CS 540 Introduction to Artificial Intelligence
Unsupervised Learning I

University of Wisconsin-Madison

Spring 2026 Sections 1 & 2

Announcements

- **Homework 3 online**:
  - Due Wednesday February 18th at 11:59PM

- Class roadmap:

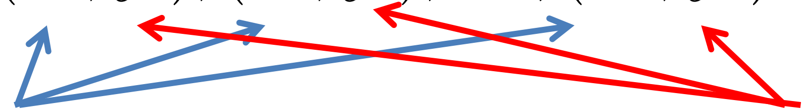
ML Unsupervised I
ML Unsupervised II
ML Linear Regression
Machine Learning: K - Nearest Neighbors & Naive Bayes

Machine Learning

Recap of Supervised/Unsupervised

Supervised learning:

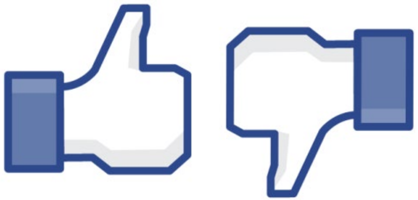
- Make predictions, classify data, perform regression
- Dataset: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$



Features / Covariates / Input

Labels / Outputs

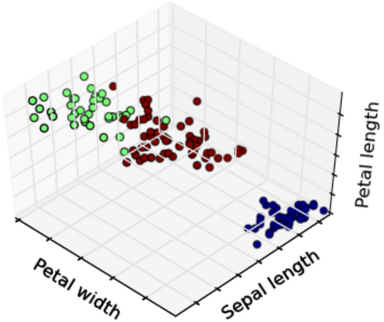
- Goal: find function $f : X \rightarrow Y$ to predict label on **new** data

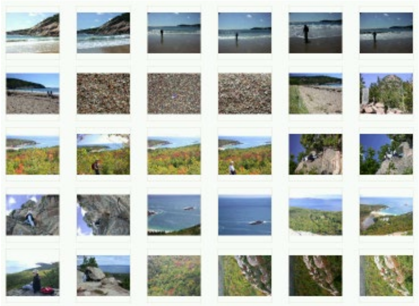


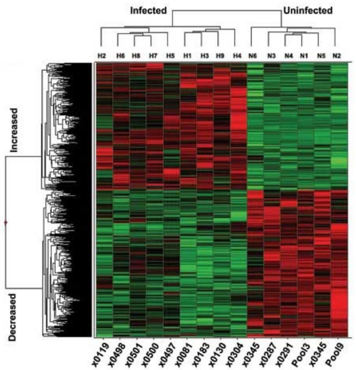
Recap of Supervised/Unsupervised

Unsupervised learning:

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







Mulvey and Gingold

Recap of Supervised/Unsupervised

Note that there are **other kinds** of ML:

- Mixtures: semi-supervised learning
  - Idea: different types of "signal"
- Reinforcement learning
  - Learn how to act in order to maximize rewards
  - Later on in course…

DeepMind

Outline

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

Unsupervised Learning & Clustering

- Note that clustering is just one type of unsupervised learning (**UL**)
  - PCA is another unsupervised algorithm
- Estimating probability distributions also UL (GANs)
- Clustering is popular & useful!

StyleGAN2 (Kerras et al ’20)

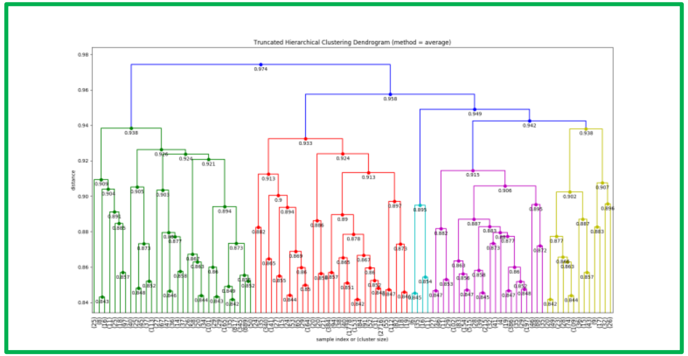
Clustering Types

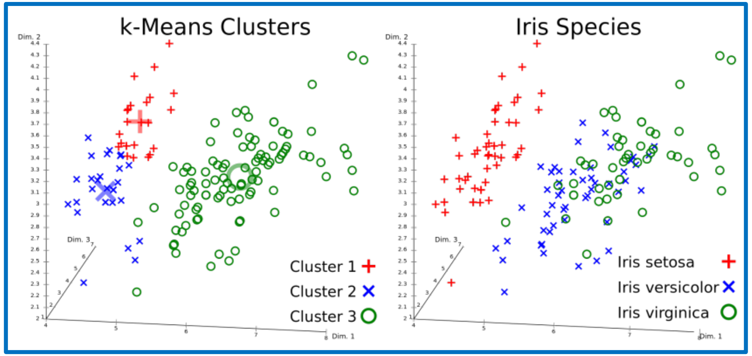
- Several types of clustering

Hierarchical
- Agglomerative
- Divisive

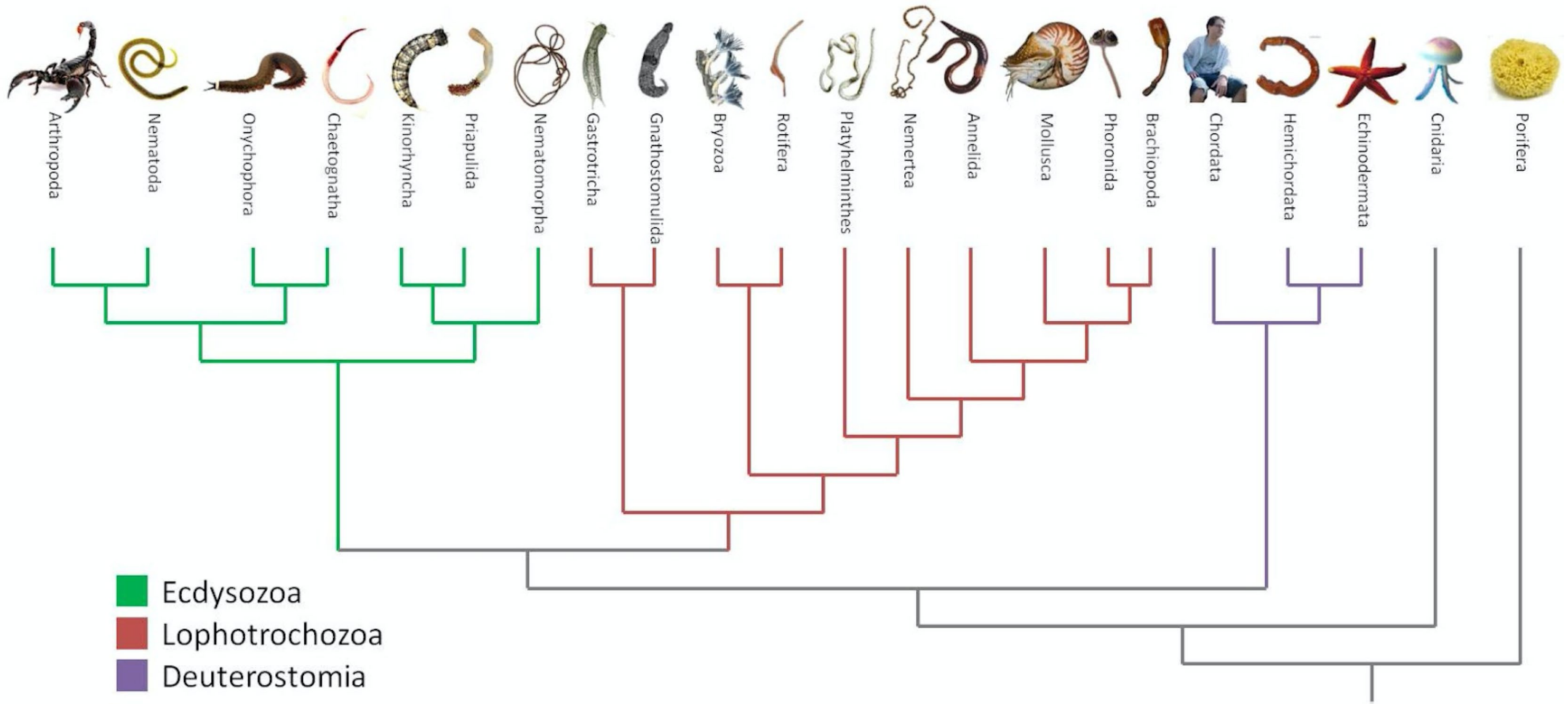
Partitional
- Center-based
- Graph-theoretic
- Spectral

Bayesian
- Decision-based
- Nonparametric





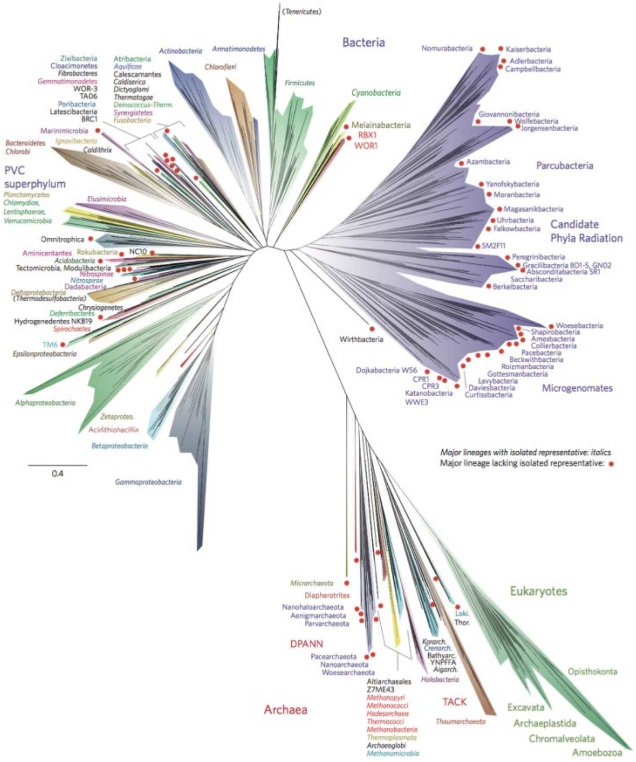
Hierarchical Clustering



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

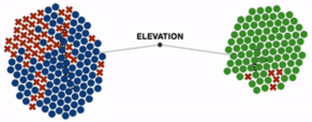


Credit: Wikipedia

Agglomerative vs Divisive

Two ways to go:

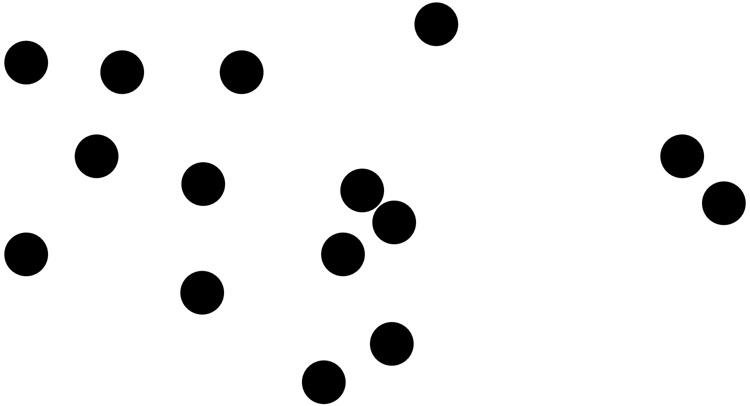
- **Agglomerative**: bottom up.
  - Start: each point a cluster. Progressively merge clusters
- **Divisive**: top down
  - Start: all points in one cluster. Progressively split clusters



Credit: r2d3.us

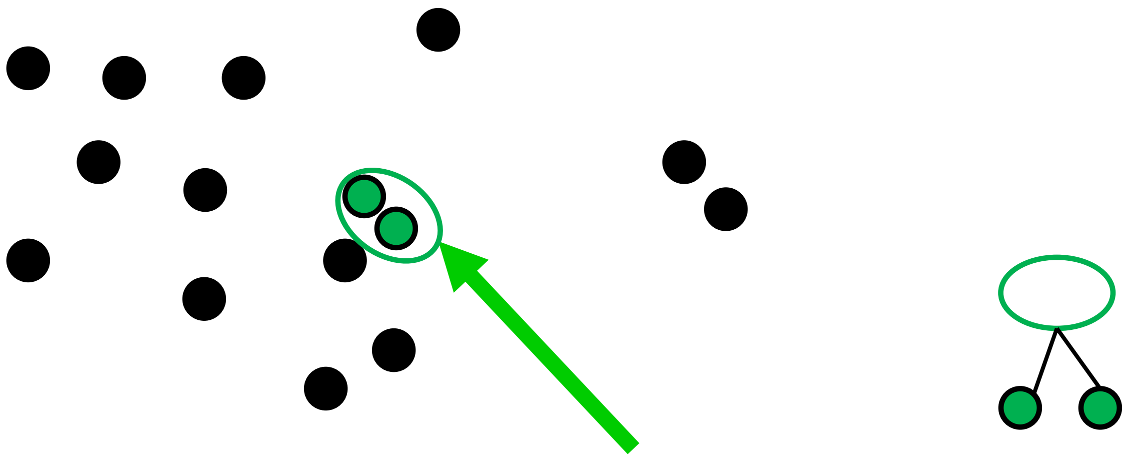
Agglomerative Clustering Example

Agglomerative. Start: every point is its own cluster



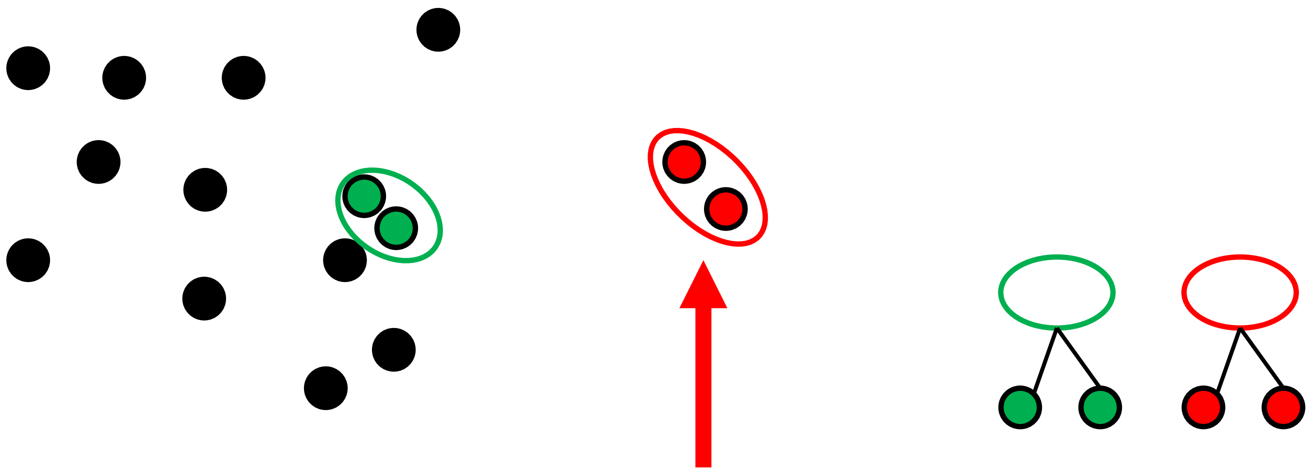
Agglomerative Clustering Example

Get pair of clusters that are closest and merge



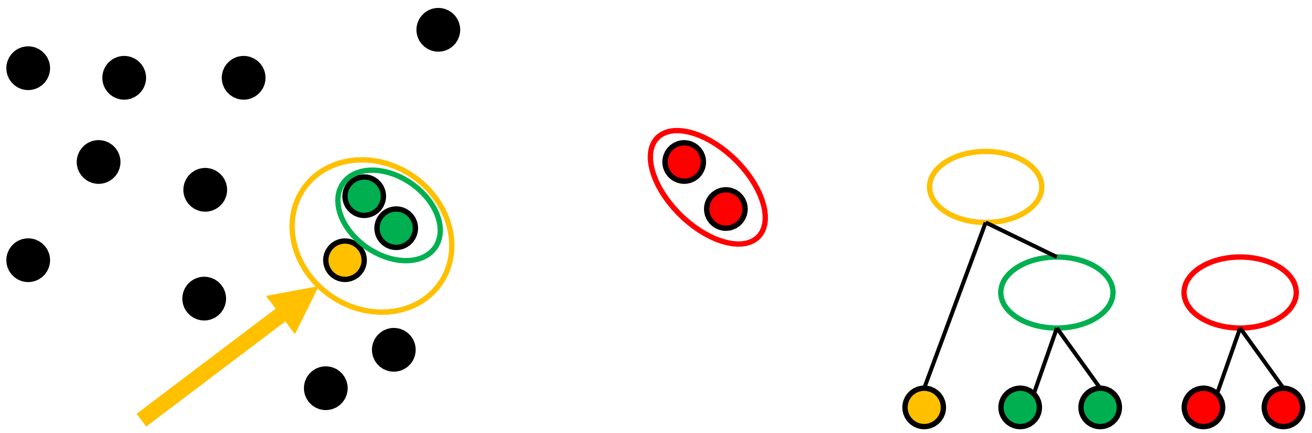
Agglomerative Clustering Example

Repeat: Get pair of clusters that are closest and merge



Agglomerative Clustering Example

Repeat: Get pair of clusters that are closest and merge



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

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

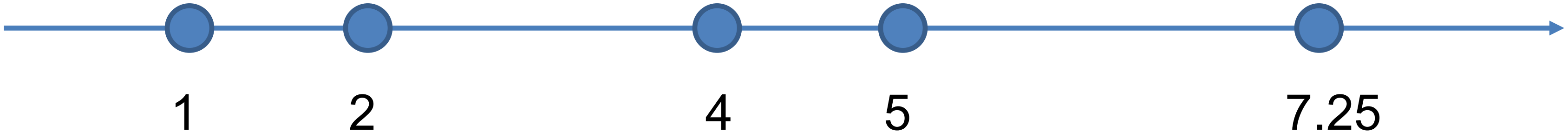
- Average-linkage

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

Single-linkage Example

We'll merge using single-linkage

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

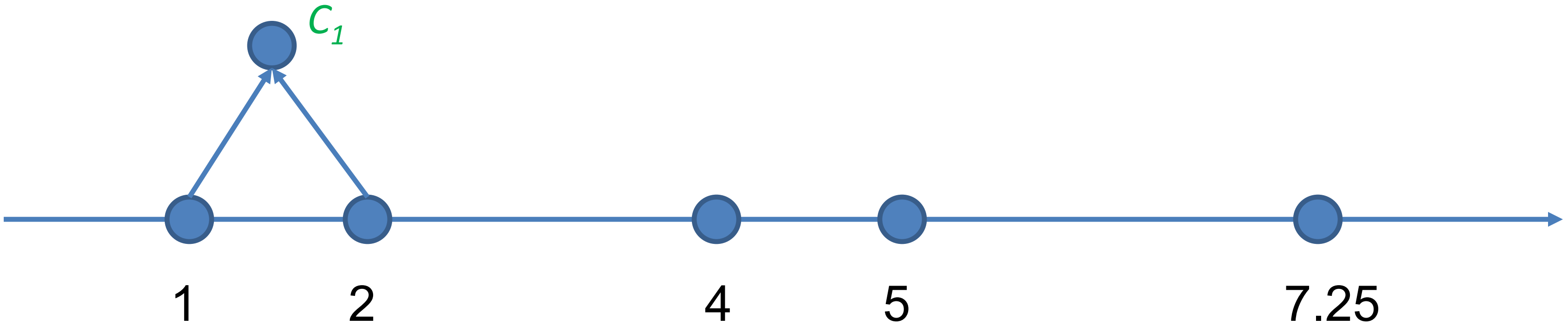


Single-linkage Example

We'll merge using single-linkage

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

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

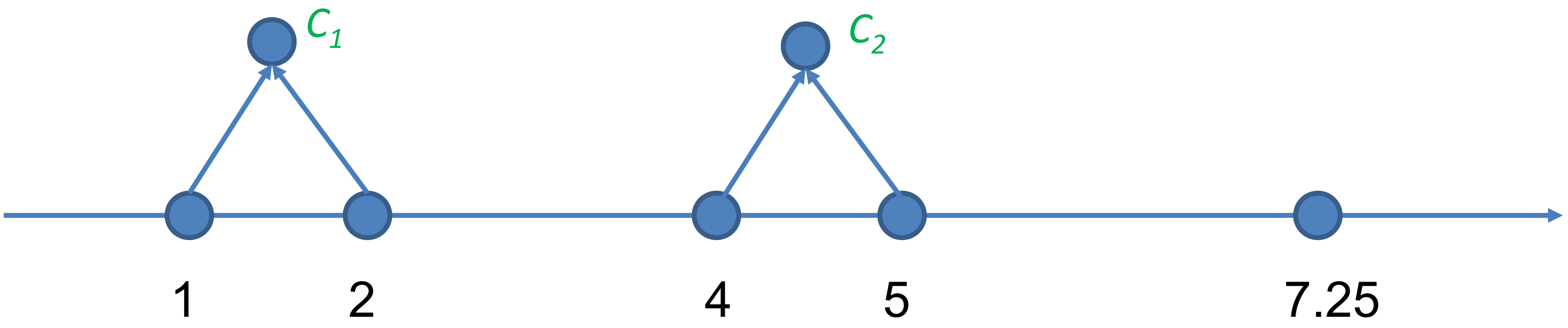


Single-linkage Example

Continue…

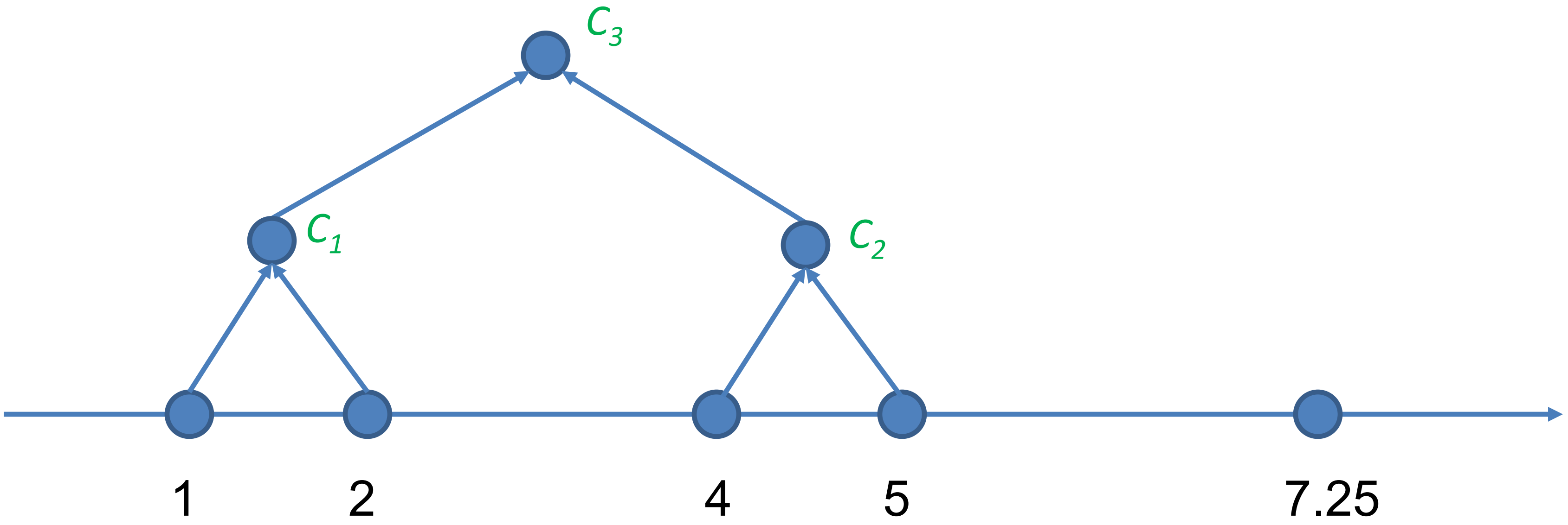
$$d(C_1, C_2) = d(2, 4) = 2$$

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

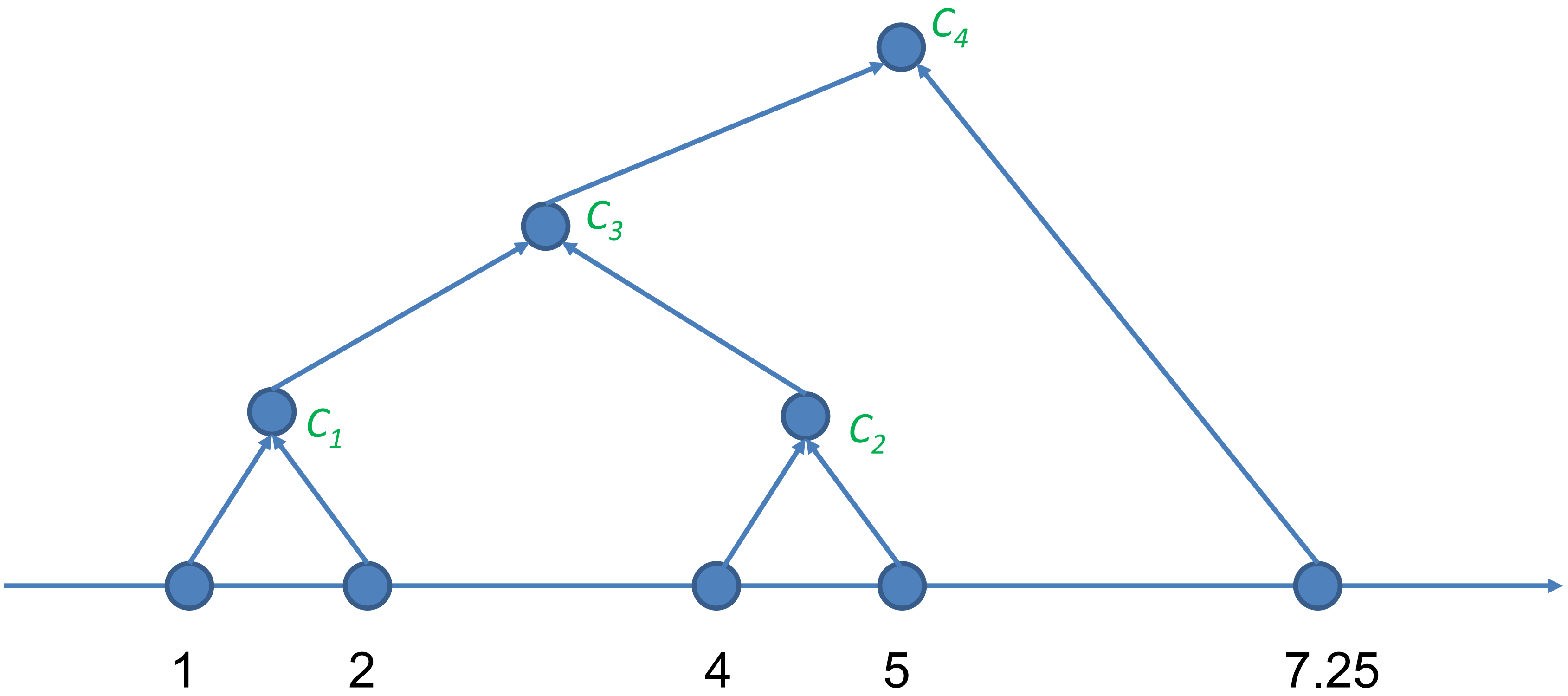


Single-linkage Example

Continue…



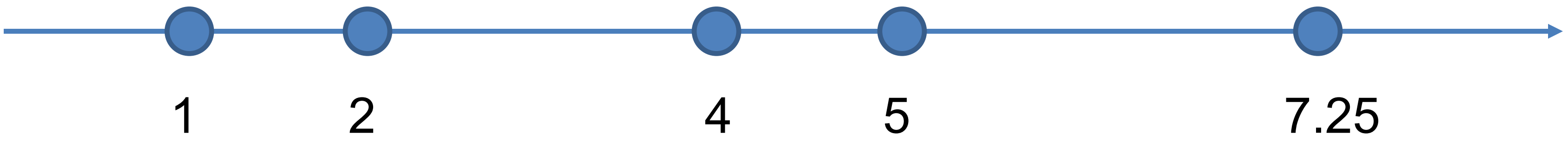
Single-linkage Example



Complete-linkage Example

We'll merge using complete-linkage

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

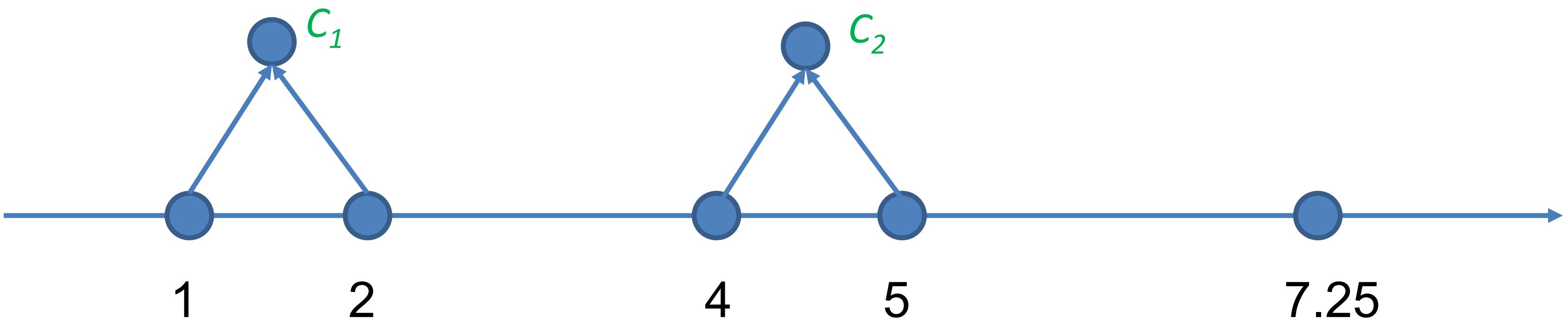


Complete-linkage Example

Beginning is the same…

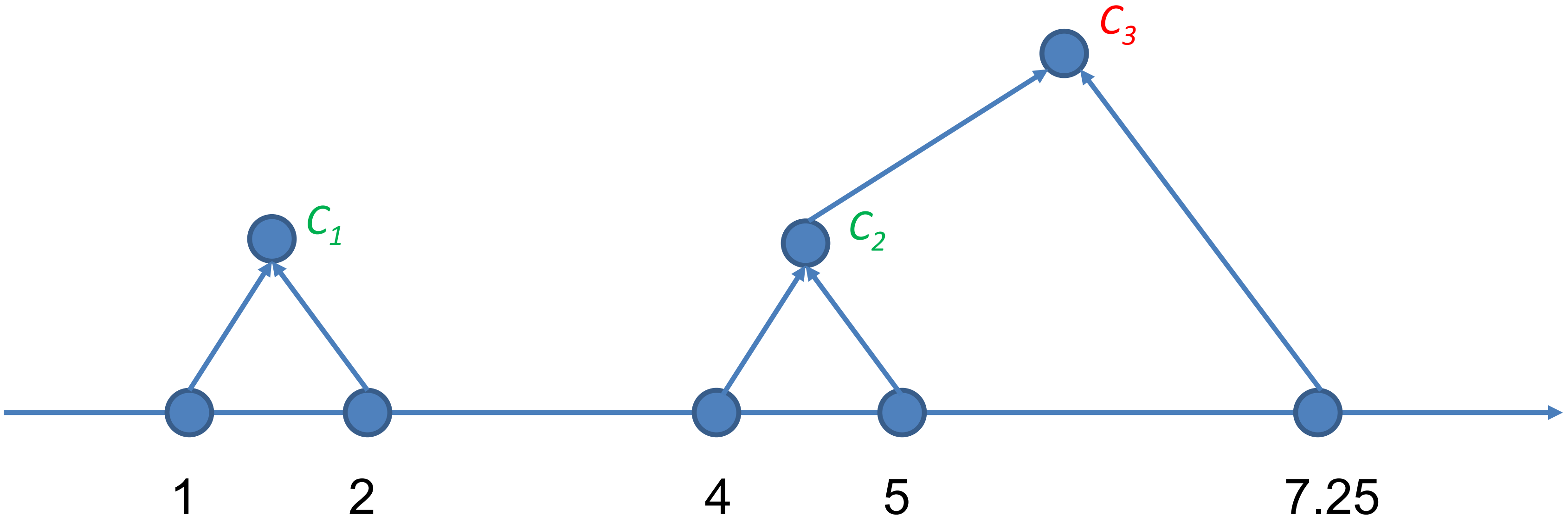
$$d(C_1, C_2) = d(1, 5) = 4$$

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

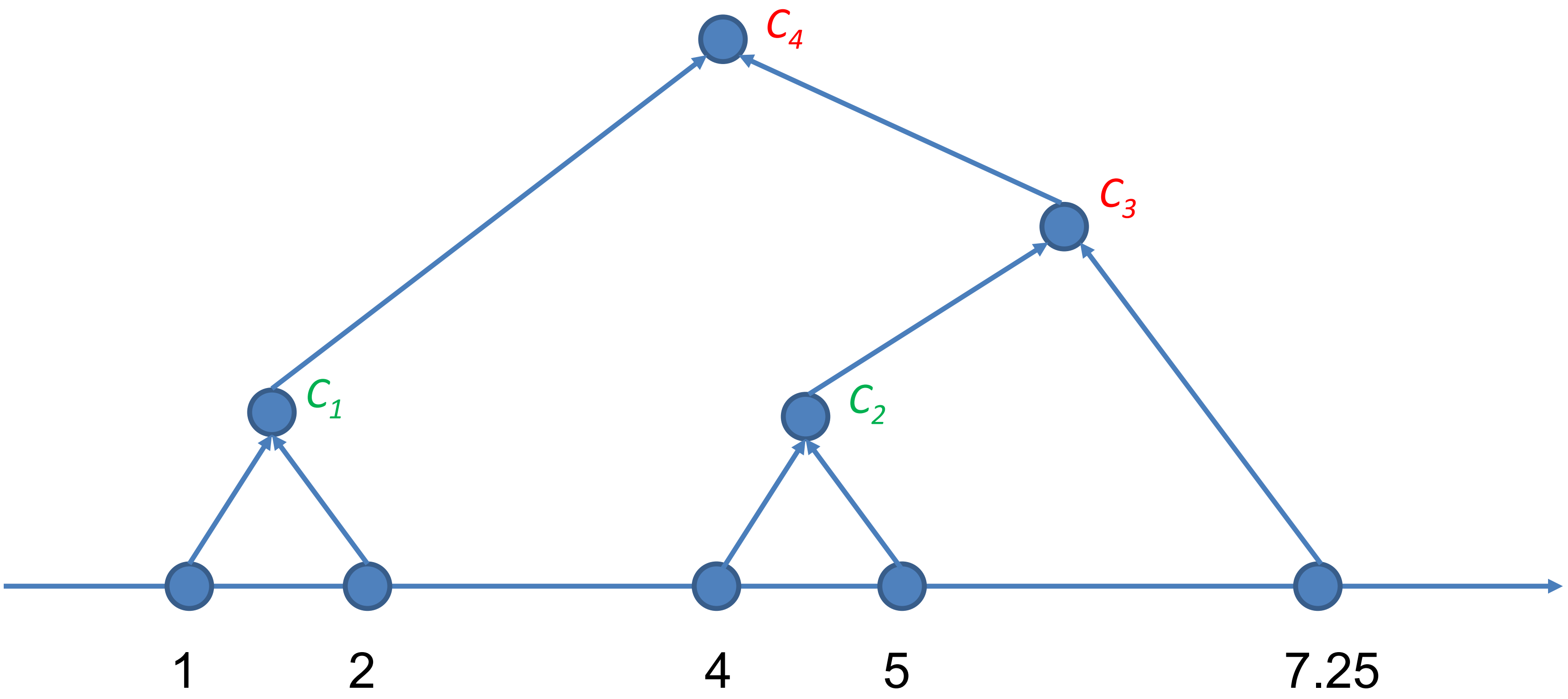


Complete-linkage Example

Now we diverge:



Complete-linkage Example

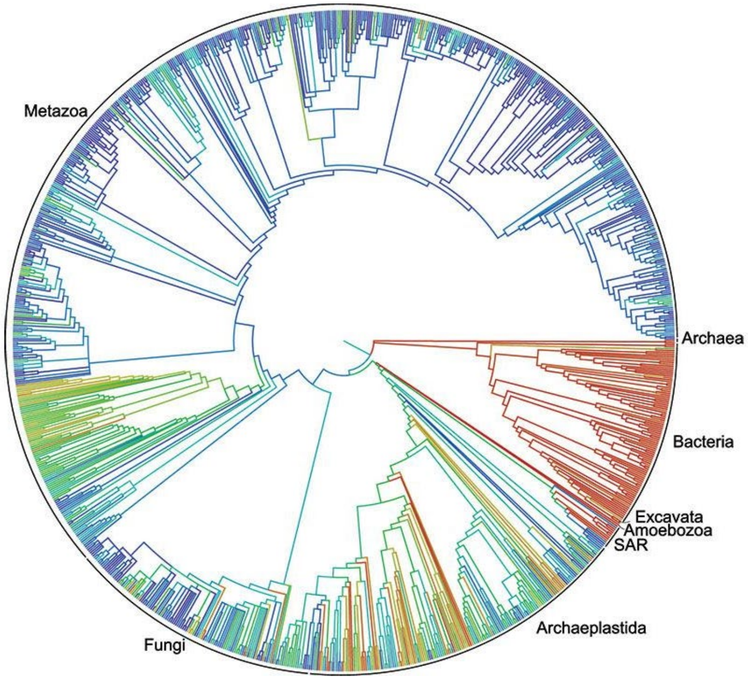


When to Stop?

No simple answer:

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

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

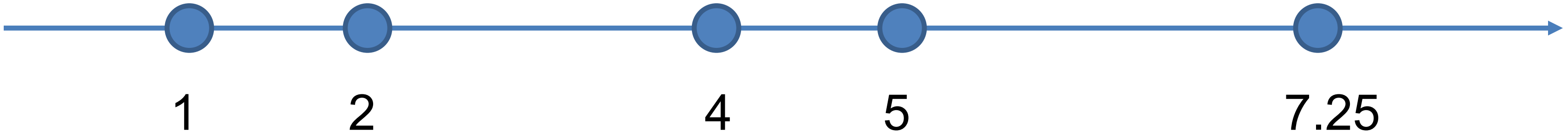


http://opentreeoflife.org/

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}



Break & Quiz

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

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

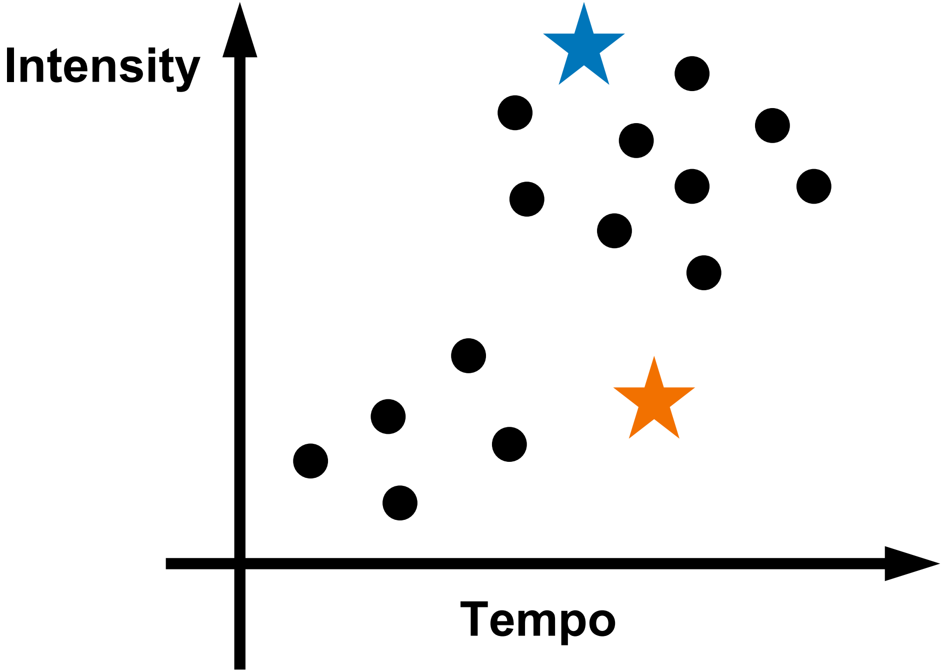
$$x_1, x_2, \dots, x_n$$

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

K-means clustering

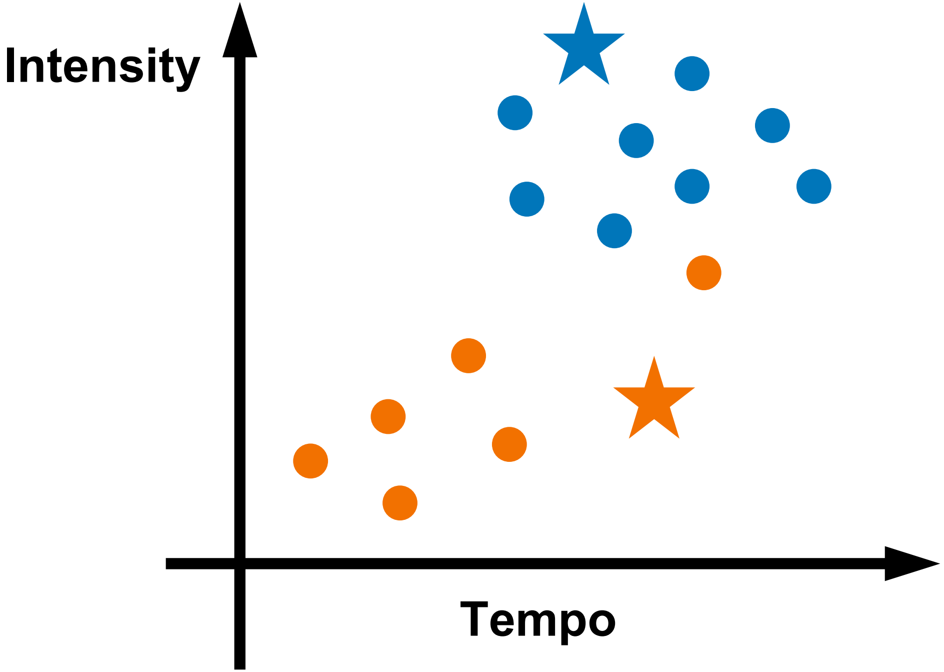
Step 1: **Randomly** picking 2 positions as initial cluster centers

(not necessarily a data point)



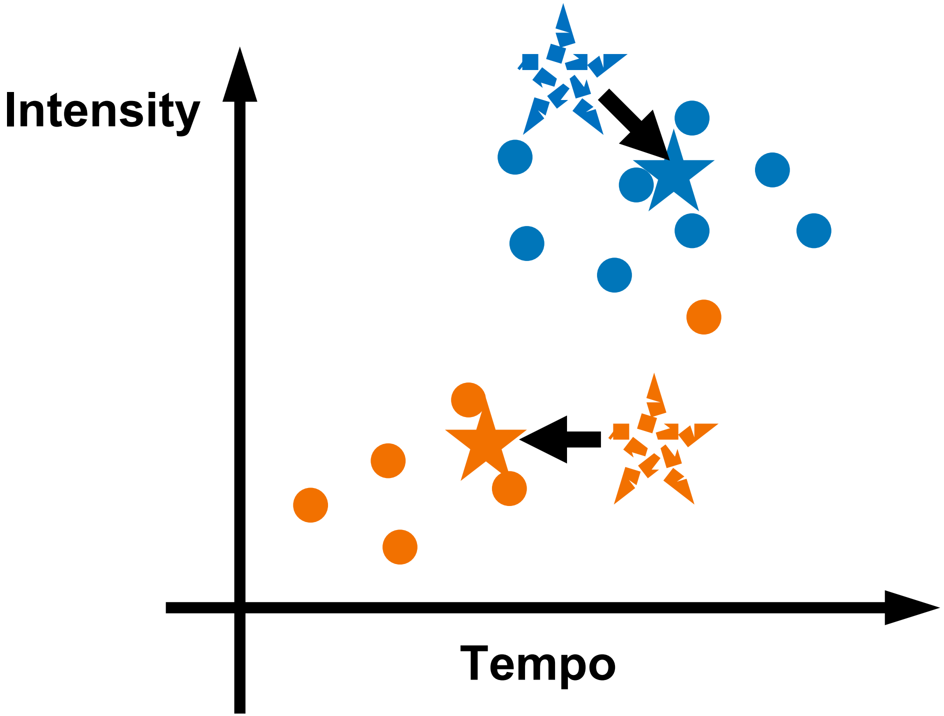
K-means clustering

Step 2: for each point x, determine its cluster: find the closest center in Euclidean space



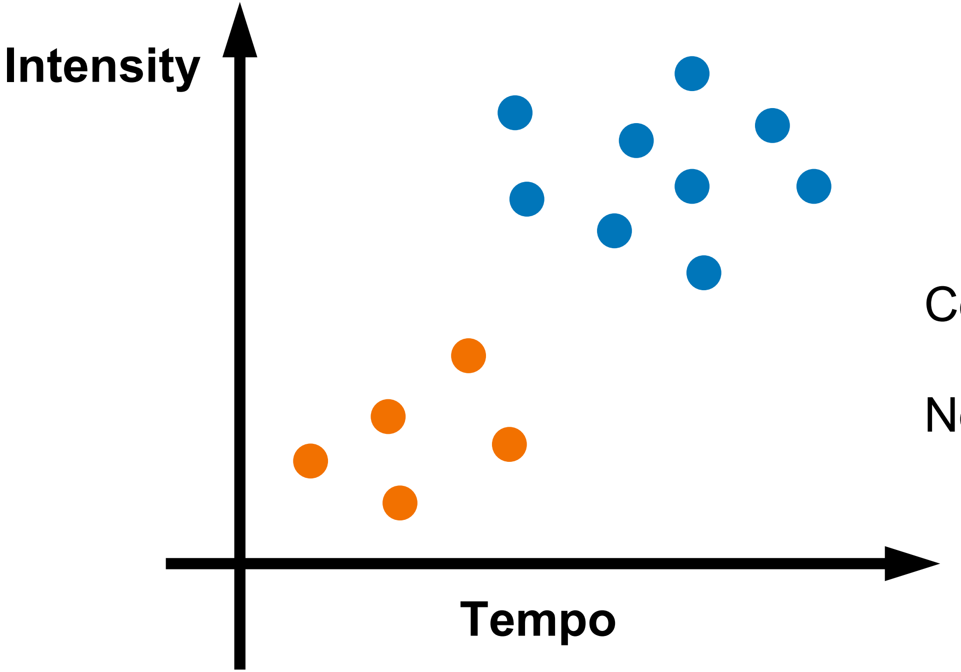
K-means clustering

Step 3: update all cluster centers as the centroids



K-means clustering

Repeat step 2 & 3 until convergence

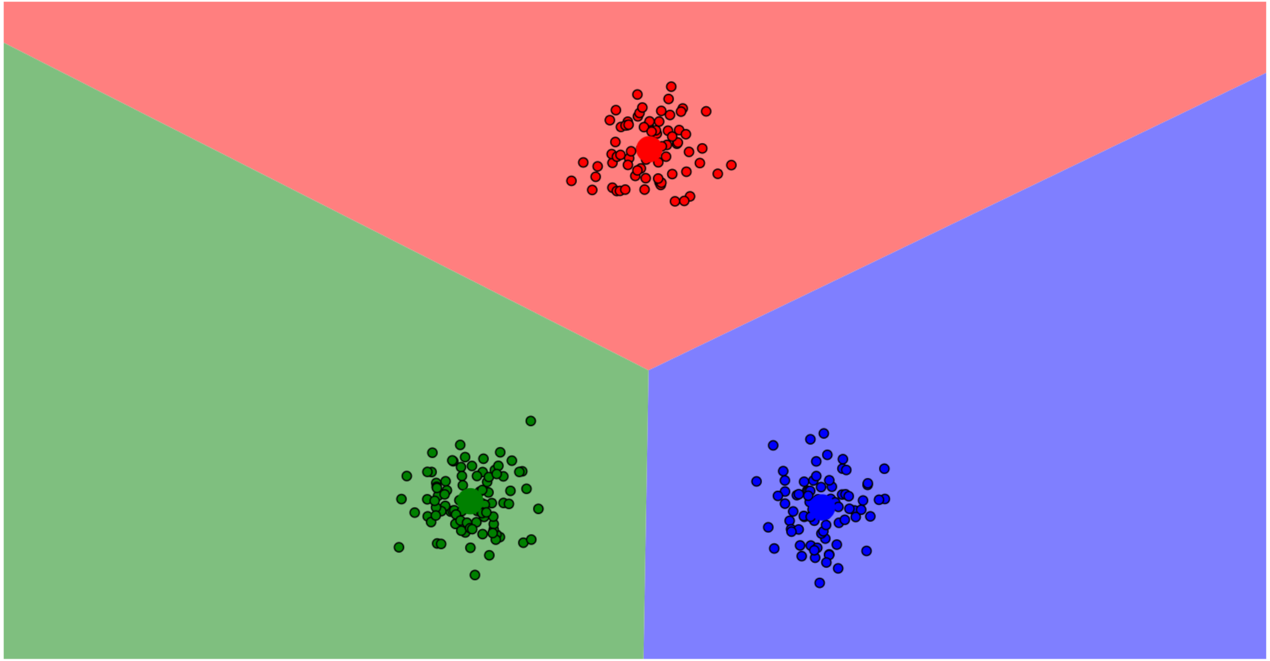


Converged solution!

No labels required!

K-means clustering: A demo

https://www.naftaliharris.com/blog/visualizing-k-means-clustering/



K-means algorithm

- Input: $x_1, x_2, \ldots, x_n, k$
- Step 1: select k cluster centers $c_1, c_2, \ldots, c_k$
- 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

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.

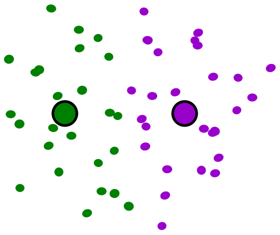
These steps **always reduce or keep the same** the objective function (sum of squared distance), ensuring termination.

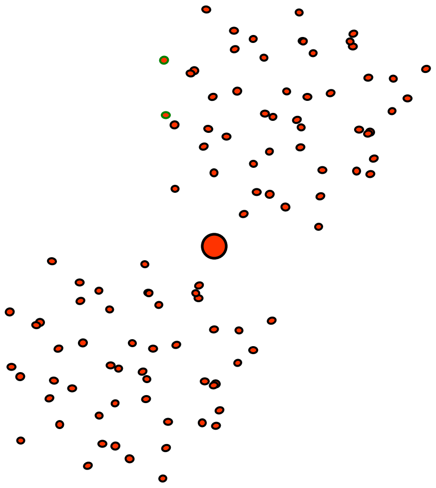
Questions on k-means

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

Questions on k-means

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





Questions on k-means

How to pick starting cluster centers?

- Randomly
- Kmeans++ (improving initialization)

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.

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 2.2: 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

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

Thanks!