CS 540 Introduction to Artificial Intelligence
Machine Learning Overview

University of Wisconsin–Madison
Fall 2025, Section 3
September 22, 2025

Announcements

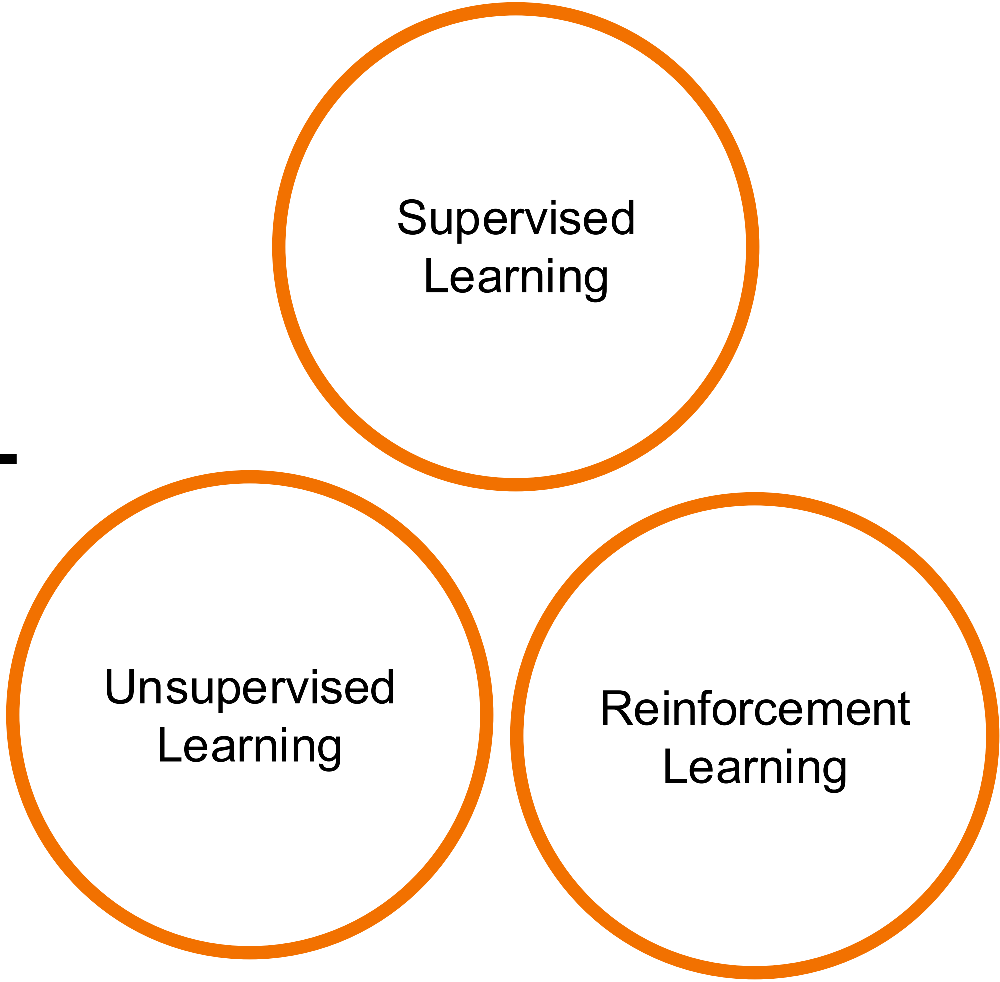
- HW2 due on Friday, September 26th at 11:59 PM
- HW3 released on Friday

- Class roadmap:

ML Introduction
ML Unsupervised I
ML Unsupervised II
ML Supervised: Linear Regression

Machine Learning

Taxonomy of ML



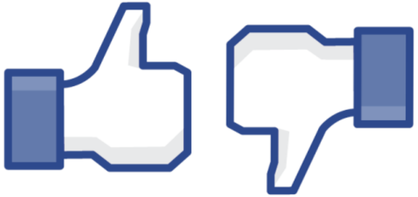
Recap of Supervised/Unsupervised

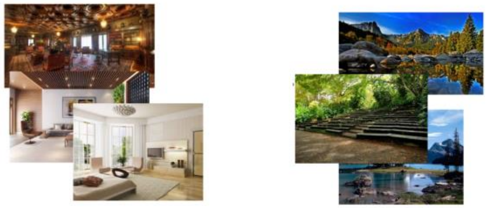
Supervised learning:

- Make predictions, classify data, perform regression
- Dataset: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

Features / Input   Labels / Outputs

- Goal: find function $f : X \rightarrow Y$ to predict label on **new** data



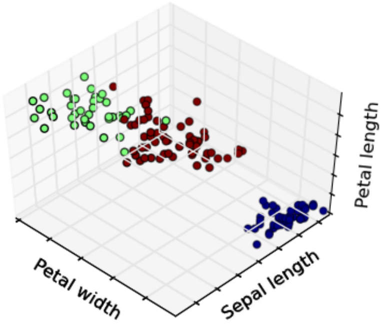


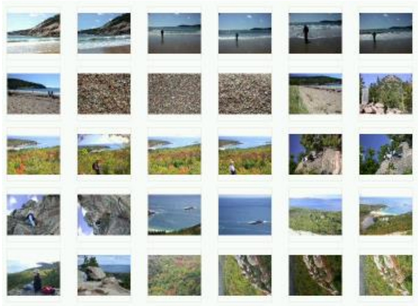
indoor outdoor

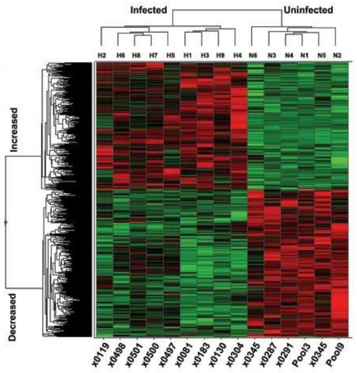
Recap of Supervised/Unsupervised

Unsupervised learning:

- No labels; usually don't make predictions
- Dataset: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$
- Goal: find patterns & structures that help better understand data.







Mulvey and Gingold

Outline

- Intro to Clustering
  - Clustering Types
- Hierarchical Clustering
  - Divisive, agglomerative, linkage strategies
- Centroid-based Clustering
  - k-means

Unsupervised Learning & Clustering

- Clustering is just one type of unsupervised learning
- Other examples:
  - PCA
  - Estimating probability distributions

StyleGAN2 (Kerras et al ’20)

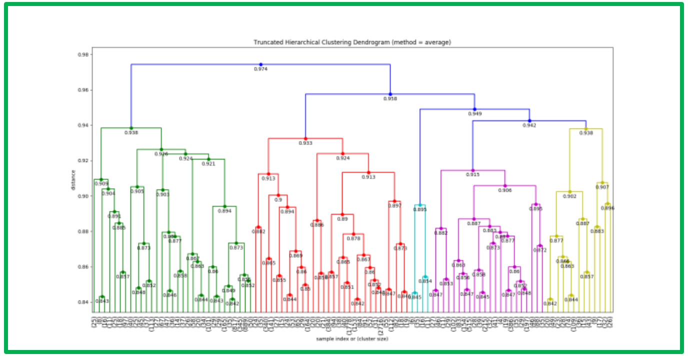
Clustering Types

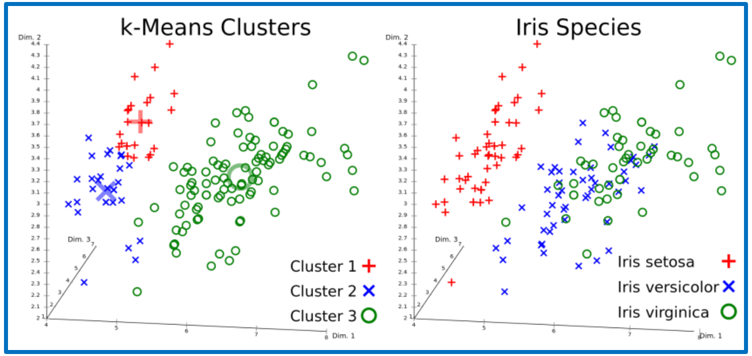
- Several types of clustering

Hierarchical
- Agglomerative
- Divisive

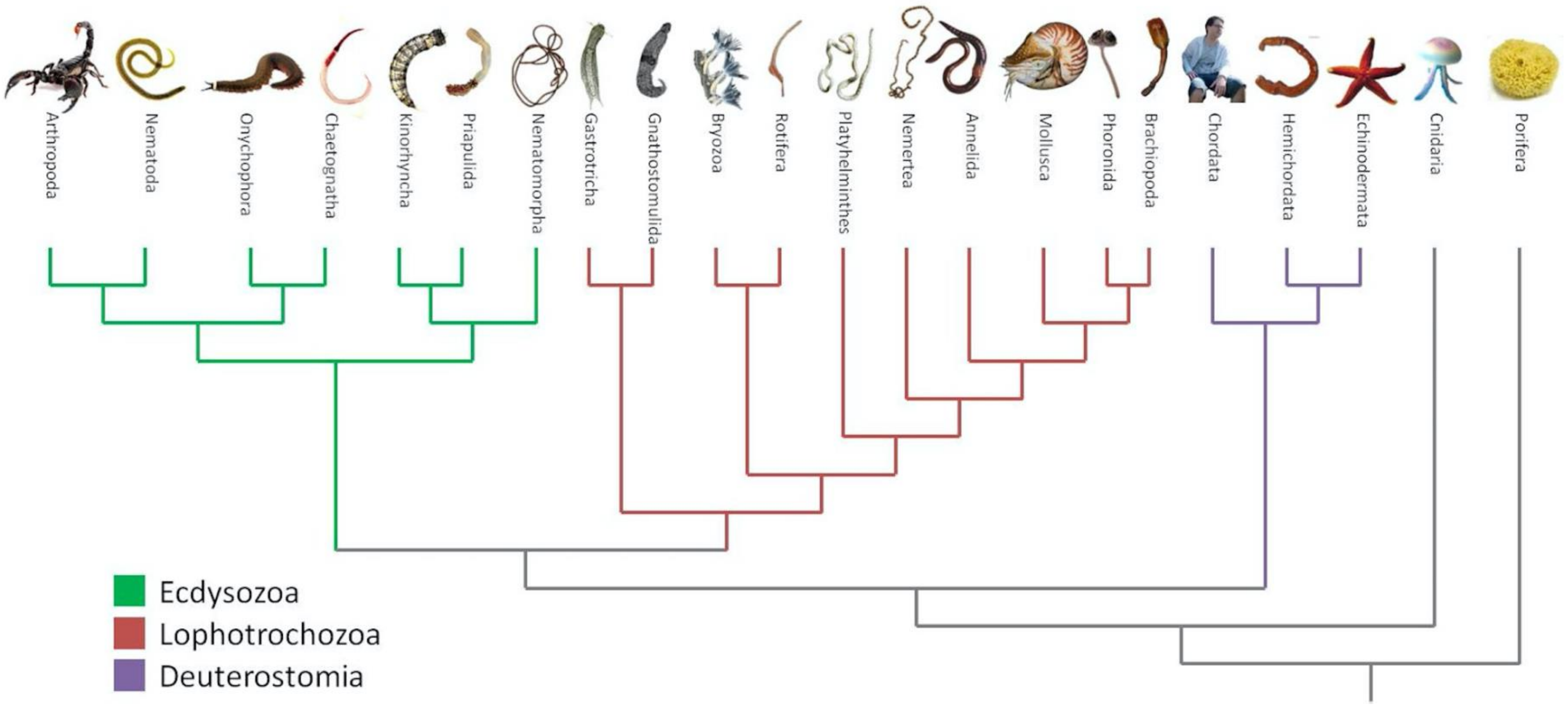
Partitional
- Center-based
- Graph-theoretic
- Spectral

Bayesian
- Decision-based
- Nonparametric





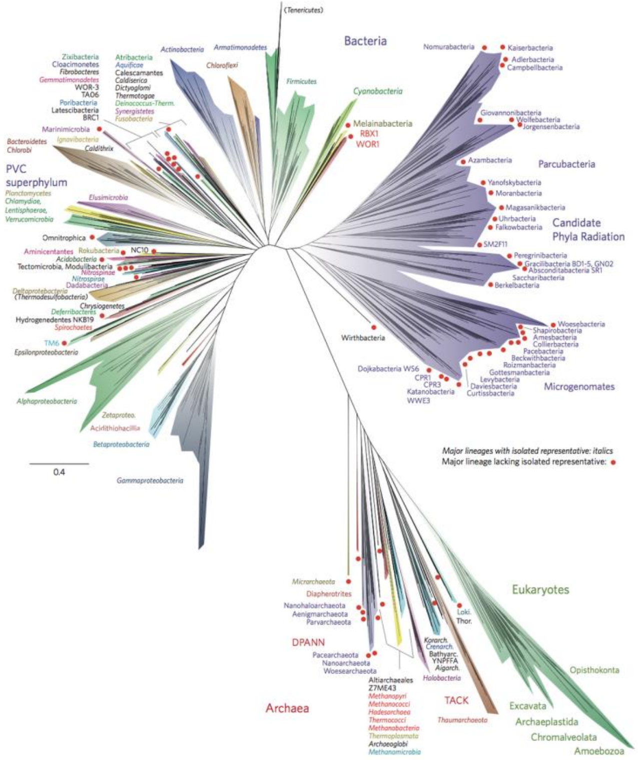
Hierarchical Clustering



Hierarchical Clustering

Basic idea: build a “hierarchy”

- Want: arrangements from specific to general
- One advantage: no need for k, number of clusters.
- **Input**: points. **Output**: a hierarchy
  - A binary tree

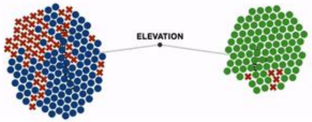


Credit: Wikipedia

Agglomerative vs Divisive

Two ways to go:

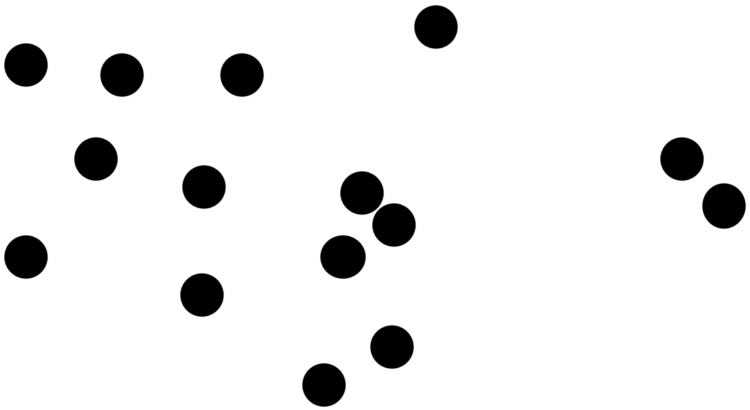
- **Agglomerative**: bottom up.
  - Start: each point a cluster. Progressively merge clusters
- **Divisive**: top down
  - Start: all points in one cluster. Progressively split clusters



Credit: r2d3.us

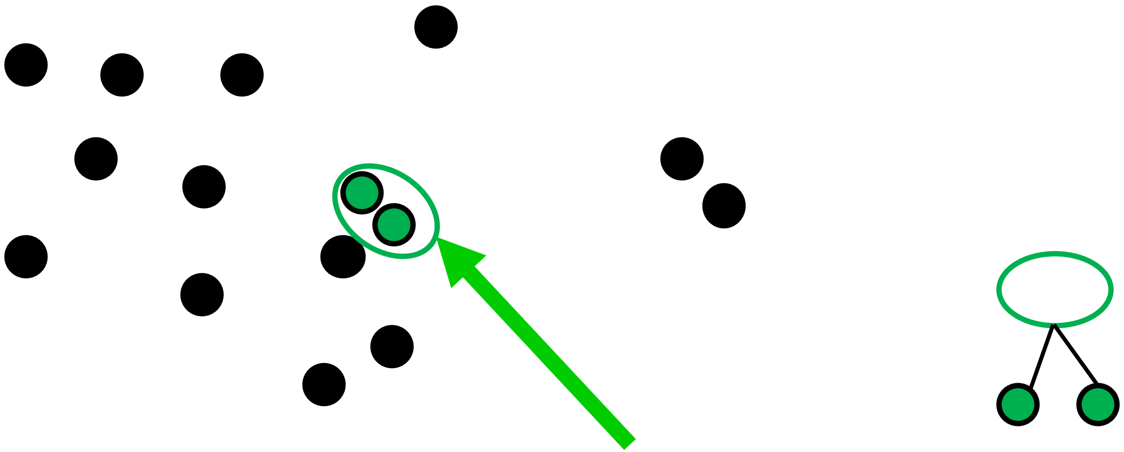
Agglomerative Clustering Example

Agglomerative. Start: every point is its own cluster



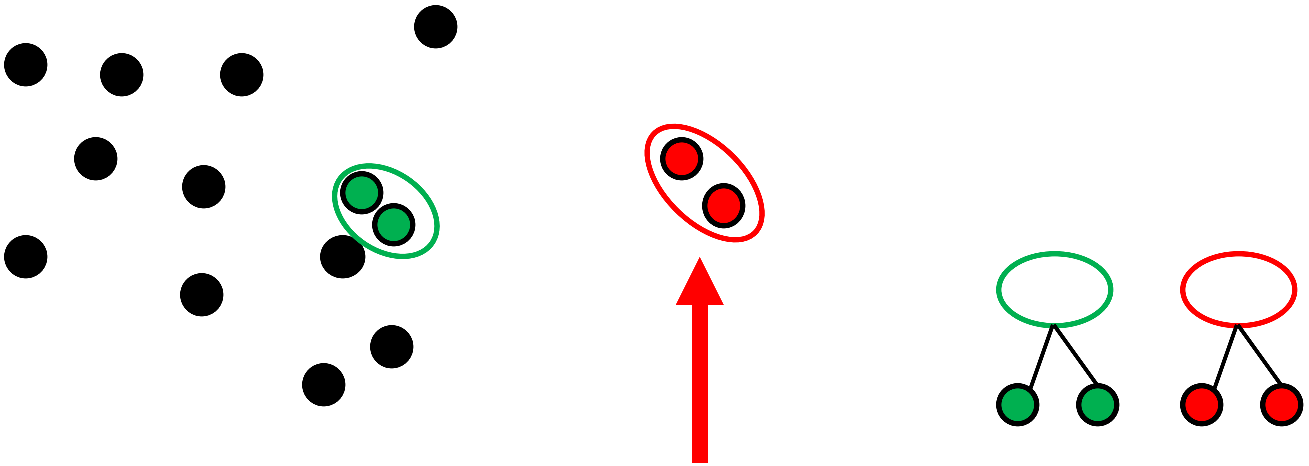
Agglomerative Clustering Example

Get pair of clusters that are closest and merge



Agglomerative Clustering Example

Repeat: Get pair of clusters that are closest and merge



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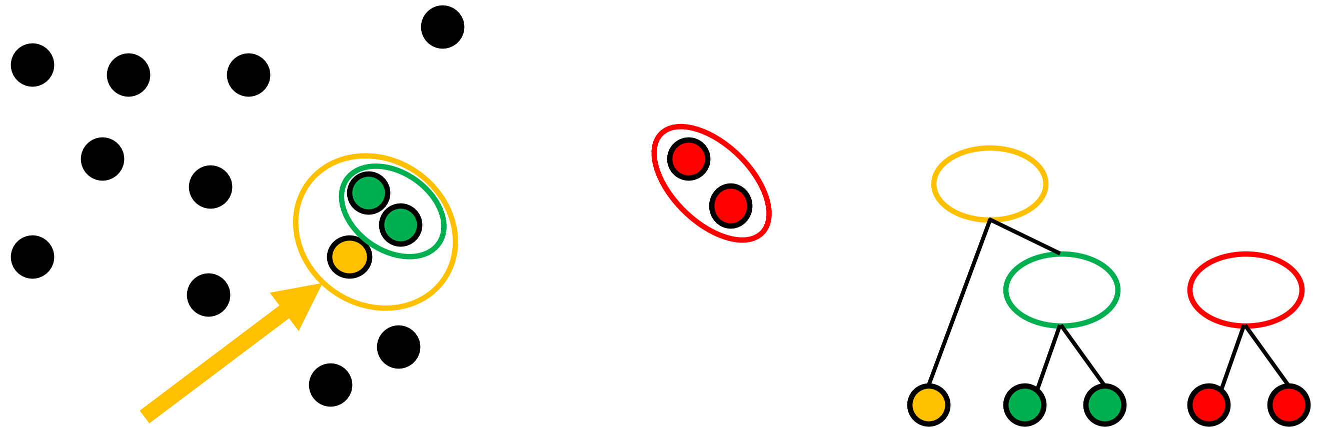


Merging Criteria

Merge: use closest clusters. Define closest?

- Single-linkage

$$d(A, B) = \min_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

- Complete-linkage

$$d(A, B) = \max_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

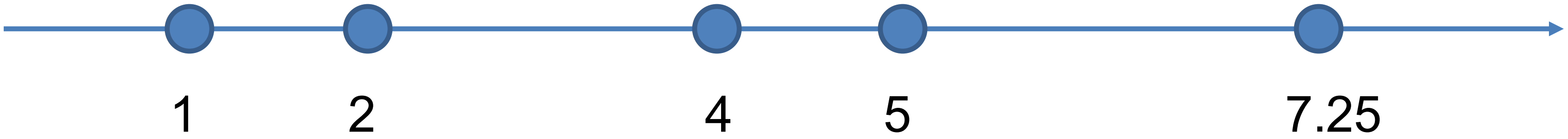
- Average-linkage

$$d(A, B) = \frac{1}{|A||B|} \sum_{x_1 \in A, x_2 \in B} d(x_1, x_2)$$

Single-linkage Example

We'll merge using single-linkage

- 1-dimensional vectors.
- Initial: all points are clusters

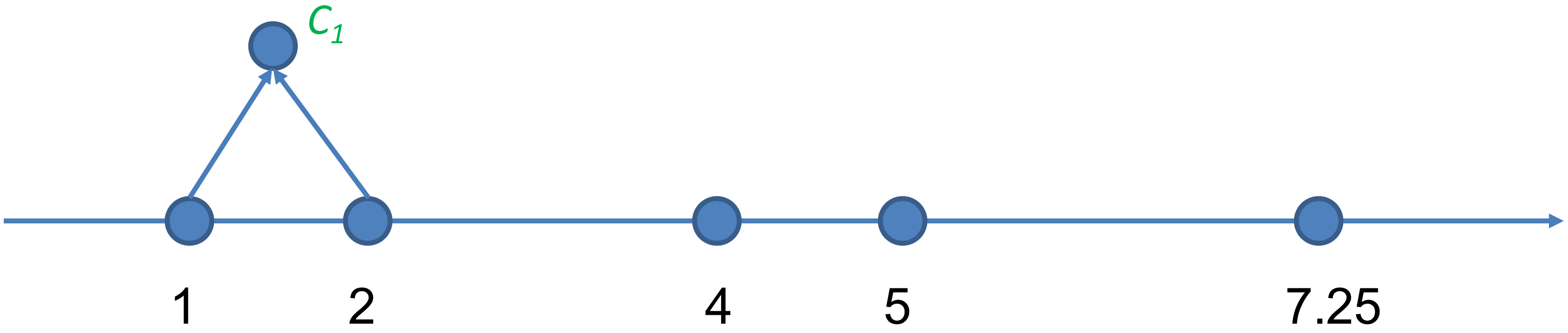


Single-linkage Example

We'll merge using single-linkage

$$d(C_1, \{4\}) = d(2, 4) = 2$$

$$d(\{4\}, \{5\}) = d(4, 5) = 1$$

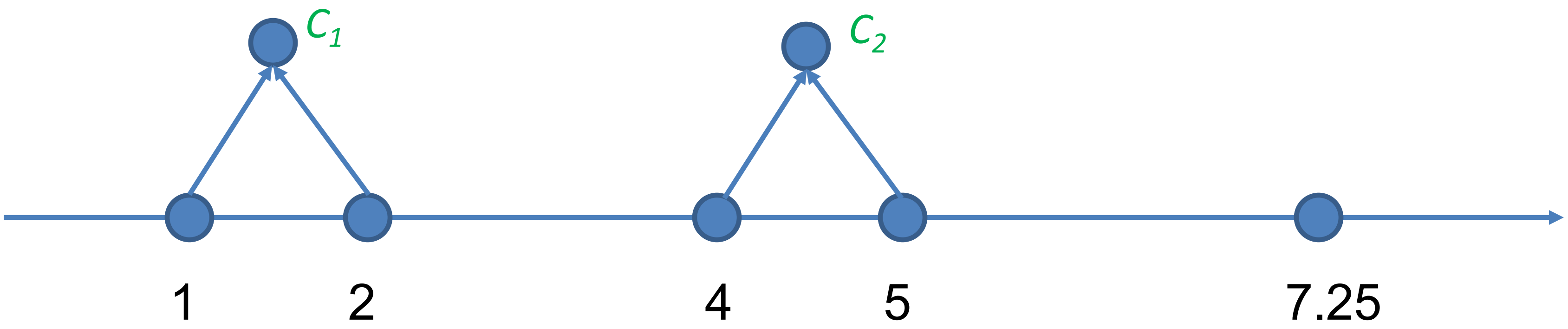


Single-linkage Example

Continue…

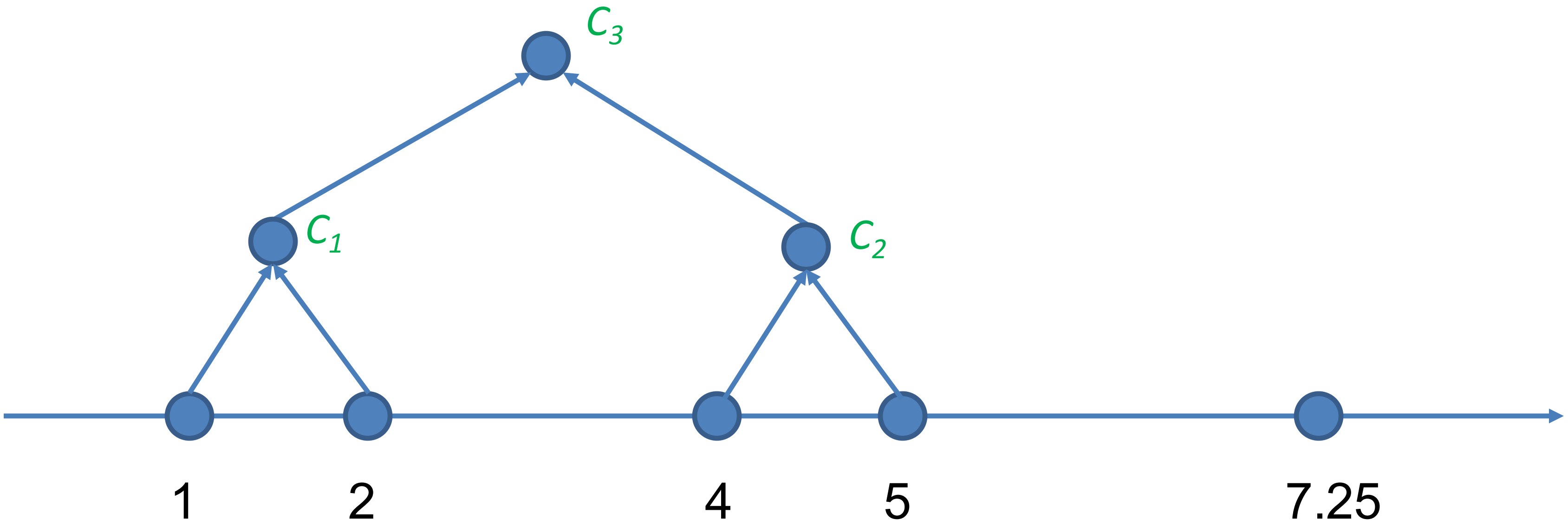
$$d(C_1, C_2) = d(2, 4) = 2$$

$$d(C_2, \{7.25\}) = d(5, 7.25) = 2.25$$

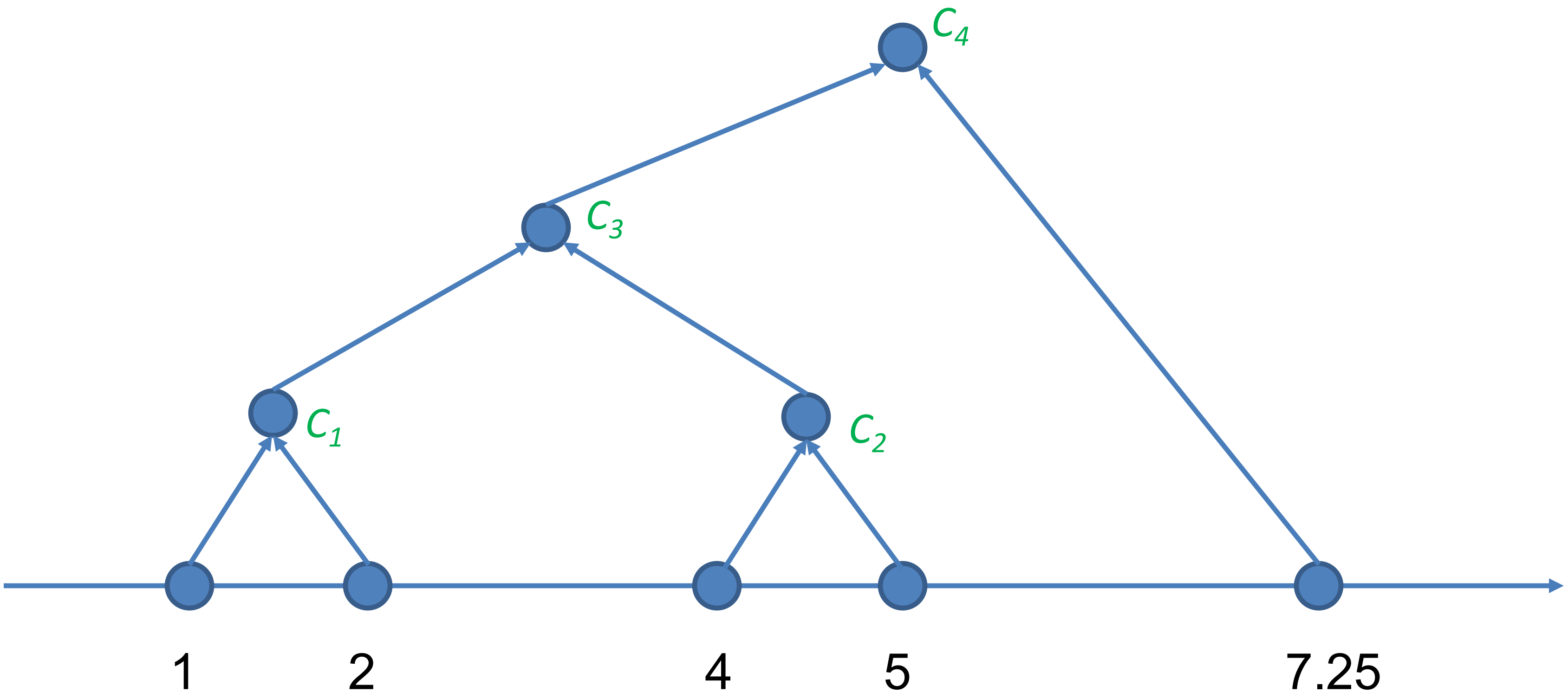


Single-linkage Example

Continue…



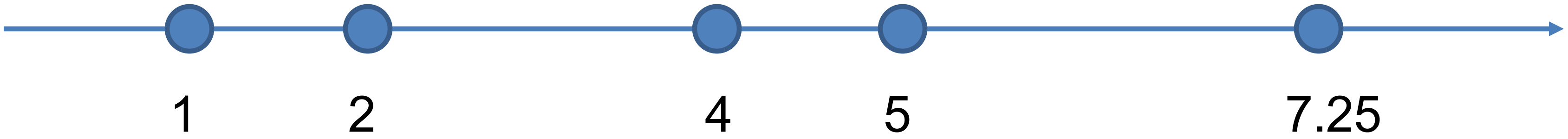
Single-linkage Example



Complete-linkage Example

We’ll merge using complete-linkage

- 1-dimensional vectors.
- Initial: all points are clusters

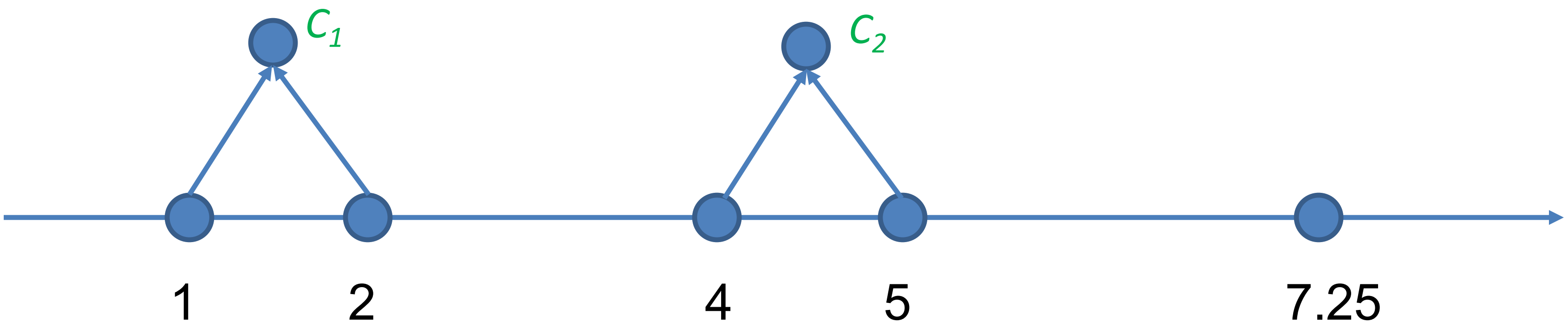


Complete-linkage Example

Beginning is the same…

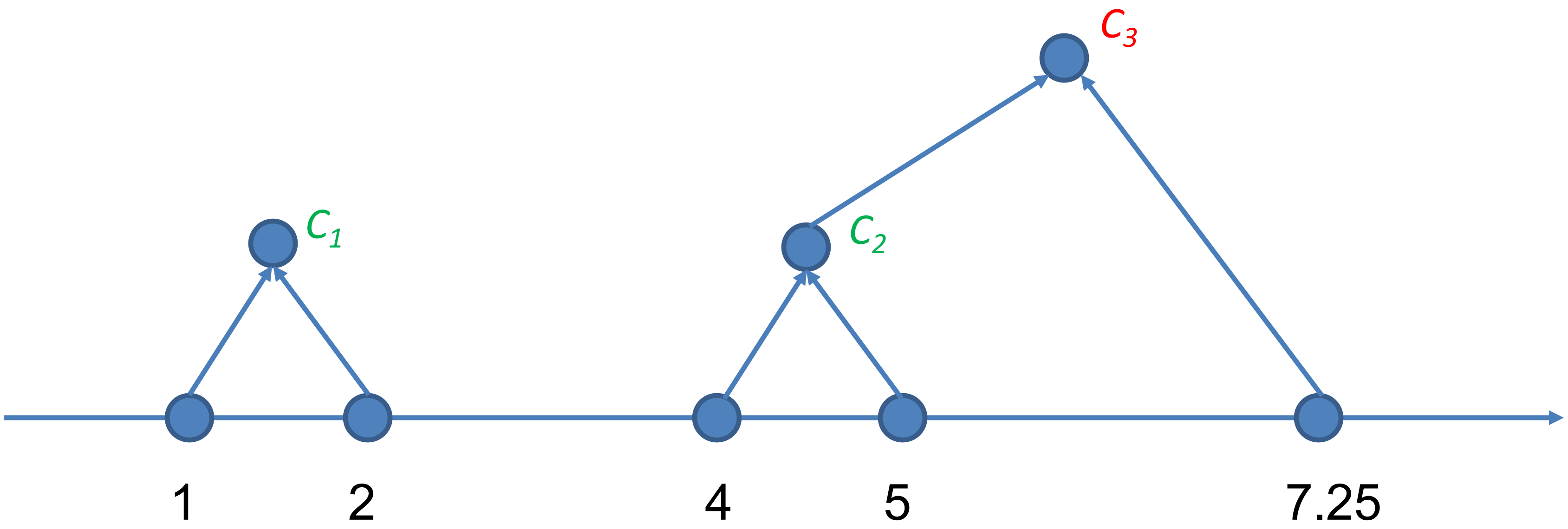
$$d(C_1, C_2) = d(1, 5) = 4$$

$$d(C_2, \{7.25\}) = d(4, 7.25) = 3.25$$

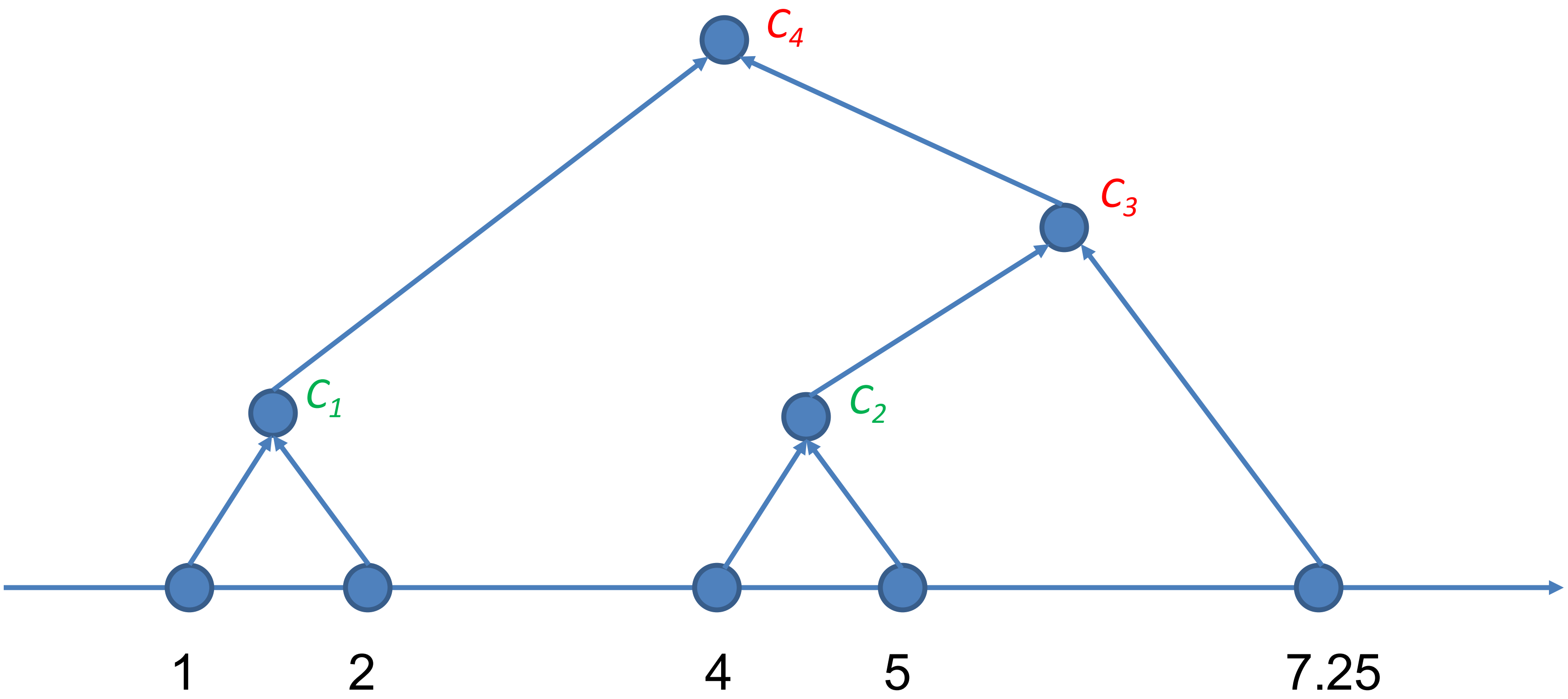


Complete-linkage Example

Now we diverge:



Complete-linkage Example

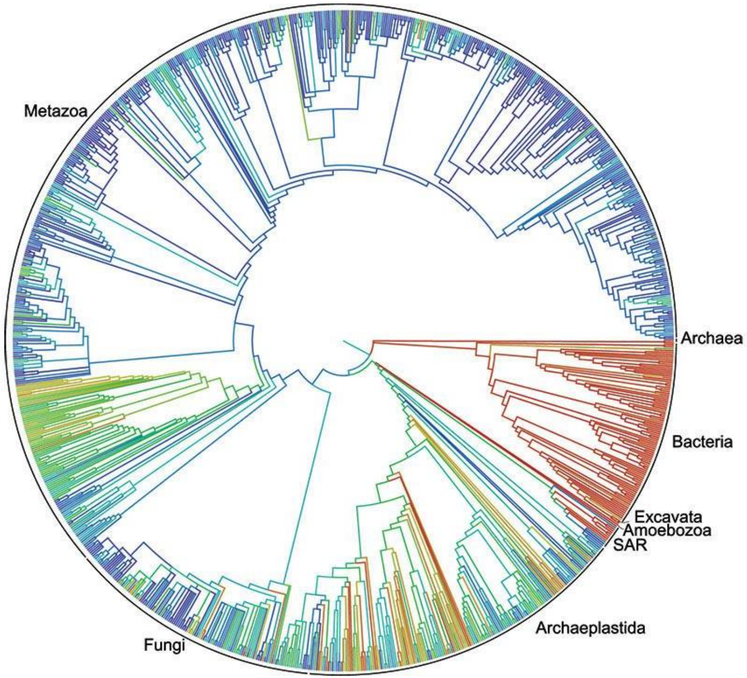


When to Stop?

No simple answer:

- Use the binary tree
  (a **dendogram**)

- Cut at different levels (get different heights/depths)

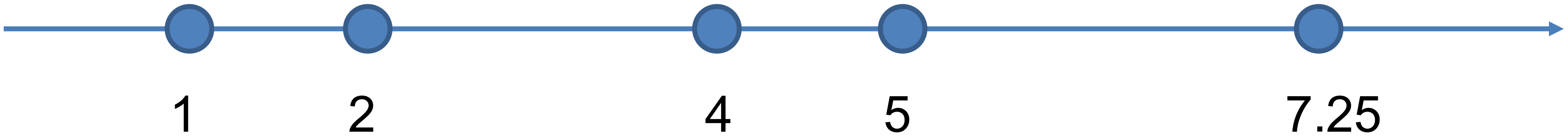


http://opentreeoflife.org/

Break & Quiz

Q 1.1: Let's do hierarchical clustering for two clusters with average linkage on the dataset below. What are the clusters?

- A. {1}, {2,4,5,7.25}
- B. {1,2}, {4, 5, 7.25}
- C. {1,2,4}, {5, 7.25}
- D. {1,2,4,5}, {7.25}



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Iteration 1: merge 1 and 2
Iteration 2: merge 4 and 5
Iteration 3: Now we have clusters {1,2}, {4,5}, {7.25}.
distance({1,2}, {4,5})= 3
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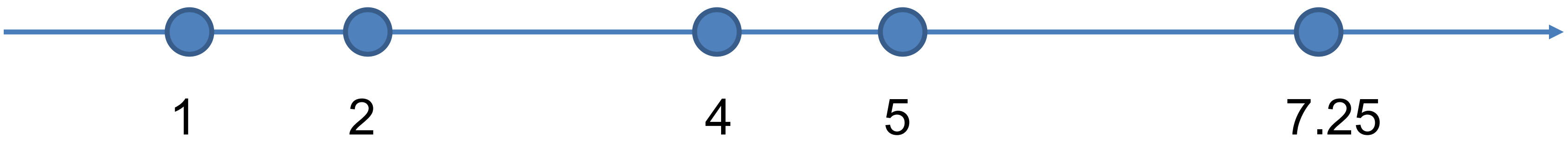

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Q 1.2: If we do hierarchical clustering on n points, the maximum depth of the resulting tree is

- A. 2
- B. log n
- C. $n/2$
- D. n-1

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Denote the points as x_1, x_2, …, x_n
Suppose:
in iteration 1, we merge points x_1 and x_2
in iteration 2, we merge {x_1, x_2} with x_3
…
in iteration t, we merge {x_1, x_2, …, x_t} with x_{t+1}
…
in iteration n-1, we merge {x_1, x_{n-1}} with x_n

Then we will get a tree with depth n-1.

Center-based Clustering

- k-means is an example of a partitional, **center-based clustering algorithm.**
- Specify a desired number of clusters, k; run k-means to find k clusters.

K-means clustering

- Very popular clustering method

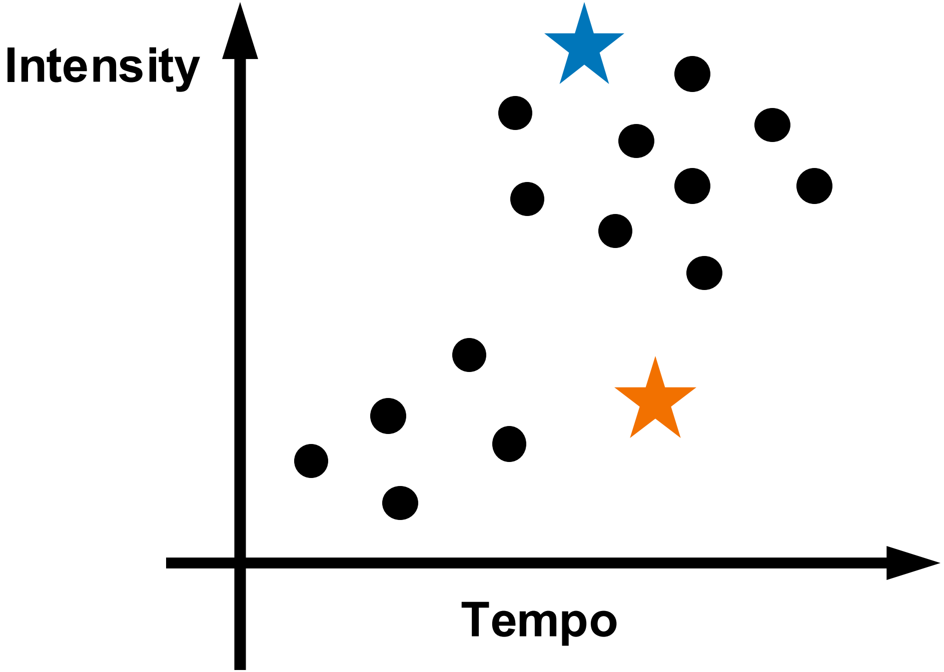
$$x_1, x_2, \ldots, x_n$$

- Input: a dataset, and assume the number of clusters **k** is given

K-means clustering

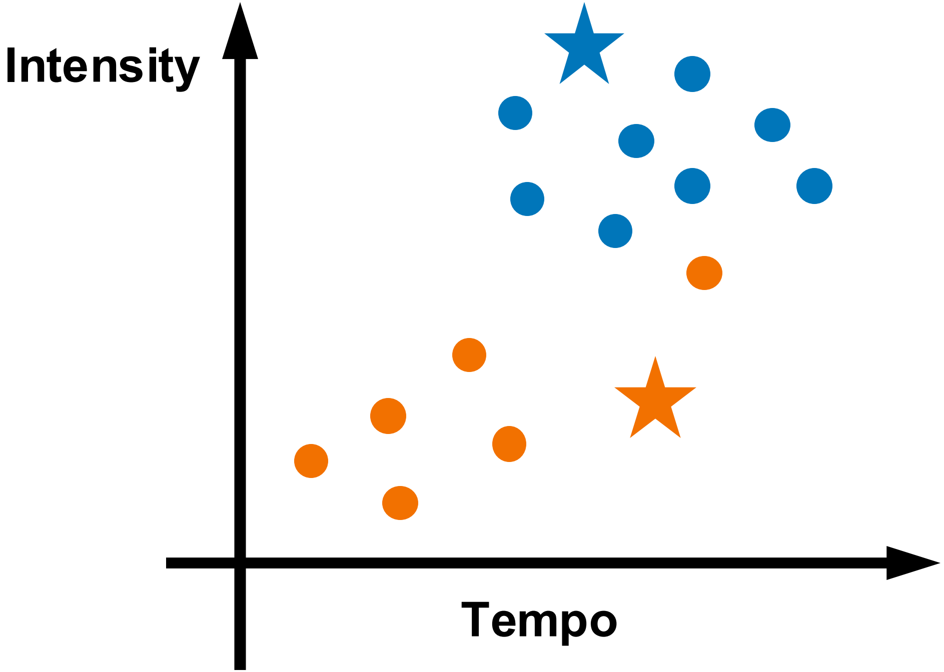
Step 1: **Randomly** picking 2 positions as initial cluster centers

(not necessarily a data point)



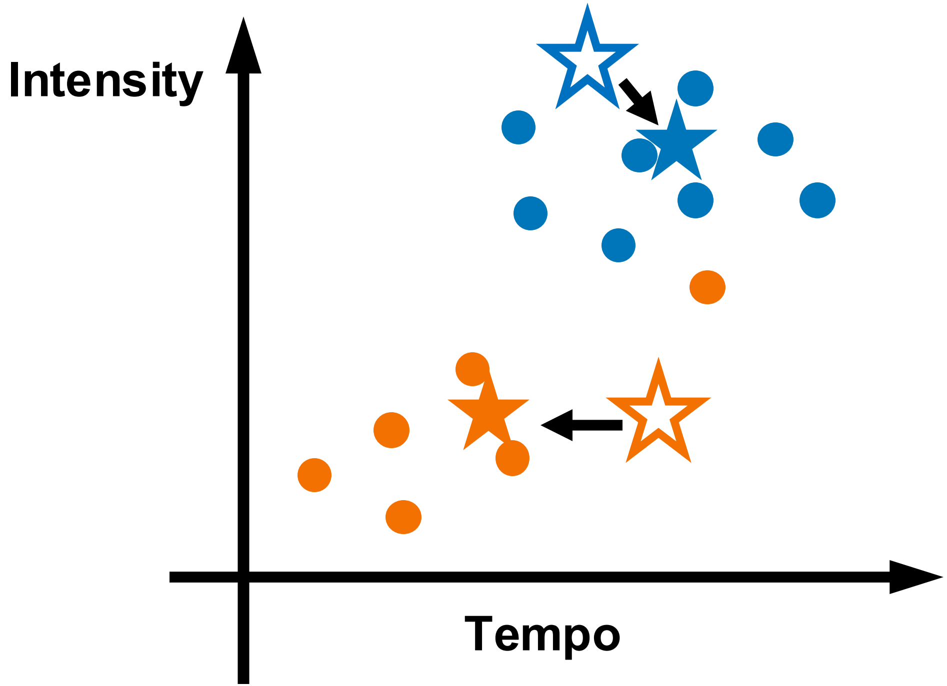
K-means clustering

Step 2: for each point x_i, determine its cluster: find the closest center



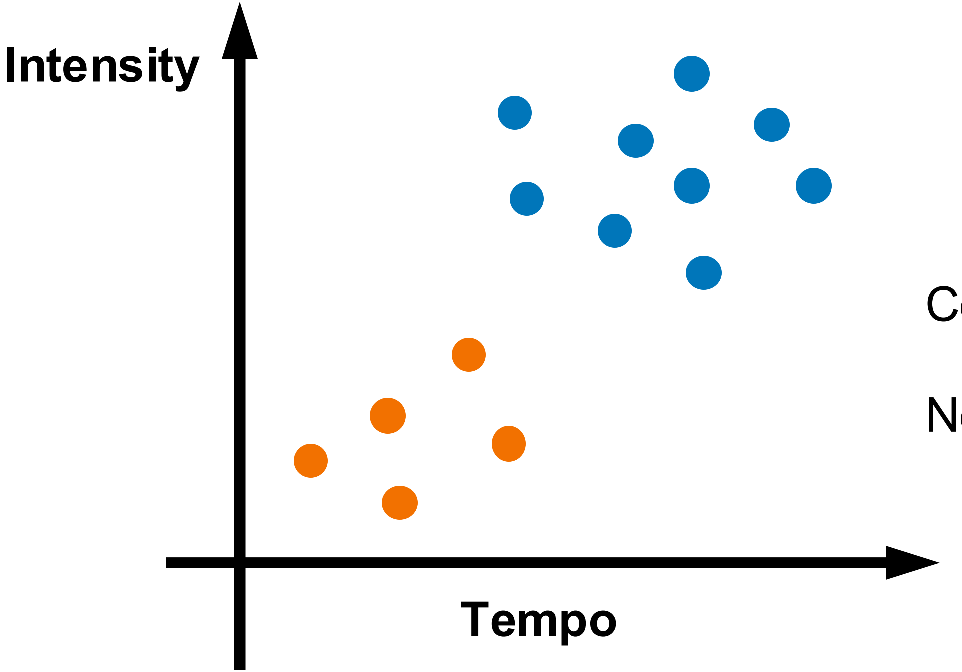
K-means clustering

Step 3: update all cluster centers as the centroids



K-means clustering

Repeat step 2 & 3 until convergence



Converged solution!

No labels required!

K-means algorithm

- Input: $x_1, x_2, \dots, x_n, k$
- Step 1: select k cluster centers $c_1, c_2, \dots, c_k$
- Step 2: for each point x_i, assign it to the closest center in Euclidean distance:

$$y(x_i) = \text{argmin}_j \; ||x_i - c_j||$$

- Step 3: update all cluster centers as the centroids:

$$c_j = \frac{\sum_{x:y(x)=j} x}{\sum_{x:y(x)=j} 1}$$

- Repeat Step 2 and 3 until cluster centers no longer change

Empty Clusters

- Can clusters ever become empty?
  - Yes: https://user.ceng.metu.edu.tr/~tcan/ceng465_f1314/Schedule/KMeansEmpty.html
  - Even if cluster centers are initialized at data points
- How do implementations deal with this?
  - Move cluster center to a random point
  - Randomly split an existing (large) cluster

Questions to Ponder

- Will k-means stop/converge?
- Could we prove guarantees about its performance?
- Can we view k-means as optimizing some objective?
- How to pick starting cluster centers?
- How many clusters should we use?

Questions on k-means

- What is k-means trying to optimize?
- Will k-means stop (converge)?
- Will it find a global or local optimum?
- How to pick starting cluster centers?
- How many clusters should we use?

The optimization problem of k-means

- What is k-means trying to optimize?

$$\min_{c,y} \sum_{i=1}^{n} ||x_i - c_{y(x_i)}||^2$$

Questions on k-means

Will k-means stop (converge)? Yes

Given a fixed dataset and a fixed number of clusters, there are only a **finite number of ways** to assign data points to clusters.

Each iteration consists of:

- Assignment Step: Assign each data point to the closest centroid.
- Update Step: Recompute centroids as the mean of assigned points.

These steps **always reduce or keep the same** the objective function (sum of squared distance), ensuring termination.

Questions on k-means

Will it find a global or local optimum? (sadly no guarantee)

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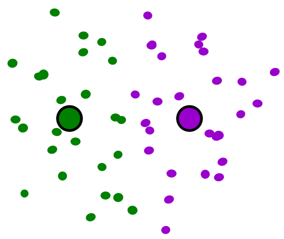

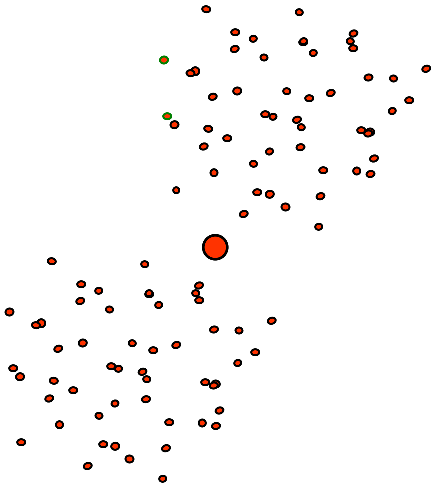

Questions on k-means

How many clusters should we use?

- Difficult problem
- Domain knowledge
- Elbow Method
  - Compute the within-cluster sum of squares (WCSS) for different values of k.
  - Plot WCSS vs. k and look for the **elbow point** where the reduction in WCSS slows down. The optimal k is typically at this elbow.

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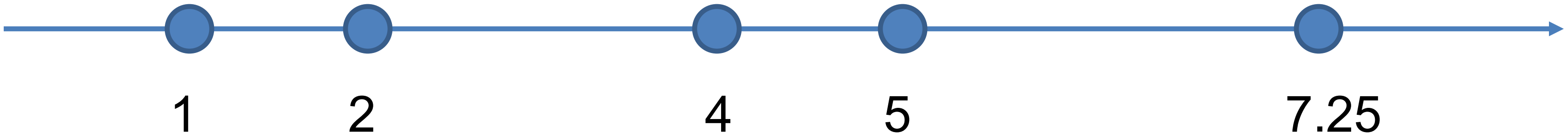

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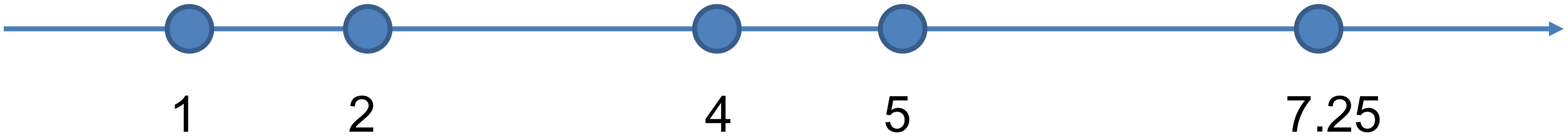

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Then we will get a tree with depth n-1.

Break & Quiz

Q 2.1: You have seven 2-dimensional points. You run 3-means on it, with initial clusters

$$C_1 = \{(2,2),(4,4),(6,6)\}, C_2 = \{(0,4),(4,0)\}, C_3 = \{(5,5),(9,9)\}$$

Cluster centroids are updated to?

- A. C_1: (4,4), C_2: (2,2), C_3: (7,7)
- B. C_1: (6,6), C_2: (4,4), C_3: (9,9)
- C. C_1: (2,2), C_2: (0,0), C_3: (5,5)
- D. C_1: (2,6), C_2: (0,4), C_3: (5,9)

Break & Quiz

Q 2.1: You have seven 2-dimensional points. You run 3-means on it, with initial clusters

$$C_1 = \{(2,2),(4,4),(6,6)\}, C_2 = \{(0,4),(4,0)\}, C_3 = \{(5,5),(9,9)\}$$

Cluster centroids are updated to?

- **A. C_1: (4,4), C_2: (2,2), C_3: (7,7)**
- B. C_1: (6,6), C_2: (4,4), C_3: (9,9)
- C. C_1: (2,2), C_2: (0,0), C_3: (5,5)
- D. C_1: (2,6), C_2: (0,4), C_3: (5,9)

The average of points in C1 is (4,4).
The average of points in C2 is (2,2).
The average of points in C3 is (7,7).

Break & Quiz

Q 2.2: We are running 3-means again. We have 3 centers, C_1 (0,1), C_2, (2,1), C_3 (-1,2). Which cluster assignment is possible for the points (1,1) and (-1,1), respectively? Ties are broken arbitrarily:

(i) C_1, C_1 (ii) C_2, C_3 (iii) C_1, C_3

- A. Only (i)
- B. Only (ii) and (iii)
- C. Only (i) and (iii)
- D. All of them

Break & Quiz

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(i) C_1, C_1 (ii) C_2, C_3 (iii) C_1, C_3

- A. Only (i)
- B. Only (ii) and (iii)
- C. Only (i) and (iii)
- **D. All of them**

For the point (1,1): square-Euclidean-distance to C1 is 1, to C2 is 1, to C3 is 5

So it can be assigned to C1 or C2

For the point (-1,1): square-Euclidean-distance to C1 is 1, to C2 is 9, to C3 is 1

So it can be assigned to C1 or C3

Break & Quiz

Q 2.3: If we run K-means clustering twice with random starting cluster centers, are we guaranteed to get same clustering results? Does K-means always converge?

- A. Yes, Yes
- B. No, Yes
- C. Yes, No
- D. No, No

Break & Quiz

Q 2.3: If we run K-means clustering twice with random starting cluster centers, are we guaranteed to get same clustering results? Does K-means always converge?

- A. Yes, Yes
- **B. No, Yes**
- C. Yes, No
- D. No, No

The clustering from k-means will depend on the initialization. Different initialization can lead to different outcomes.

K-means will always converge on a finite set of data points:

1. There are finite number of possible partitions of the points
2. The assignment and update steps of each iteration will only decrease the sum of the distances from points to their corresponding centers.
3. If it run forever without convergence, it will revisit the same partition, which is contradictory to item 2.

Thanks!