Applied Machine Learning

Unsupervised Learning

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Supervised v.s. Unsupervised Learning

1. Supervised learning: learning from examples (**labeled** data)
   - regression, classification $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^{N}$
   - e.g. predict if patient has cancer based on different tests/measurements, learn from previous diagnosis cases (previous cancer/no cancer cases)
2. Unsupervised learning: inferring from patterns (**unlabeled** data)
   - clustering $\mathcal{D} = \{x^{(n)}\}_{n=1}^{N}$
   - e.g. find different types of patients based on different tests/measurements

In many practical cases we do not have labels, and unsupervised techniques could be useful as a first option to understand our data or might be sufficient on their own based on the task

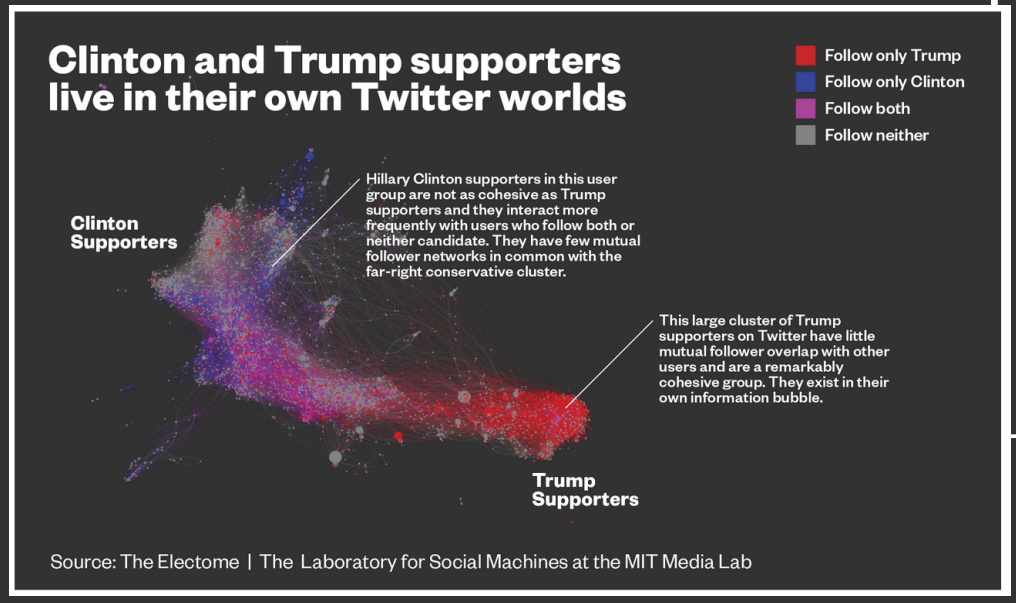
Learning objectives

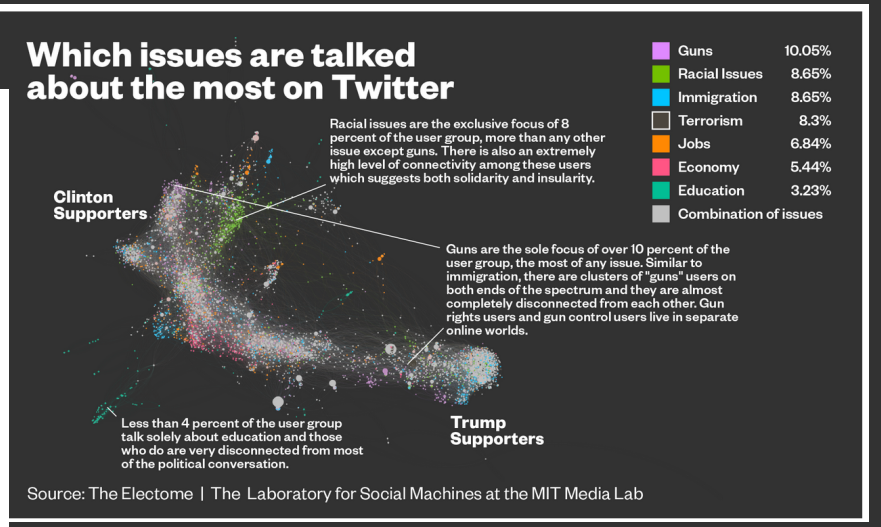
- what is clustering and when is it useful?
- what are the different types of clustering?
- some clustering algorithms:
  - k-means, k-medoid, DB-SCAN, hierarchical clustering

Clustering Examples

for many applications we want to classify the data without having any labels

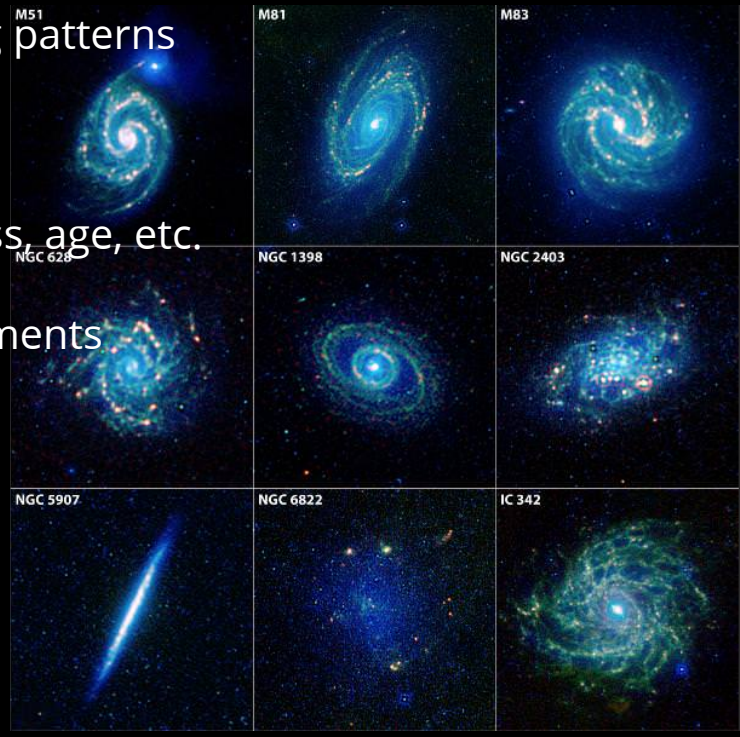
- categories of shoppers or items based on their shopping patterns
- communities in a social network





Clustering Examples

- categories of shoppers or items based on their shopping patterns
- communities in a social network
- categories of stars or galaxies based on light profile, mass, age, etc.
- categories of minerals based on spectroscopic measurements
- categories of webpages in meta-search engines
- categories of living organisms based on their genome
- ...



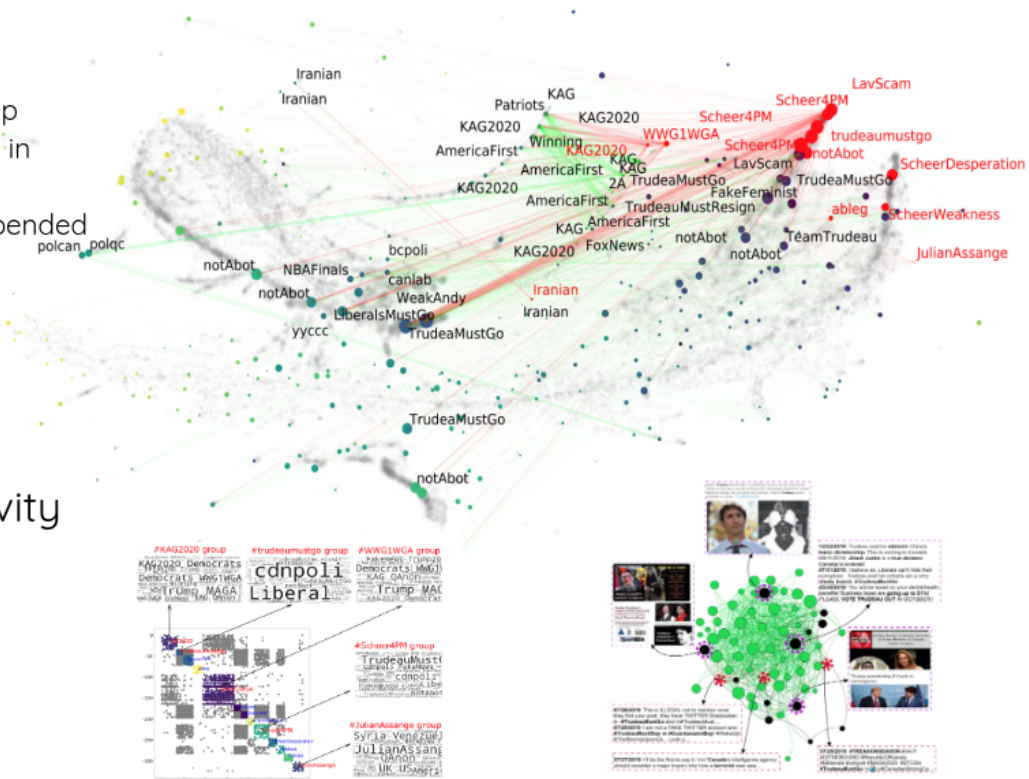
Clustering Examples in My Group

Spotting Coordinated Groups in Social Media

- 60 thousand user accounts with 3.4 million followership connections, and 1.3 million unique hashtags engaged in twitter around the 2019 Canadian Federal Elections
- users in coordinated groups 4x more likely to get suspended
- hashtags which characterize their creed linked to misinformation campaigns

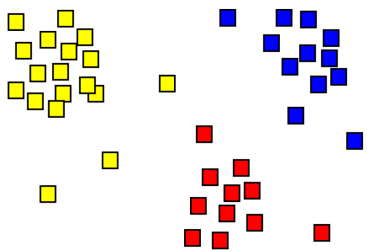
Understanding Troll behavior

Studying Polarization and Polarizing Activity



Wang J, Levy S, Wang R, Kulshrestha A, Rabbany R. SCG: Spotting Coordinated Groups in Social Media. arXiv preprint arXiv:1910.07130. 2019 Oct 16.

What is a cluster?



a **subset** of entities that are similar to each other and different from other entities

we can try and organize clustering methods based on

- form of input data
- types of cluster / task
- general methodology

Common Types of input

1. features $X \in \mathbb{R}^{N \times D}$

2. pairwise distances or similarities $D \in \mathbb{R}^{N \times N}$

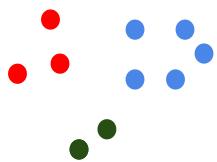
- we can often produce similarities from features
- infeasible for very large D

3. graphs with attributes on nodes $X \in \mathbb{R}^{N \times D}, A \in \mathbb{R}^{N \times N}$

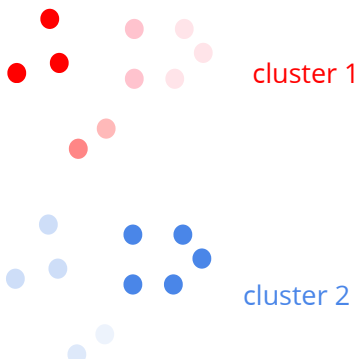
- node attribute is similar to feature in the first family
- edge attribute can represent similarity or distance

Types of cluster / task

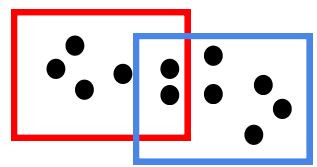
partitioning or hard clusters



soft fuzzy membership



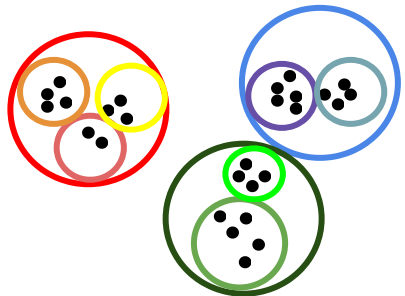
overlapping



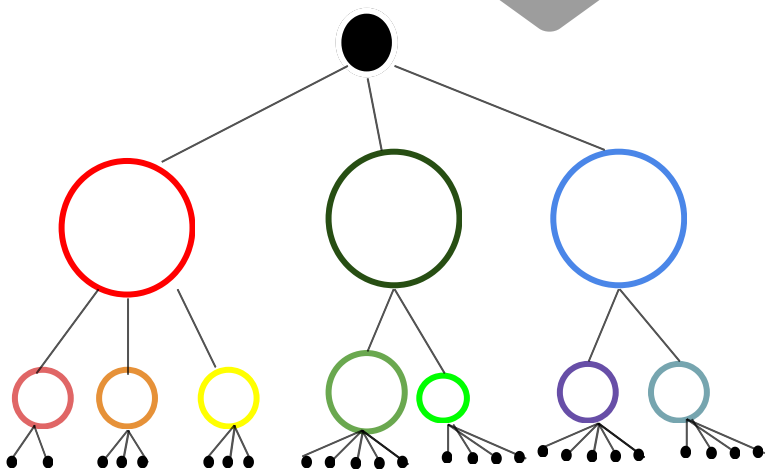
Types of cluster / task

other categories!

hierarchical clustering with
hard, soft, or overlapping membership

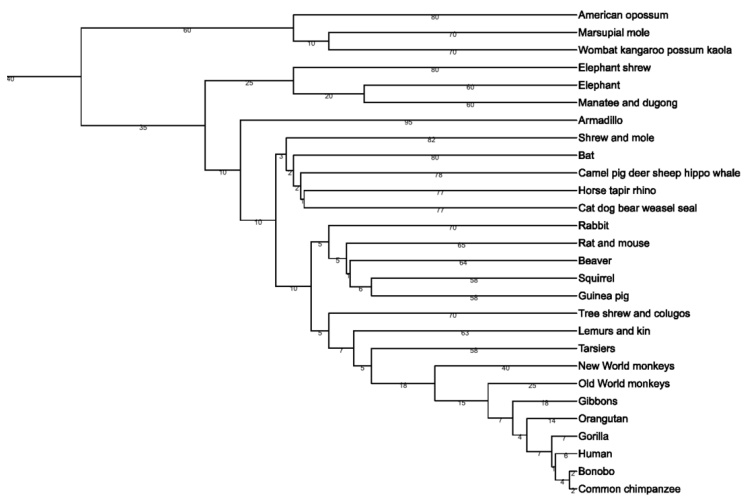


it is customary to use a **dendrogram** to represent hierarchical clustering



example

tree of life (clustering of genotypes)

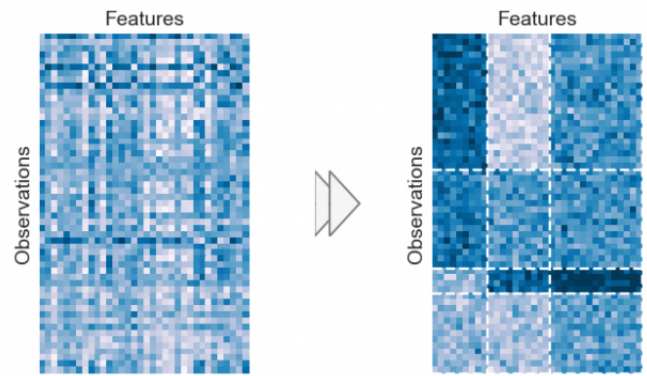


Types of cluster / task

other categories!

co-clustering or biclustering:

simultaneous clustering of instances and features



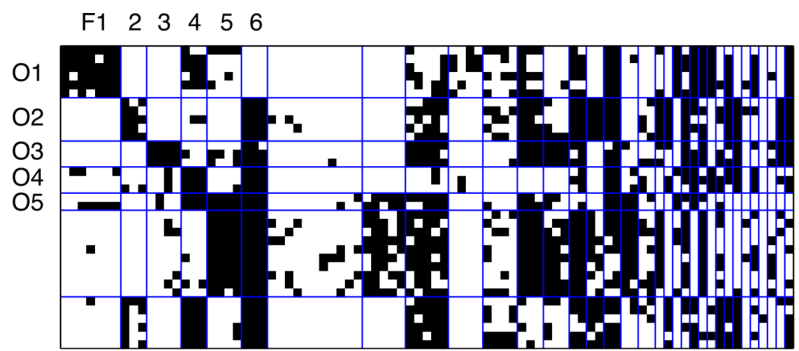
we can re-order the rows of X such that points in the same cluster appear next to each other. Same for the features.

examples

- co-clustering of user-items in online stores
- conditions and gene expressions ...
- below: co-clustering if mammals and their features

O1 killer whale, blue whale, humpback, seal, walrus, dolphin
O2 antelope, horse, giraffe, zebra, deer
O3 monkey, gorilla, chimp
O4 hippo, elephant, rhino
O5 grizzly bear, polar bear

F1 flippers, strain teeth, swims, arctic, coastal, ocean, water
F2 hooves, long neck, horns
F3 hands, bipedal, jungle, tree
F4 bulbous body shape, slow, inactive
F5 meat teeth, eats meat, hunter, fierce
F6 walks, quadrapedal, ground



Centroid methods

identify the centers, prototypes or exemplars of clusters

early use of clustering in psychology

each cluster is
represented by its center

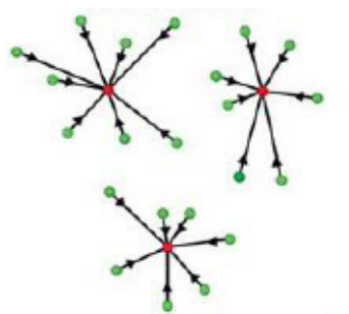
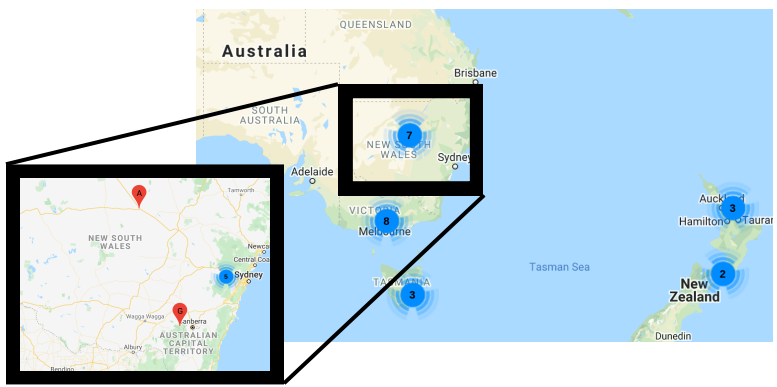


image: Frey & Dudek'00

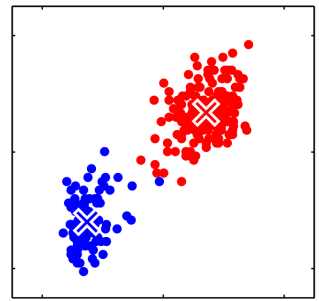
example

cluster centers are shown on the map
a hierarchical clustering with level of hierarchy depending on the zoom level



K-means is an example of a centroid method

K-means clustering: objective



idea partition the data into K-clusters to minimize the sum of distance to the cluster mean/center

equivalent to minimizing the within cluster distances

K is a hyperparameter

cost function

number of points *number of clusters*

$$J(\{r_{n,k}\}, \{\mu_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{n,k} ||x^{(n)} - \mu_k||_2^2$$

cluster center (mean) $\mu_k = \frac{\sum_n x^{(n)} r_{n,k}}{\sum_n r_{n,k}}$

cluster membership $r_{n,k} = \begin{cases} 1 & \text{point n belongs to cluster k} \\ 0 & \text{otherwise} \end{cases}$

we need to find **cluster memberships** and **cluster centers**

how to minimize the cost?

K-means clustering: algorithm

idea: iteratively update cluster memberships and cluster centers

start with some cluster centers $\{\mu_k\}$

repeat until convergence:

assign each point to the closest center: $r_{n,k} \leftarrow \begin{cases} 1 & k = \arg\min_c ||x^{(n)} - \mu_c^t||_2^2 \\ 0 & \text{otherwise} \end{cases}$

re-calculate the center of the cluster: $\mu_k \leftarrow \frac{\sum_n x^{(n)} r_{n,k}}{\sum_n r_{n,k}}$

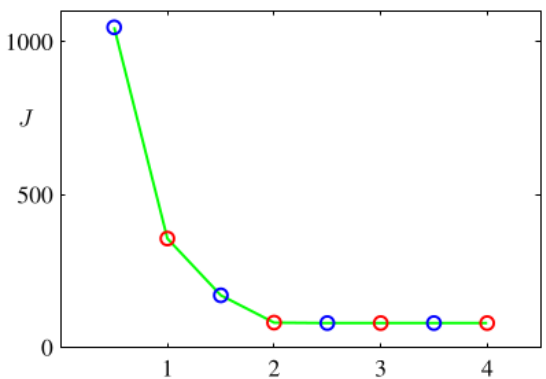
since each iteration can only reduce the cost, the algorithm has to stop

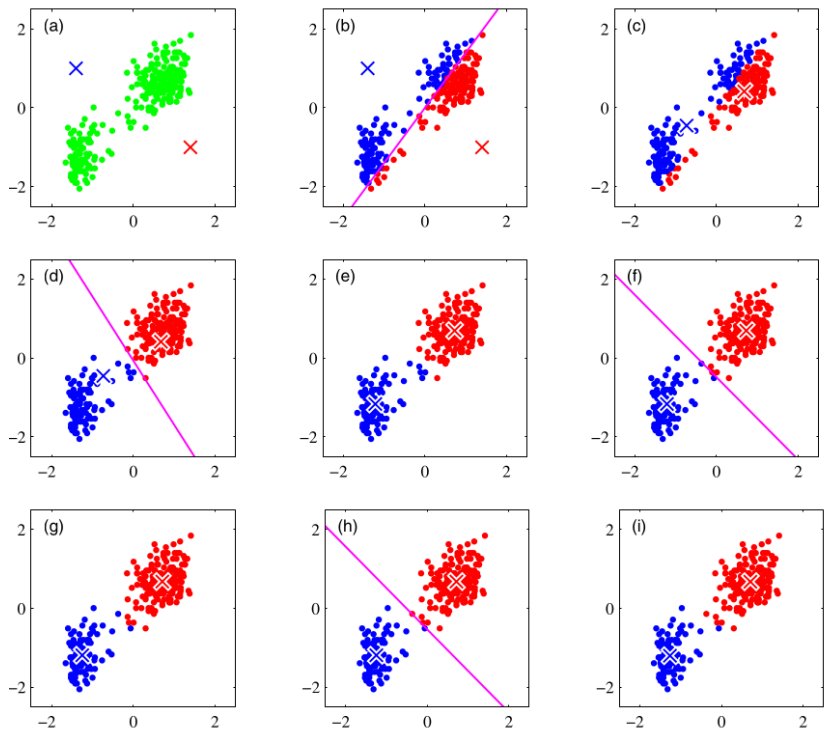
K-means clustering: algorithm

example iterations of k-means (K=2) for 2D data.

Two steps in each iteration are shown.

the cost decreases at each step





K-means clustering: derivation

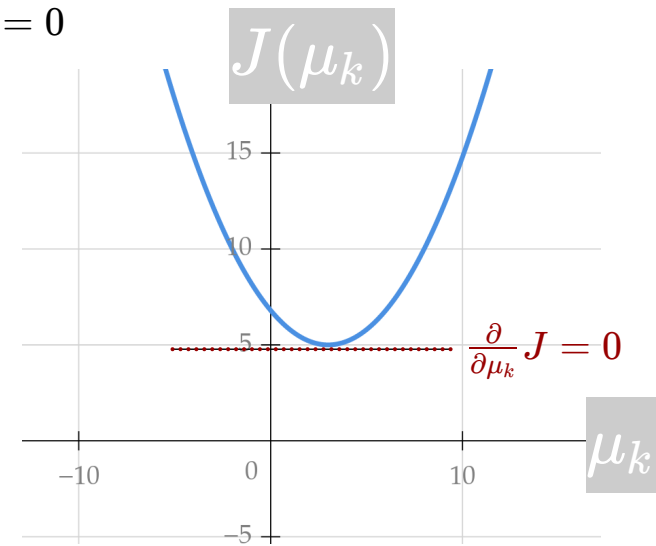
why this procedure minimizes the cost? $J(\{r_{n,k}\},\{\mu_k\}) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{n,k}||x^{(n)} - \mu_k||_2^2$

1. fix memberships $\{r_{n,k}\}$ and optimize centers $\{\mu_k\}$

set the derivative wrt μ_k to zero: $\frac{\partial}{\partial \mu_k} J = \frac{\partial}{\partial \mu_k} \sum_n r_{n,k}||x^{(n)} - \mu_k||_2^2 = 0$

$2\sum_n r_{n,k}(x^{(n)} - \mu_k) = 0$

$\mu_k = \frac{\sum_n x^{(n)} r_{n,k}}{\sum_n r_{n,k}}$ ✓



2. fix centers $\{\mu_k\}$ and optimize memberships $\{r_{n,k}\}$

finding the "closest" center minimizes the cost

$$r_{n,k} \leftarrow \begin{cases} 1 & k = \arg\min_c ||x^{(n)} - \mu_c||_2^2 \\ 0 & \text{otherwise} \end{cases}$$ ✓

3. repeat 1 & 2 until convergence

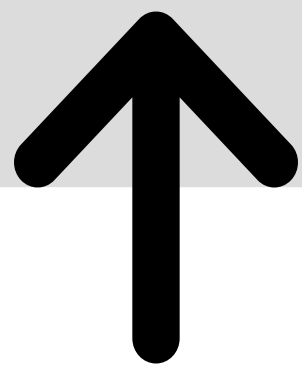
K-means clustering: complexity

start with some cluster centers $\{\mu_k\}$

repeat until convergence:

assign each point to the closest center: $r_{n,k} \leftarrow \begin{cases} 1 & k = \arg\min_c ||x^{(n)} - \mu_c||_2^2 \\ 0 & \text{otherwise} \end{cases}$

re-calculate the center of the cluster: $\mu_k \leftarrow \frac{\sum_n x^{(n)} r_{n,k}}{\sum_n r_{n,k}}$



calculating the mean of all cluster $\mathcal{O}(ND)$

calculating distance of a node to center $\mathcal{O}(D)$, number of features

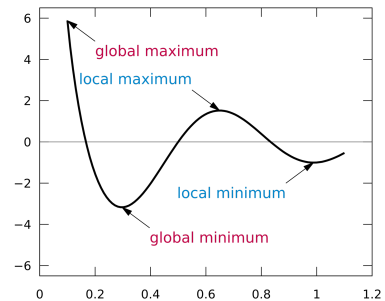
we do this for each point (n) and each center (k)

total cost is $\mathcal{O}(NKD)$

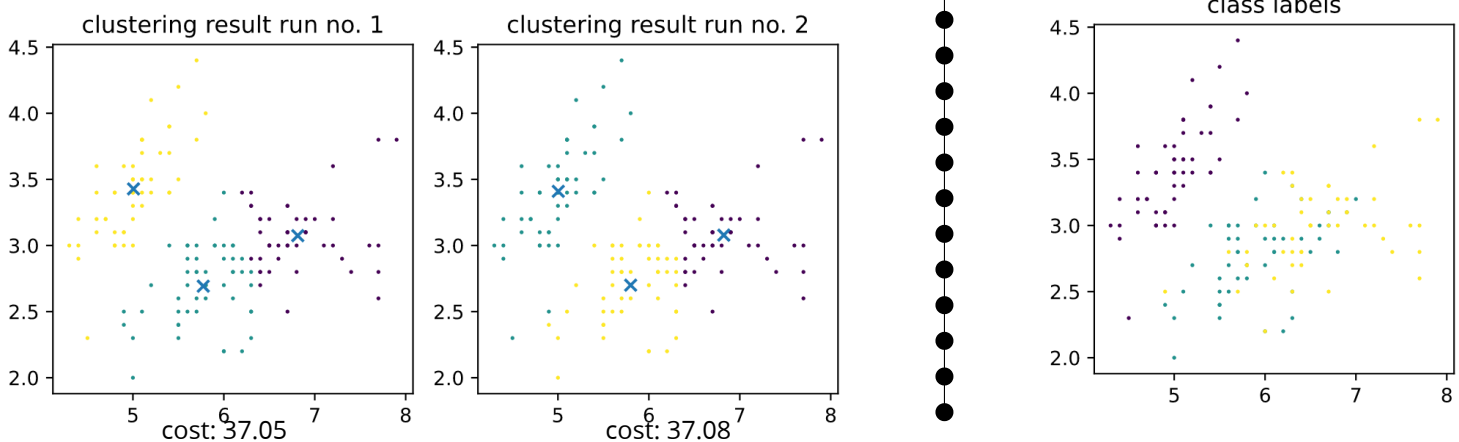
K-means clustering: performance

K-means' alternating minimization finds a **local** minimum

different **initialization** of cluster centers gives different clustering



example: Iris flowers dataset (also interesting to compare to true class labels)



even if the clustering is the same we could swap cluster indices (colors)

optional

K-means clustering: initialization

K-means' alternative minimization finds a **local** minimum

different **initialization** gives different clustering:

- run many times and pick the clustering with the lowest cost
- use good heuristics for initialization:

K-means++ initialization

- pick a random data-point to be the first center
- calculate the distance of each point to the nearest center d_n
- pick a new point as a new center with prob $p(n) = \frac{d_n^2}{\sum_i d_i^2}$

often faster convergence to better solutions

the clustering is within $\mathcal{O}(\log(K))$ x optimal solution

Application: vector quantization

given a dataset $\mathcal{D} = \{x^{(1)}, \ldots, x^{(N)}\}$ of vectors $x^{(n)} \in \mathbb{R}^D$

storage $\mathcal{O}(NDC)$ *C is the number of bits for a scalar (e.g., 32bits)*

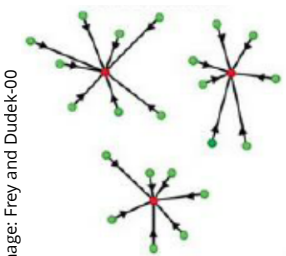
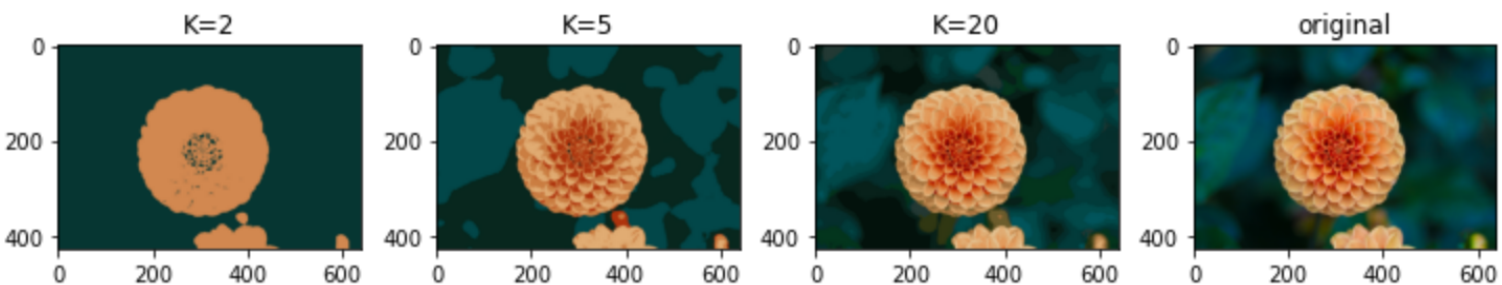


image: Frey and Dudek-00

compress the data using k-means:

- replacing each data-point with its cluster center
- store only the cluster centers and memberships $\mathcal{O}(KDC + N\log(K))$

apply this to compress images (denote each pixel by $x^{(n)} \in \mathbb{R}^3$)



cluster the colors

K-medoids

K-means objective minimizes squared Euclidean distance

the minimizer for a set of points is given by their mean

$D(x, x') = \sum_d |x_i - x'_i|$

if we use Manhattan distance the minimizer is the median (K-medians)

for general distance functions the minimizer doesn't have a *closed form* *(computationally expensive)*

solution pick the cluster center from the points themselves (**medoids**)

K-medoid objective

$$J(\{r_{n,k}\}, \{\mu_k\}) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{n,k} dist(x^{(n)}, \mu_k) \quad \text{and} \quad \mu_k \in \{x^{(1)}, \ldots, x^{(N)}\}$$

algorithm

- assign each point to the "closest" center
- set the point with the min. overall distance to other points as the center of the cluster

K-medoids

solution pick the cluster center from the points themselves (**medeoids**)

K-medoid objective

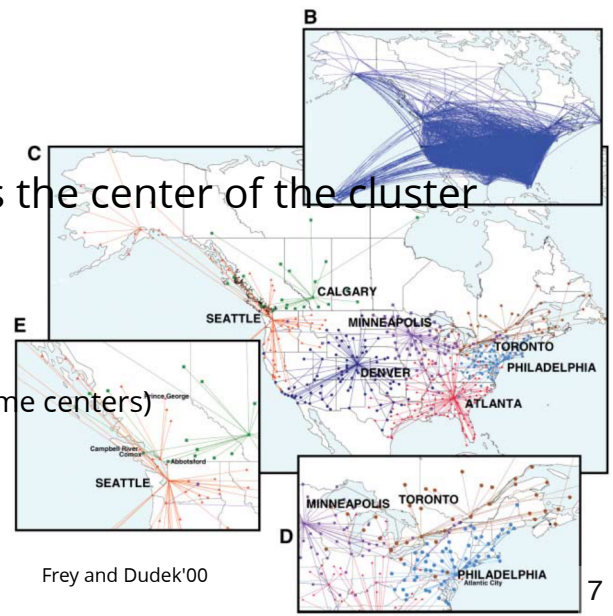
$$J(\{r_{n,k}\},\{\mu_k\}) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{n,k}\, dist(x^{(n)},\mu_k) \quad \text{and} \quad \mu_k \in \{x^{(1)},\ldots,x^{(N)}\}$$

algorithm

- assign each point to the "closest" center
- set the point with the min. overall distance to other points as the center of the cluster

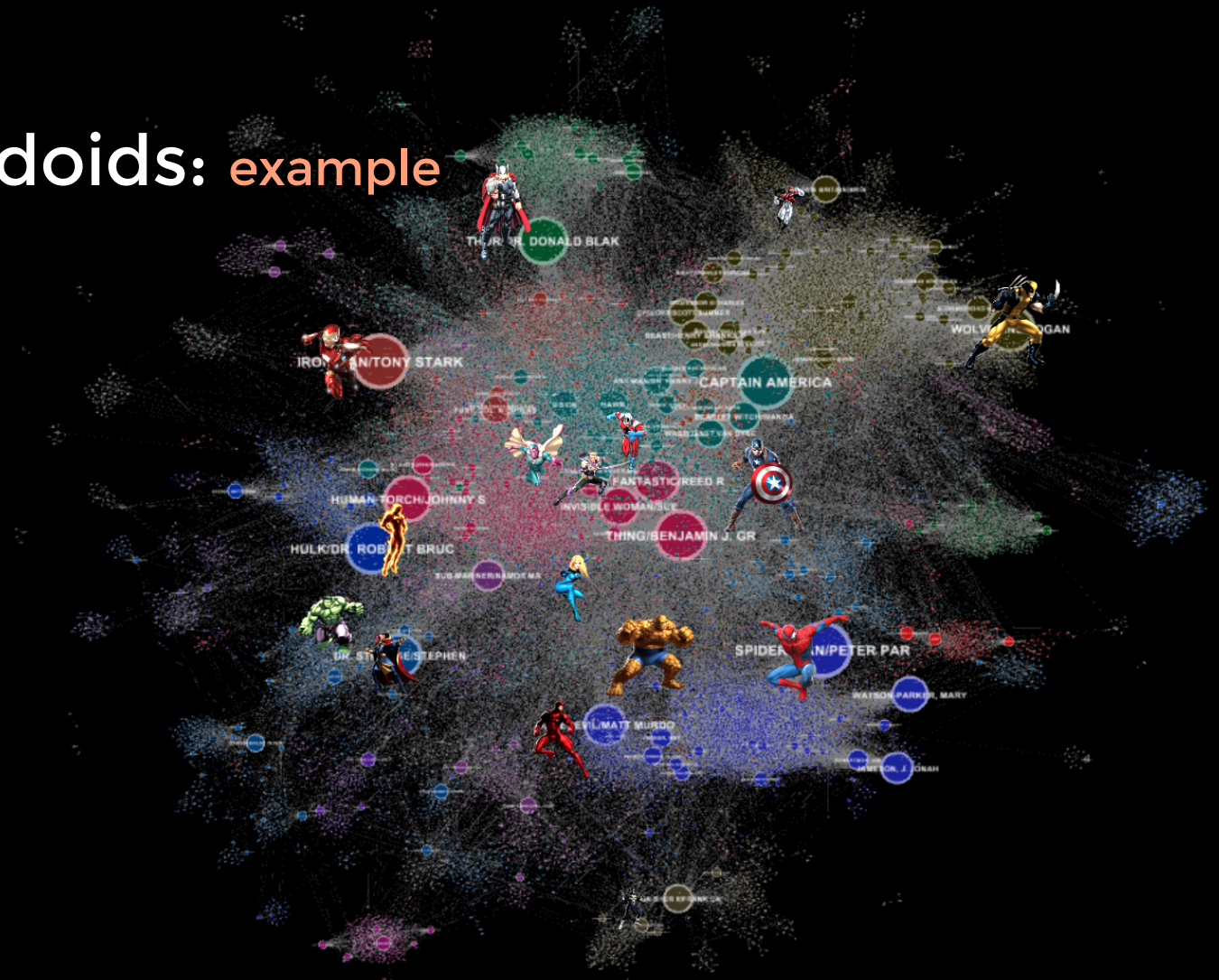
example finding key air-travel hubs (as medeoids)

K-medoid also makes sense when the input is **graph** (nodes become centers)



Frey and Dudek'00

K-medoids: example

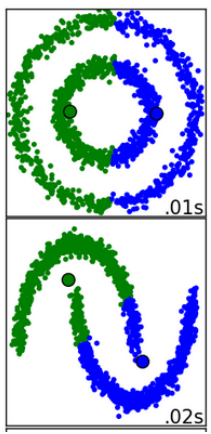


Density based methods

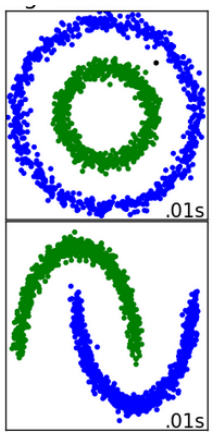
dense regions define clusters

a notable method is **d**ensity-**b**ased **s**patial **c**lustering of **a**pplications with **n**oise (**DB-SCAN**)

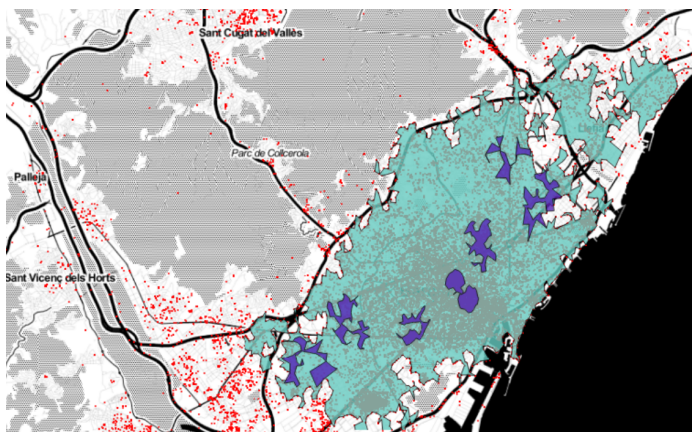
K-means



DB-SCAN



geospatial clustering



astronomical data

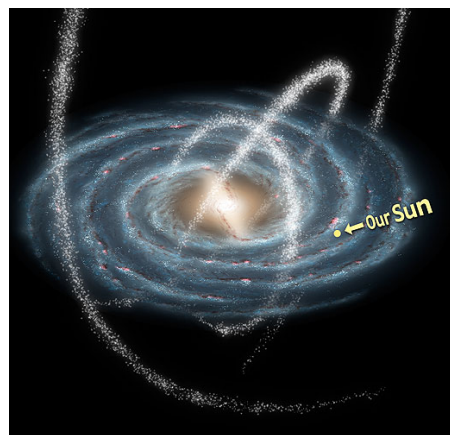


image credit: wiki, https://doublebyteblog.wordpress.com

DB-SCAN

points that have more than C neighbors in ϵ-neighborhood are called **core** points

if we connect nearby core points we get a graph

connected components of the graph give us **clusters**

all the other points are either:

- ϵ-close to a core, so belong to that cluster
- labeled as **noise**

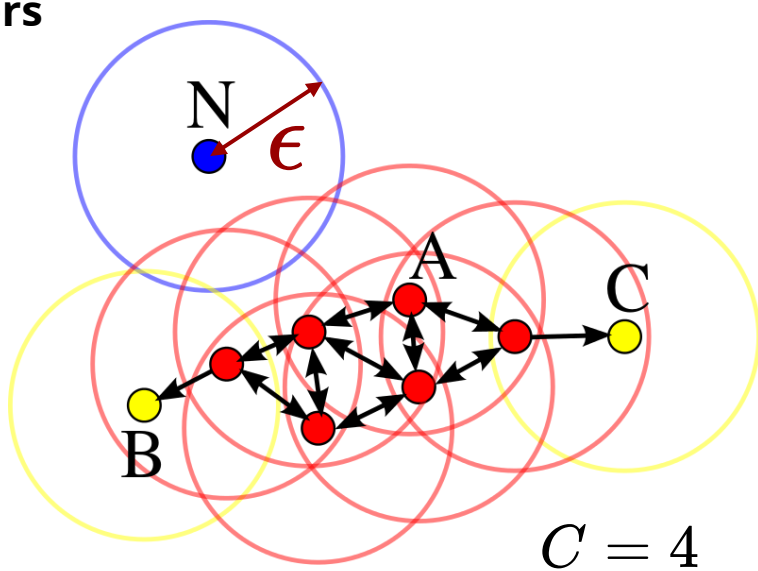


image credit: wiki

Hierarchical clustering heuristics

bottom-up hierarchical clustering (**agglomerative clustering)**

- start from each item as its own cluster
- merge most similar clusters

top-down hierarchical clustering (**divisive clustering**)

- start from having one big cluster
- at each iteration pick the "widest" cluster and split it *(e.g. using k-means)*

these methods often do not optimize a specific objective function (hence heuristics)
they are often too expensive for very large datasets

Agglomerative clustering

- start from each item as its own cluster
- merge most similar clusters

initialize clusters $\mathcal{C}_n \leftarrow \{n\}, \quad n \in \{1, \dots, N\}$

initialize set of clusters available for merging $\mathcal{A} \leftarrow \{1, \dots, N\}$

for $t = 1, \dots$

  pick two clusters that a most similar $i, j \leftarrow \arg\min_{c, c' \in \mathcal{A}} \text{distance}(c, c')$

  merge them to get a new cluster $\mathcal{C}_{t+N} \leftarrow \mathcal{C}_i \cup \mathcal{C}_j$

  if $\mathcal{C}_{t+N}$ contains all nodes, we are done!

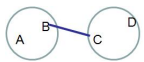
  update clusters available for merging $\mathcal{A} \leftarrow \mathcal{A} \cup \{t+N\} \backslash \{i, j\}$

  calculate dissimilarities for the new cluster $\text{distance}(t+N, n) \quad \forall n \in \mathcal{A}$

- how to define dissimilarity or distance of two clusters?

Agglomorative clustering

how to define dissimilarity of two clusters?

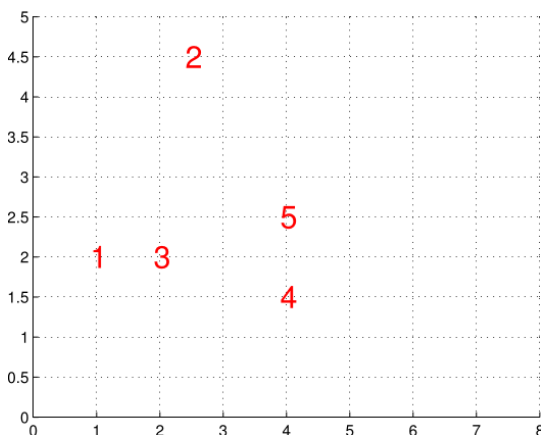


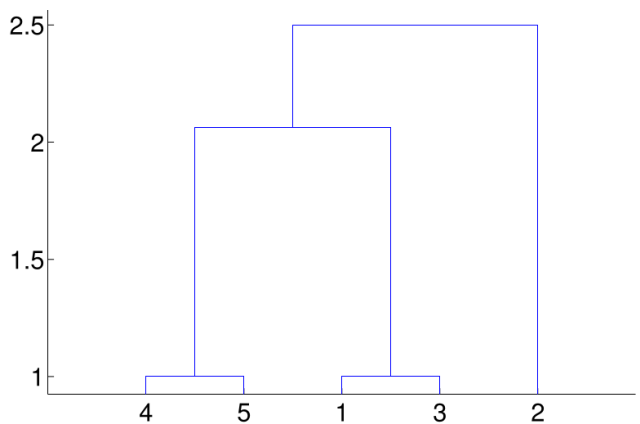
single linkage: distance between closest members

$$\text{distance}(c, c') = \min_{i \in \mathcal{C}_c, j \in \mathcal{C}_{c'}} \text{distance}(i, j)$$

example

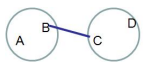
note that we can use the distance between clusters for the height of tree nodes in the dendrogram





Agglomorative clustering

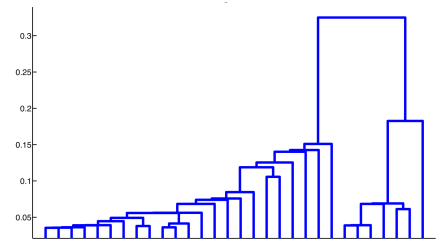
how to define dissimilarity of two clusters? some common choices:

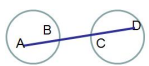


single linkage: distance between closest members

clusters can have members that are very far apart

$$\text{distance}(c, c') = \min_{i \in \mathcal{C}_c, j \in \mathcal{C}_{c'}} \text{distance}(i, j)$$

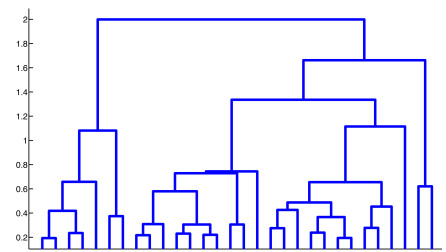


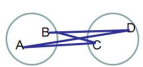


complete linkage: distance between furthest members

clusters that are more compact (all members should be close together)

$$\text{distance}(c, c') = \max_{i \in \mathcal{C}_c, j \in \mathcal{C}_{c'}} \text{distance}(i, j)$$

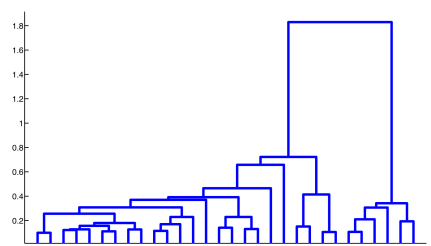




average linkage: average pairwise distance

a compromise between the above

$$\text{distance}(c, c') = \frac{1}{|\mathcal{C}_c||\mathcal{C}_{c'}|} \sum_{i \in \mathcal{C}_c, j \in \mathcal{C}_{c'}} \text{distance}(i, j)$$



How to Evaluate?

- Validate the algorithm on a set of benchmarks with known ground-truth
  - using a clustering agreement measure, e.g. **ARI**, NMI
  - useful in algorithm design

can be averaged over different datasets

$$A(C_1, G) > A(C_2, G)$$

- Measure a relative criterion to compare goodness of different algorithms or hyperparameters (e.g. k in k-means) on your dataset

meaningful only on the same dataset

  - using a clustering quality index, e.g. **silhouette** score
  - useful in practice
  - measures (in different ways) within cluster to between cluster ratio

$$I(C_1) > I(C_2)$$

Summary

clustering can help us explore and understand our data
input to clustering methods can be features, similarities or graphs
clusters can be flat, hierarchical, overlapping, fuzzy...

we saw several clustering methods:

- K-means and K-medoid define clusters using **centers** and distance to these centers
  - optimization objective
  - algorithm to perform the optimization
- DB-SCAN as an example of **density-based** methods
- some heuristic **hierarchical** clustering methods

some notable methods we did not discuss

- popular community-mining methods such as modularity optimizing methods
- spectral clustering
- probabilistic generative models of clusters