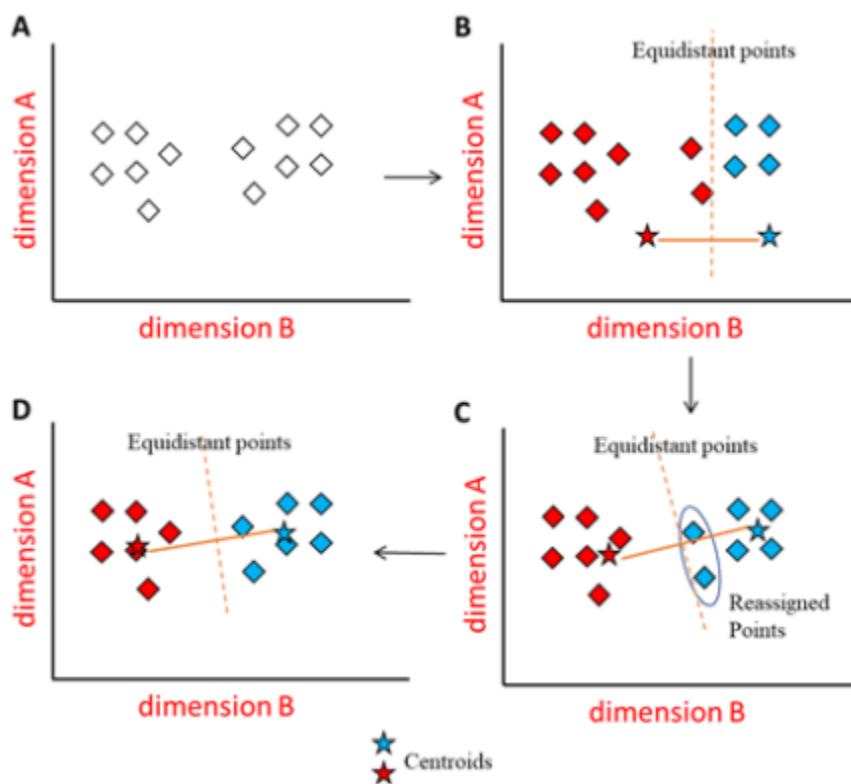
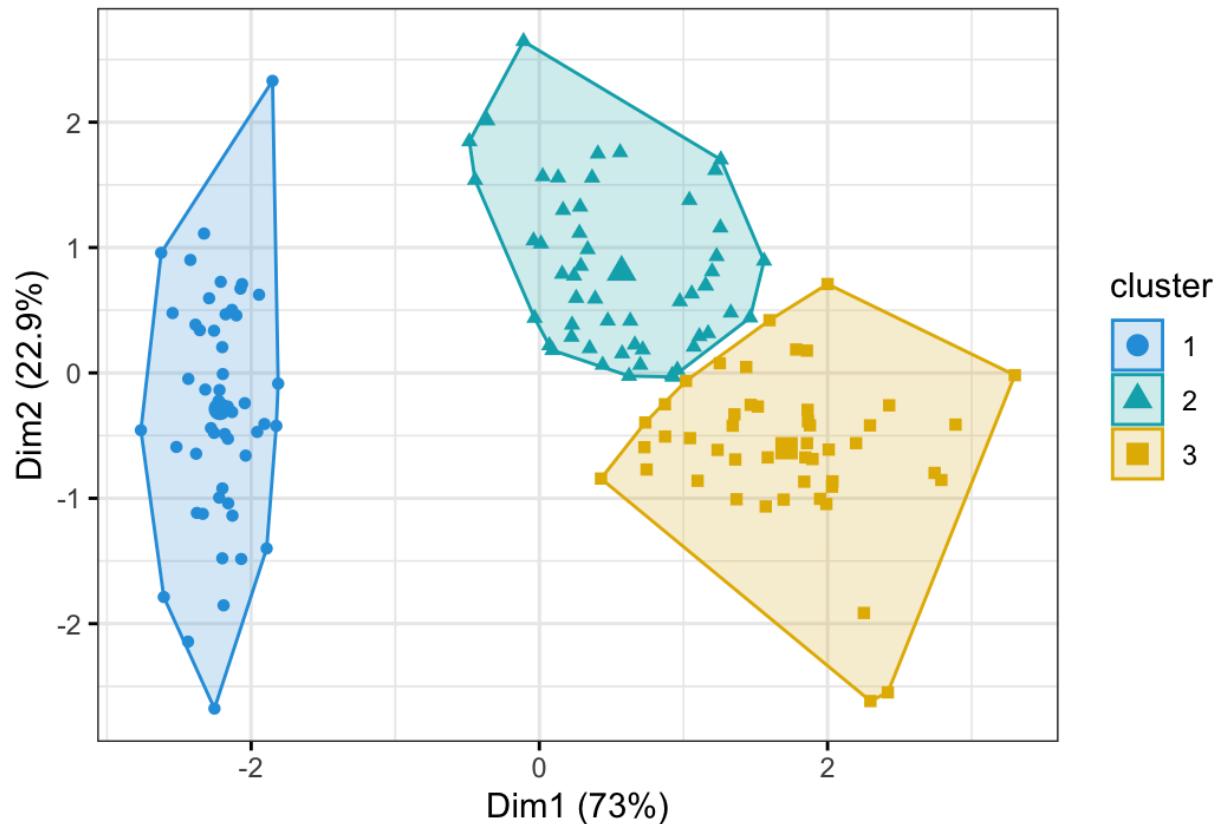
K-Means thinks completely differently:

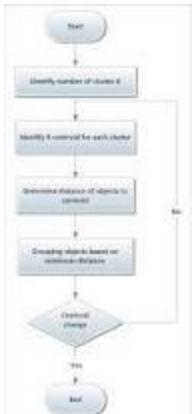
“You tell me K.  
I’ll force the data into exactly K clusters.”

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.

$$\text{Cosine Similarity} = \frac{\vec{A} \cdot \vec{B}}{\|A\| \|B\|}$$

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

💡 Think:

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

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## 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**)

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## 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 ≈ Cosine

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

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## 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.

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## 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
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## **13 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.

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## Big picture (one sentence)

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

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### Step 0 — 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}

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### Step 1 — 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**.

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## 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:

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

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

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## 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**.

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## Step 4— Linkage decides cluster distance

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

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

- ◆ **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.

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## Step 6— Final merge

Now only two clusters remain.

Compute:

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

Using single linkage:

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

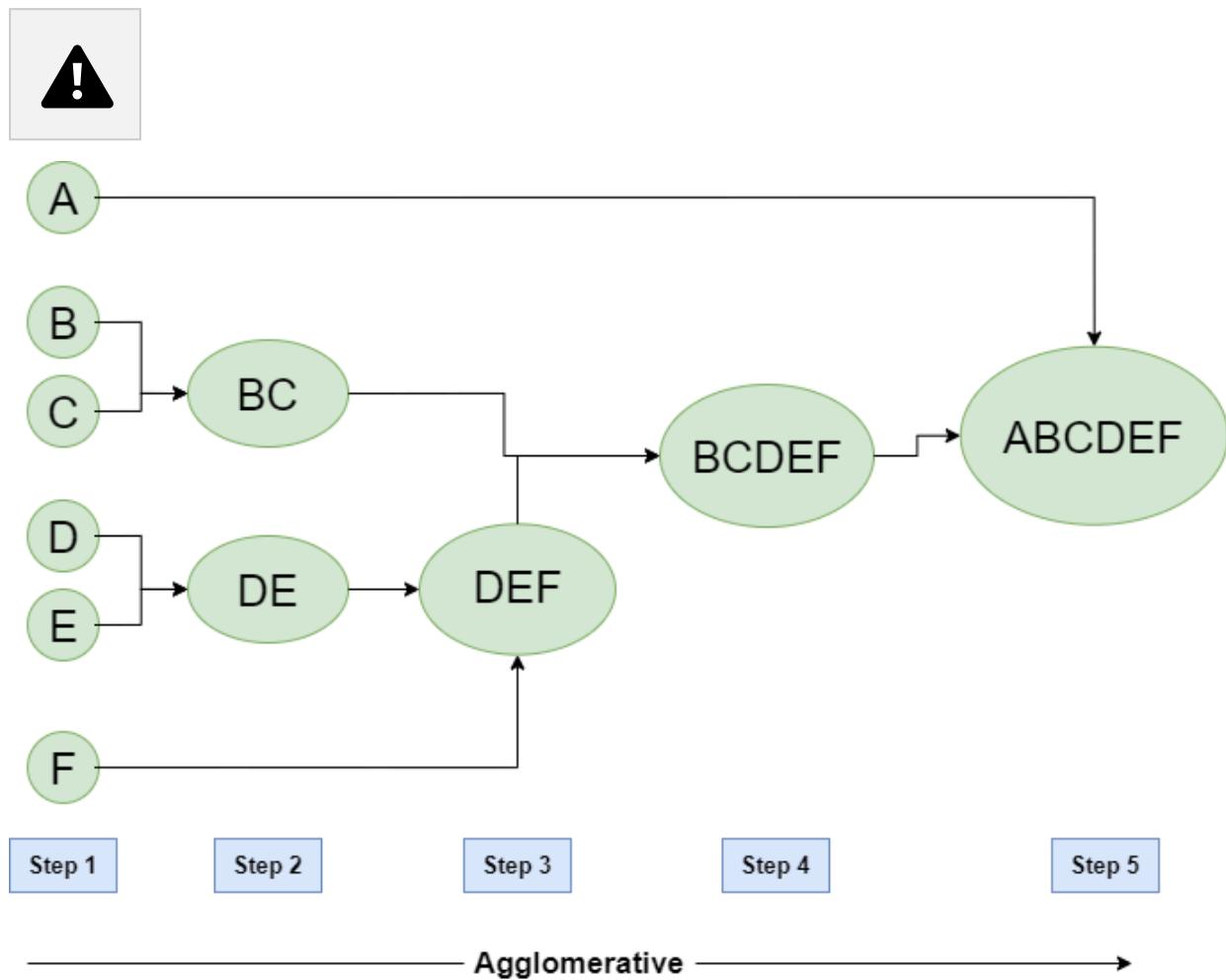
$$= \min(4, 7, 3, 6)$$

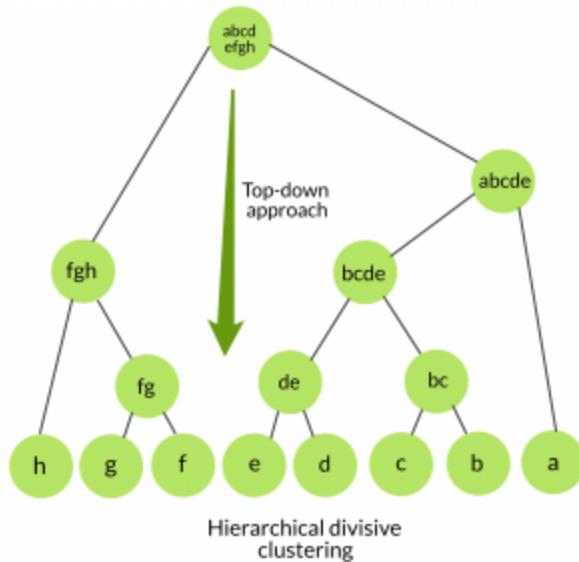
$$= 3$$

Merge them → one cluster.

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## Step 7— Build the dendrogram (result)





The dendrogram stores:

- Which clusters merged
- At what distance

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

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## 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
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## 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 ( $O(n)$ )

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## 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