NUS | Computing

National University of Singapore

CS5228: Knowledge Discovery and Data Mining

Lecture 2 — Clustering I

Course Logistics — Update

- Project — Team Formation
  - Default team size: 4 (exception maybe later if needed)
  - Final allocation at the teaching team's discretion
  - Canvas self-signup group
- Project — Deadline
  - Dataset release: Week ~3
  - Progress Report: Week ~7
  - Final Report: Week 11 (Thu, Oct 30)

Earlier submission are always welcome! :)

Quick Recap

- Data Mining — from data to knowledge

Data Selection → Data Pre-processing → Data Trans-formation → Data Mining Methods → Data Post-processing

- Nature of data
  - Types of attributes: categorical (nominal / ordinal) vs. numerical (interval / ratio)
  - Types of data and data representations
    (e.g., data matrix, transactions, graph, ordered data)
  - Data quality

Quick Recap — Data Preparation

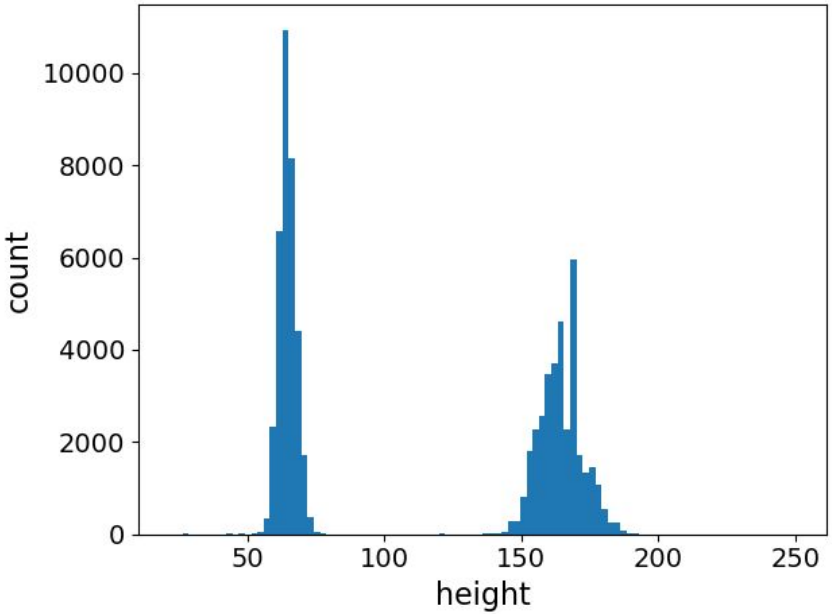
- Exploratory Data Analysis (EDA)
  - Assess data quality
  - Get to know your data
- Data Preprocessing
  - Improve data quality (*"Garbage in, garbage out!"*)
  - Generate valid input for data mining algorithms
  - Remove complexity from data to ease analysis

Example of noise: missing values

Age	Edu-cation	Marital Status	Annual Income	Credit Default
23	Masters	Single	75k	Yes
N/A	Bachelor	Married	N/A	No
26	Masters	Single	70k	Yes
41	PhD	Single	95k	Yes
18	Bachelor	Single	40k	No
55	Master	Married	N/A	No
30	Bachelor	Single	N/A	No
35	PhD	Married	60k	Yes
N/A	PhD	Married	65k	Yes

Quick Recap — Clarifications

- Suspicious EDA results $\not\Rightarrow$ errors in the data



Data may be absolutely correct

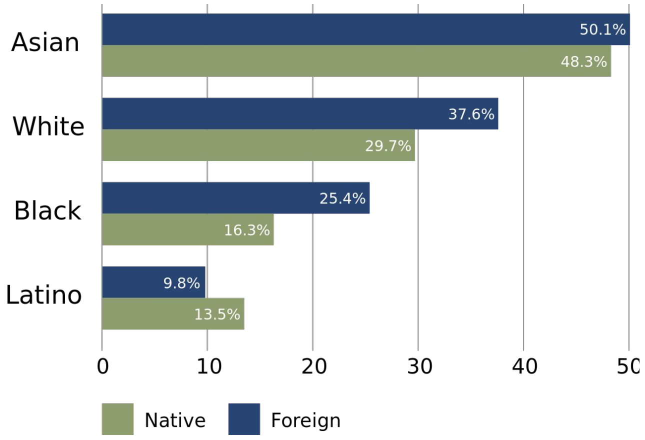
Example: infant care dataset (infants + parents)

Quick Recap — Clarifications

- Removing "questionable" attributes $\not\Rightarrow$ better results
  - e.g., removing zodiac sign from credit default prediction might lower accuracy

- Removing "questionable" attributes $\not\Rightarrow$ no biases (or perfect privacy)
  - e.g., removing ethnicity not foolproof if it correlates with other attributes

Age	Ethnicity	Edu-cation	Annual Income	Credit Approval
23	White	Masters	75k	Yes
35	Buddhist	Bachelor	50k	No
26	Asian	Masters	70k	Yes
41	Asian	PhD	95k	Yes
18	Black	Bachelor	40k	No
...	...	...	...	...

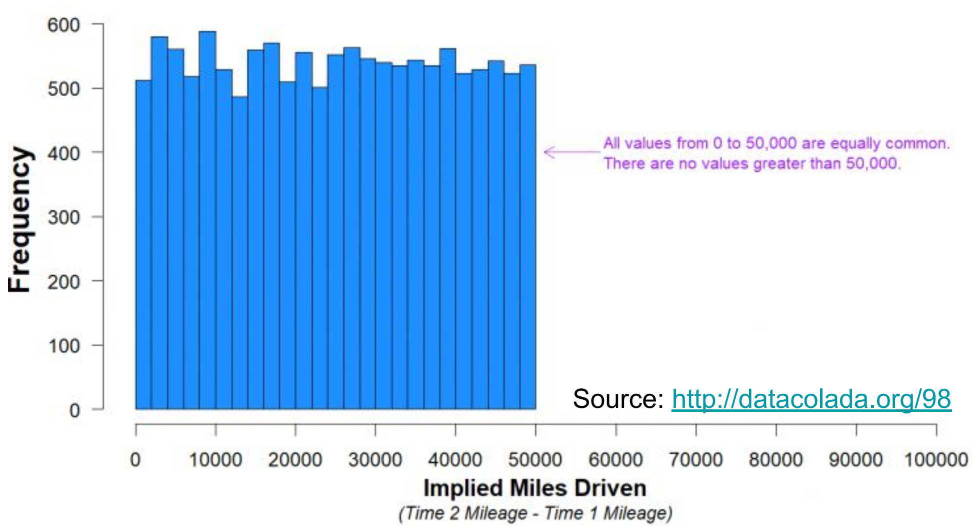


Source: https://en.wikipedia.org/wiki/Educational_attainment_in_the_United_States

Quick Recap — EDA: Additional Insights

- Manipulated / fudged data
  - Sometimes data just does not "look right"
  - Example: unexpected/unintuitive data distributions

Figure 1. Histogram of Miles Driven - Car #1 (N=13,488)



Source: http://datacolada.org/98

[Some background article]()

Outline

- **Clustering**
  - Overview
  - Applications
  - Concepts

L2

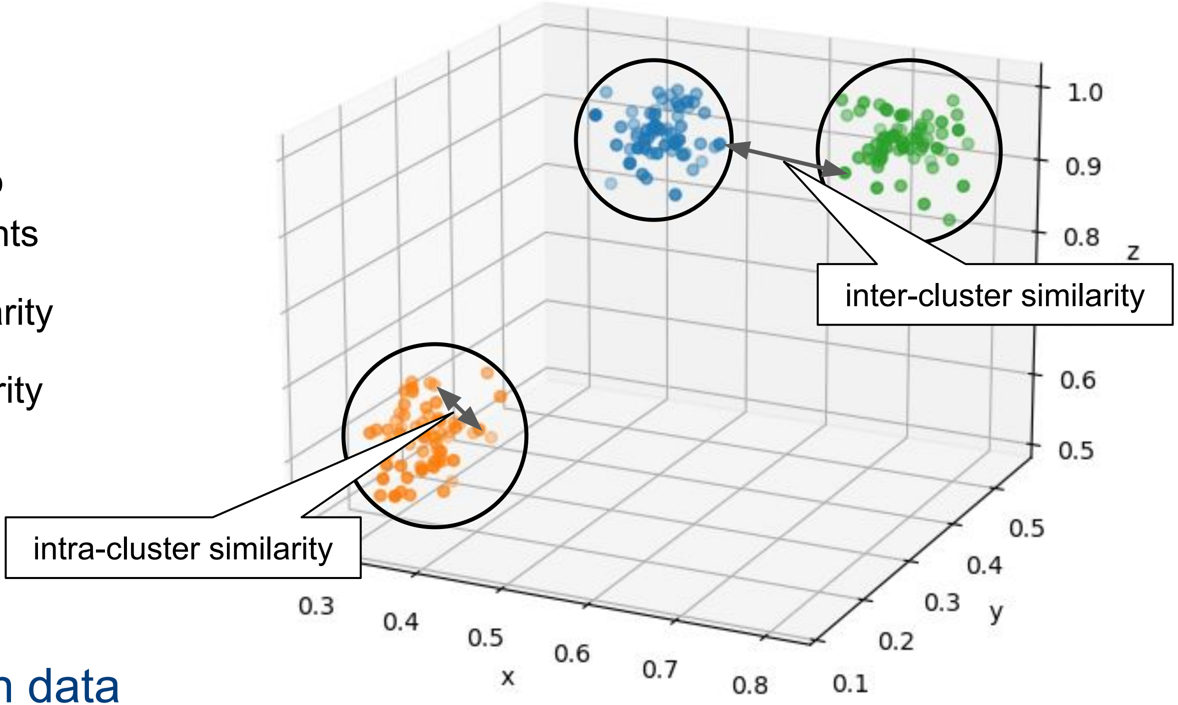
- Clustering algorithms
  - K-Means
  - DBSCAN
  - Hierarchical Clustering

L3

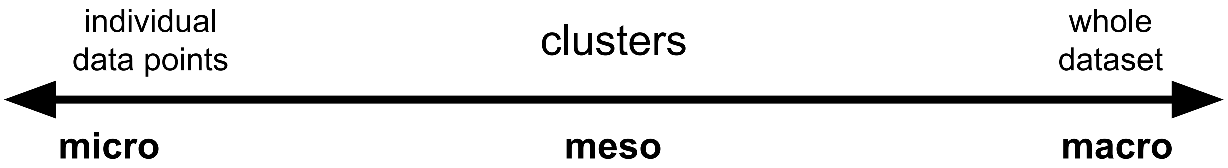
- Cluster Evaluation

What is Clustering?

- Goal of Clustering
  - Separate **unlabeled** data into groups of **similar** objects/points
  - Maximize **intra-cluster** similarity
  - Minimize **inter-cluster** similarity



- Meso-level perspective on data



Applications

- Market segmentation
  - Group customers based on behavior and/or preferences
  - Push tailored promotions to all customers in cluster

- Recommender systems
  - Group items (e.g., movies) based on their attributes (e.g., genre, length, budget)
  - Recommend movies from a cluster with movies a user liked

- Web Search Diversification
  - Group Web pages (e.g., news articles) based on content, source (type), etc.
  - Return search results from different clusters to ensure diversity

- …and many more applications

- EDA

Ingredients for Clustering

- Representation of objects, e.g.:
  - (Multidimensional) point coordinates *x*, *y*
  - Sets *A*, *B* (e.g., items in a transaction)
  - Vectors *u*, *v* (e.g., TF-IDF)

$$dist_{euclidean}(x, y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

- Similarity Measure, e.g.:
  - Euclidean Distance
  - Jaccard Similarity
  - Cosine Similarity

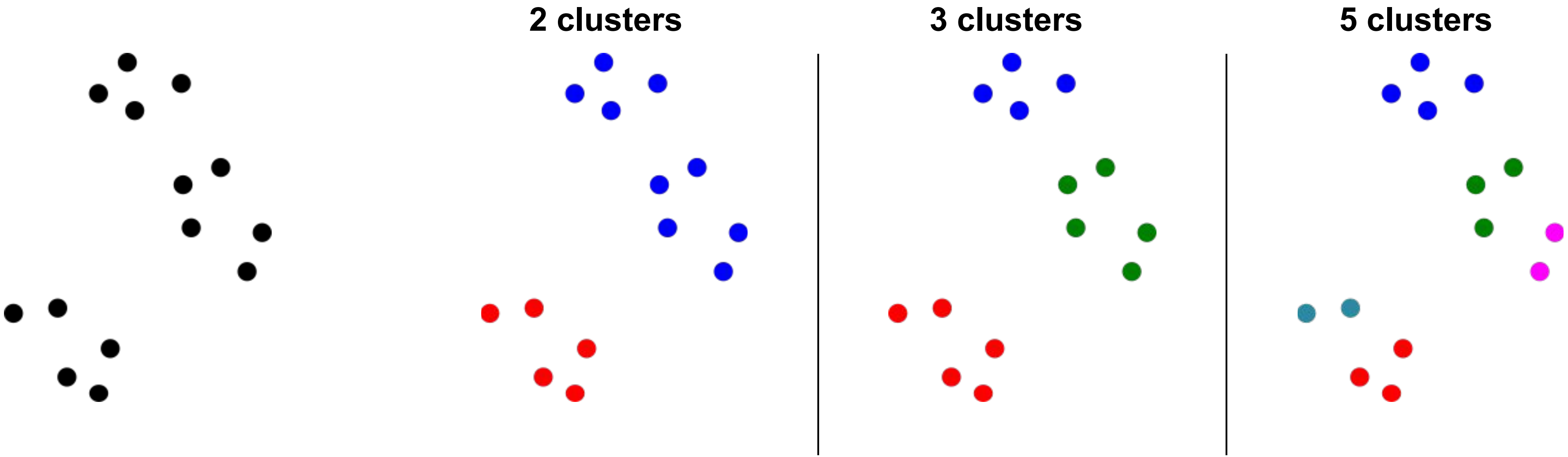
$$sim_{jaccard}(A, B) = \frac{|A \cap B|}{|A \cup B|}$$

$$sim_{cosine}(u, v) = \frac{u \cdot v}{\|u\|\|v\|}$$

- Clustering Algorithm
  - Process that determines if an object belongs to a cluster

What makes a clustering "good"?

How many clusters?



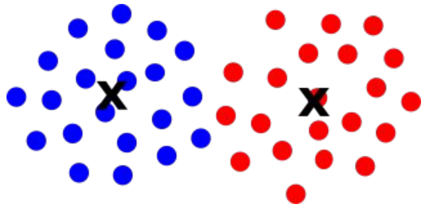
➜ Deciding on a good / meaningful / useful set of clusters not obvious

Types of Clusters

- Well-separated

  - Any object in a cluster is closer to every other object in the cluster than to any point outside the cluster

- Center-based

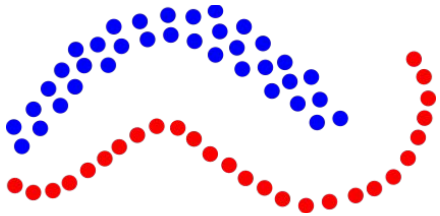


  - Any object in a cluster is closer to the "center" of a cluster than to the center of any other cluster
  - Example: mean of all data points (in Euclidean space)
  - Cluster center commonly called **centroid**

K-Means

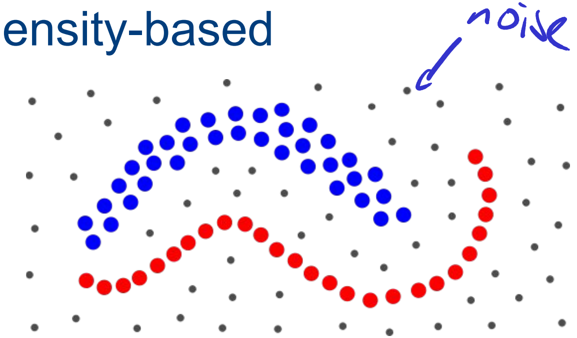
Types of Clusters

- Contiguity-based



  - 2 objects are in a cluster if they are more similar than a specified threshold
  - Each object is more similar to some object in that cluster than to any point in a different cluster

- Density-based



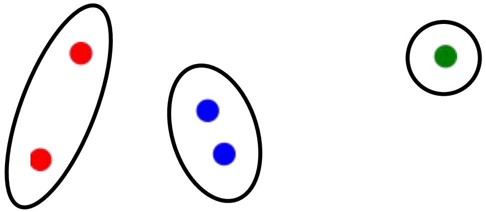
  - Cluster = dense(r) region of objects surrounded by region of low(er) density
  - Can typically address noise better than contiguity-based clusters

DBSCAN

Types of Clusterings (i.e., sets of clusters)

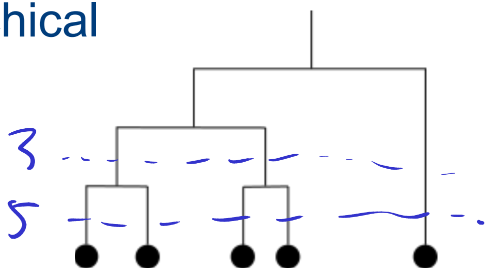
vs.

- Partitional



- Division of the set of data objects into non-overlapping subsets (i.e., clusters)
- Each object is in exactly 1 cluster (or in no cluster at all)

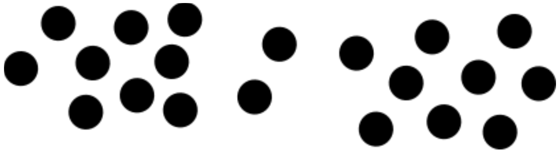
- Hierarchical



- Clusters can be nested
- A point can belong to different clusters depending on the hierarchy level

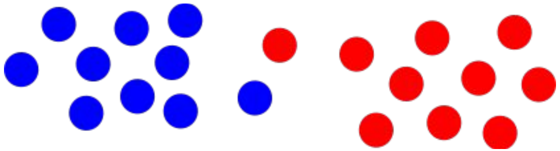
AGNES

Types of Clusterings (i.e., sets of clusters)



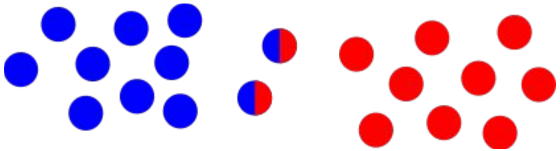
vs.

- Exclusive



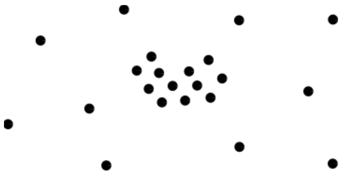
  - Each object belongs to 1 cluster

- Non-exclusive / overlapping



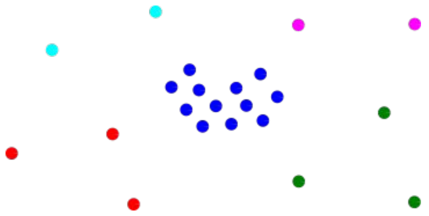
  - An object can belong to more than 1 cluster at a time
  - Fuzzy clustering: each object belongs to all clusters with a certain probability

Types of Clusterings (i.e., sets of clusters)



vs.

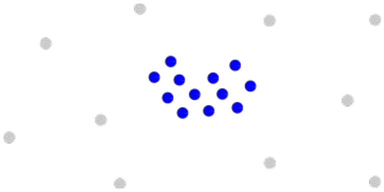
- Complete



  - Every object is assigned to (at least) 1 cluster

K-Means, AGNES

- Partial



  - An object might not belong to a cluster
  - Examples: noise, outliers

DBSCAN

Quick Quiz

In what situation can I **NOT** apply clustering on a dataset?

A All attributes of my dataset are nominal attributes

B My dataset is 1-dimensional, i.e., there is only one attribute

C The values of the attributes are not normally distributed

D ✓ There is no similarity or distance between the data points defined

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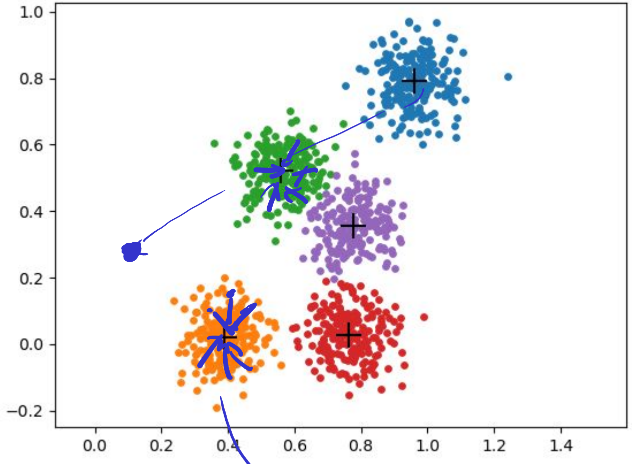
  - Overview
  - Applications
  - Concepts
- **Clustering Algorithms**
  - **K-Means**
  - DBSCAN
  - Hierarchical Clustering
- Cluster Evaluation

K-Means

- Basic characteristics
  - Clusters: centroid-based
  - Clustering: partitional, exclusive, complete



- Inputs (for d-dimensional Euclidean space)
  - $(x_1, x_2, \ldots, x_N), \;\; x_i \in R^d$
  - Number of clusters K ➜ $c_1, c_2, \ldots, c_K$ cluster centers

- Optimization objective
  - Minimize Sum of Squared Error
  - Finding optimal solution is NP-hard

    $O(N^{Kd+1})$

➜ Greedy solutions

$$SSE = \sum_{i=1}^{K} \underbrace{\sum_{x \in C_i}}_{\text{set of points in i-th cluster}} \overbrace{||x - c_i||^2}^{\text{squared distance between data point and center}}$$

K-Means — How to Define the Centroid of a Cluster?

- Simple case in Euclidean space $SSE = \sum_{i=1}^{K} \sum_{x \in C_i} ||x - c_i||^2$

$$\frac{\delta}{\delta c_k} SSE = \frac{\delta}{\underline{\delta c_k}} \cancel{\sum_{i=1}^{K}} \sum_{x \in C_i} (x - c_i)^2$$

$$= \cancel{\sum_{i=1}^{K}} \sum_{x \in C_i} \frac{\delta}{\delta c_k} (x - c_i)^2$$

$$\Rightarrow \sum_{x \in C_k} 2 \cdot (x - c_k) \stackrel{!}{=} 0$$

K-Means — How to Define the Centroid of a Cluster?

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$$\sum_{x \in C_k} 2 \cdot (x - c_k) \stackrel{!}{=} 0$$

$$\Rightarrow \sum_{x \in C_k} x - \sum_{x \in C_k} c_k = 0$$

$$\Rightarrow m_k c_k = \sum_{x \in C_k} x$$

$$\Rightarrow c_k = \frac{1}{m_k} \sum_{x \in C_k} x$$

➜ **Centroid of cluster = Mean of all points in that cluster**

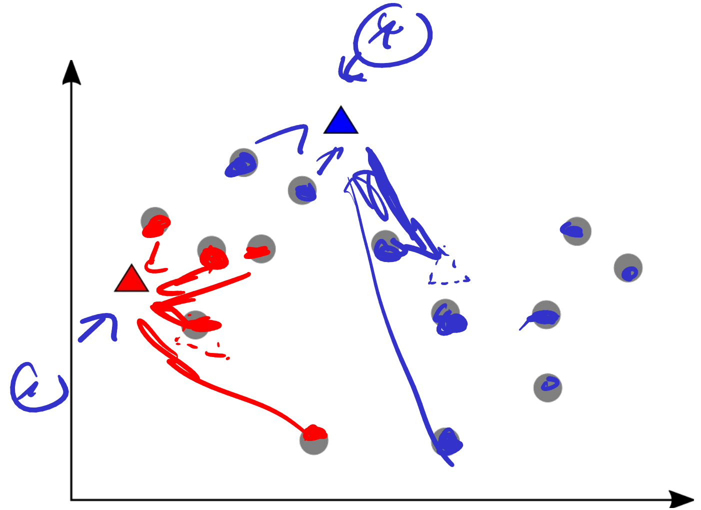
K-Means — Basic Algorithm (Lloyd's Algorithm)

1. Initialization: Select K points as initial centroids $c_1, c_2, \ldots, c_K$
2. Repeat

   2a) **Assignment**: assign each point to nearest cluster (i.e., centroid)

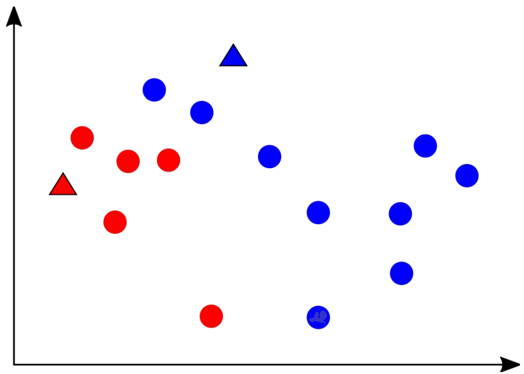
   2b) **Update**: move each centroid to the average of its assigned points

   Until no change in assignments

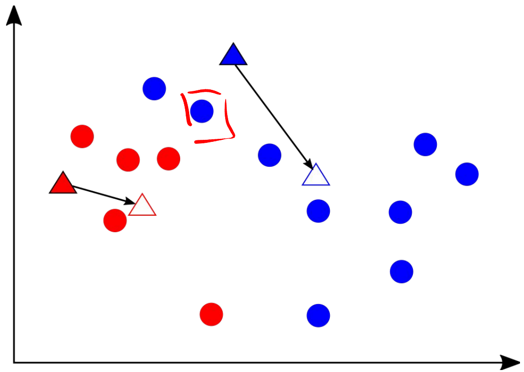


Example: K=2, after initialization

K-Means — Repeated Steps

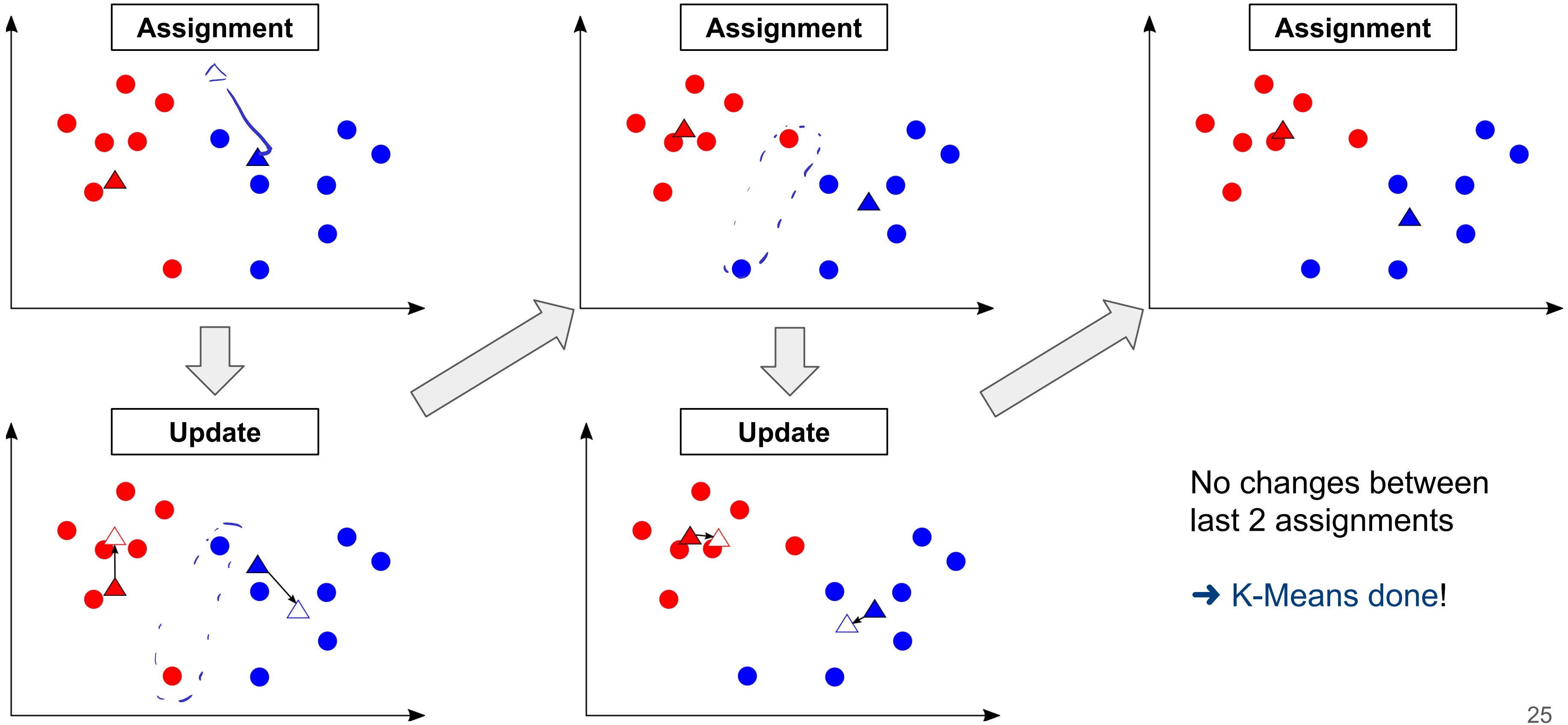


- Assignment
  - For each data point x , find nearest centroid c_i
  - Assign x to cluster i



- Update
  - Calculate mean of all data points of cluster i
  - Set centroid c_i to mean of cluster i

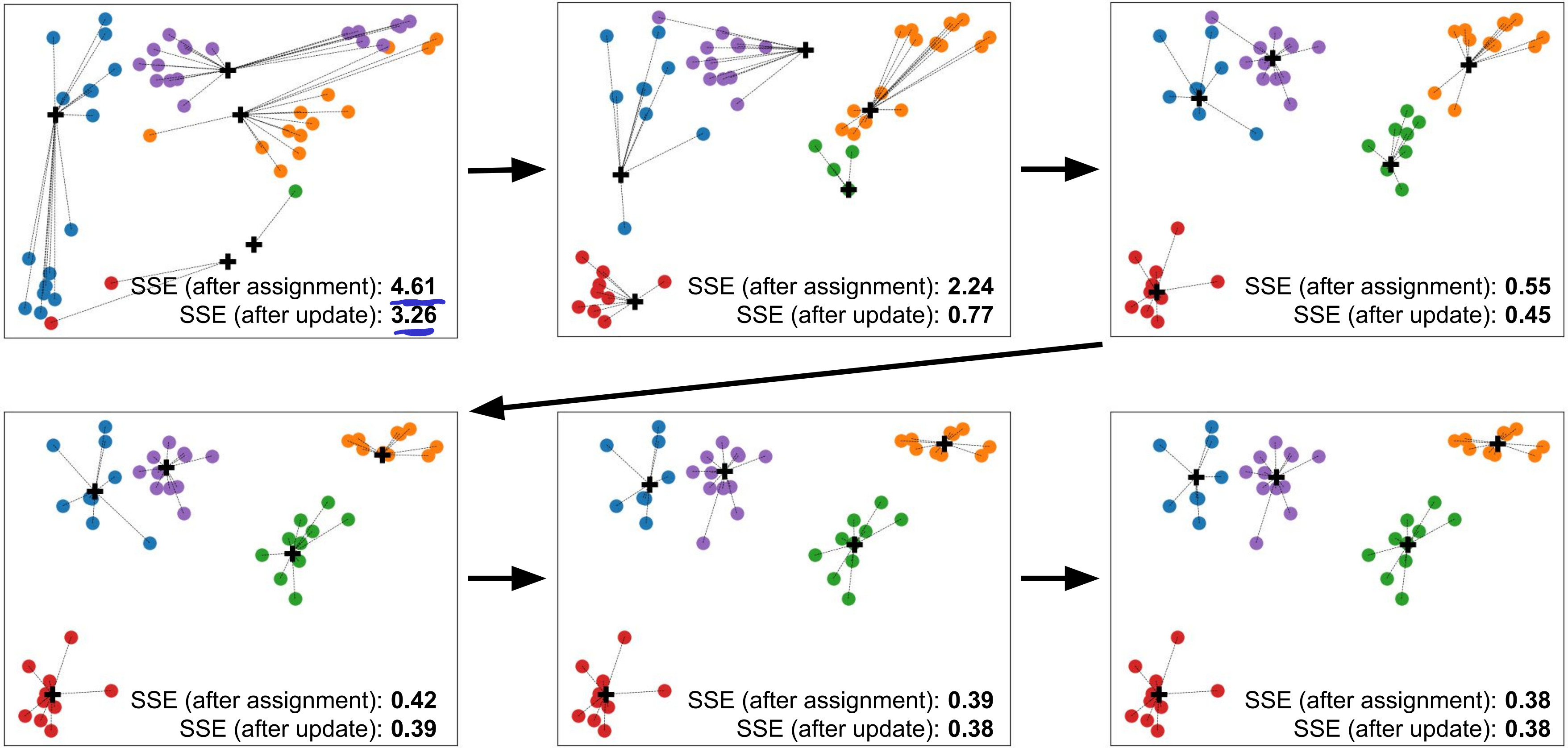
K-Means — Iteration until Convergence



No changes between last 2 assignments

➜ K-Means done!

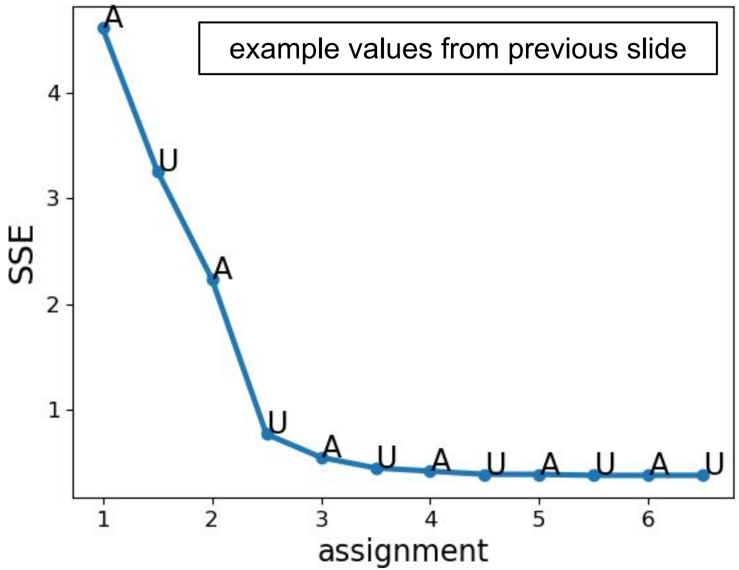
K-Means — Convergence



K-Means — Convergence

- Good news: K-Means always converges!
  - Both assignment (A) and update (U) reduce SSE (or no changes)
  - Most improvement during the first iterations

- Bad news
  - Lloyd's algorithm returns a **local optimum**, not necessarily a global optimum
  - Important: initialization of centroids
    (discussed in more detail later)

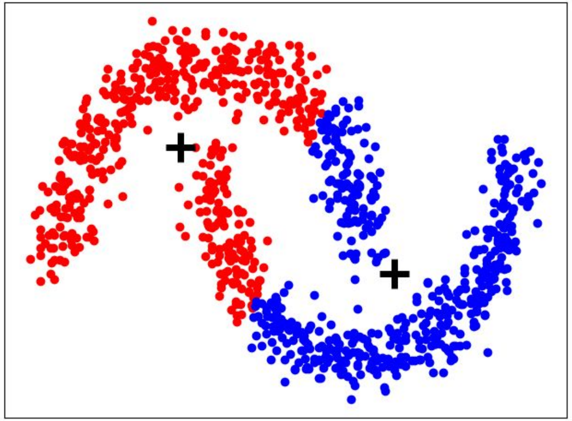


K-Means — Limitations (Data Distribution)

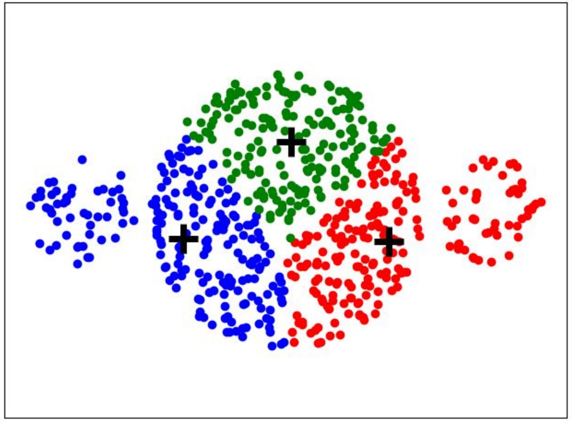
- K-Means is susceptible to "natural" clusters

non-blob-like

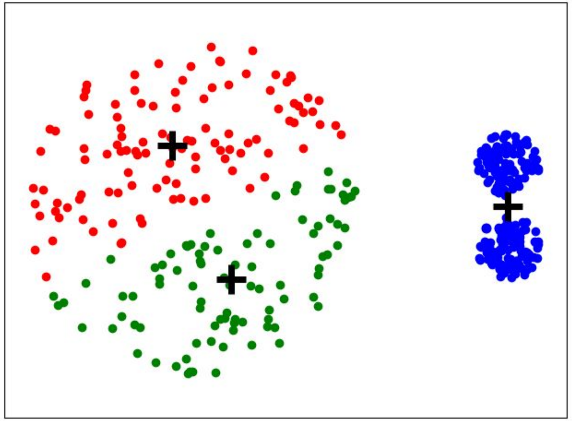
Non-Spherical Clusters



Clusters of different sizes

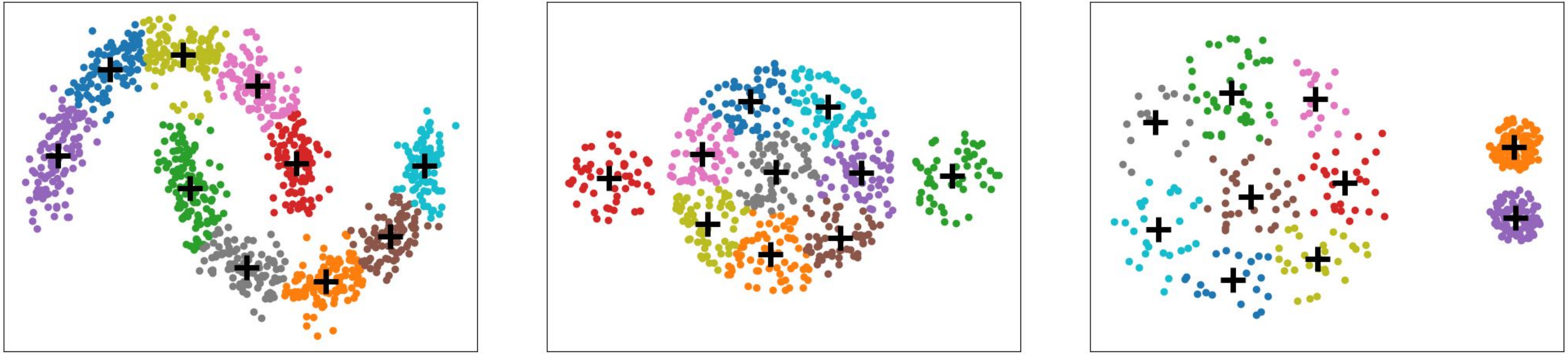


Clusters of different densities



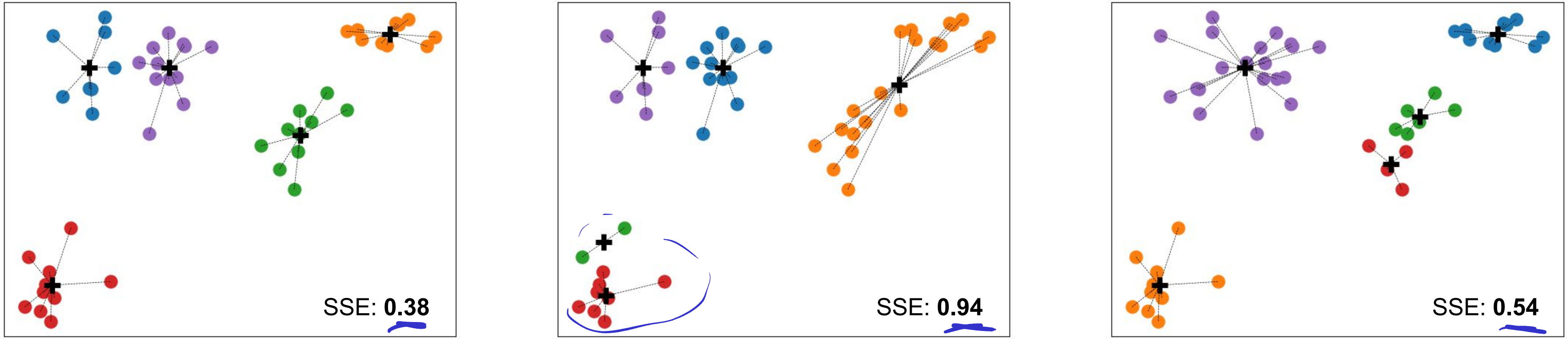
K-Means — Limitations (Data Distribution)

- Potential workaround: Choose large(r) value for K
  - Intuition: split natural clusters into multiple "well-behaved" (blob-like) subclusters
  - Apply suitable postprocessing steps to merge subclusters



K-Means — Limitations (Initial Centroids Issue)

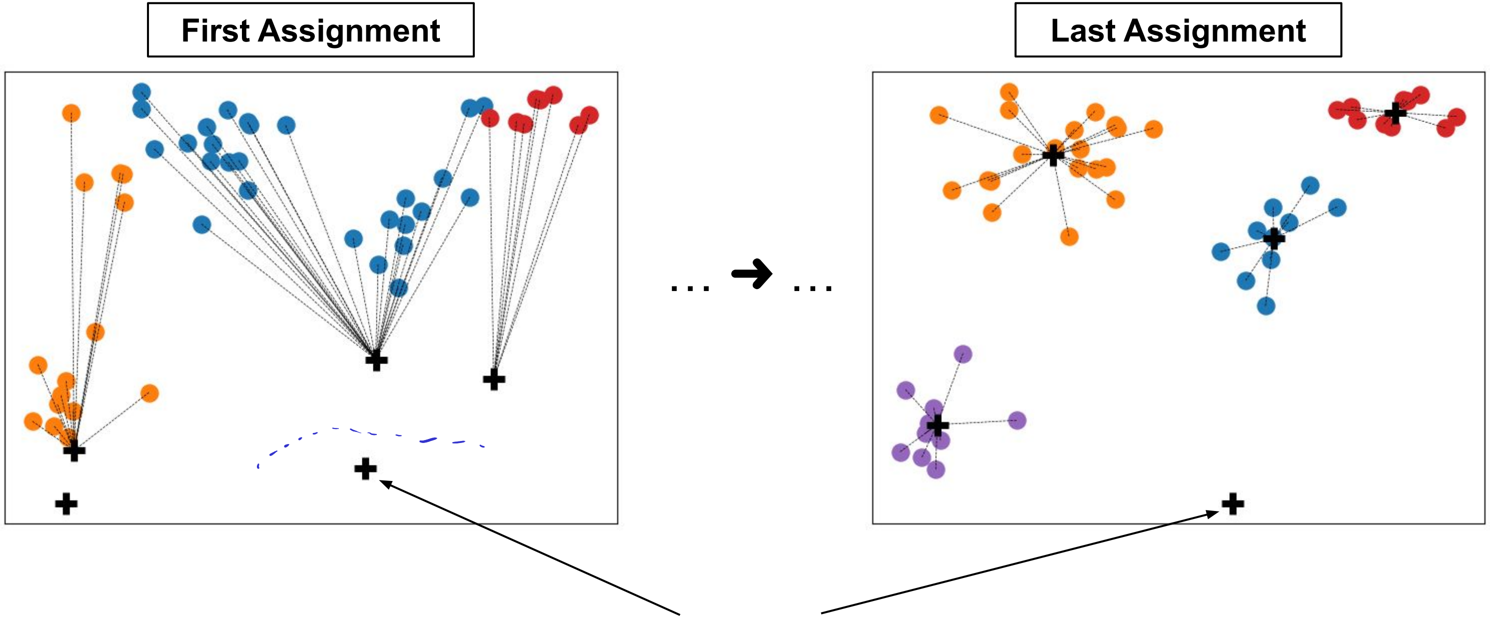
- Different initializations of centroids may yield different clusterings
  - Different clusterings typically have different SSEs ➜ global minimum!



k=5

K-Means — Limitations (Initial Centroids Issue)

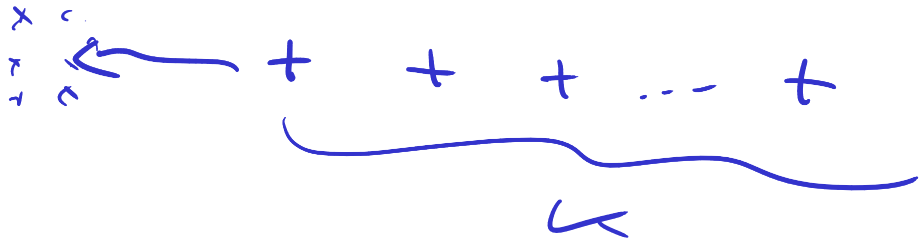
- Some initialization of centroids can yield empty clusters
  - Occurs when a centroid is "blocked off" data points by other centroids



(same centroid location; shift caused by autoscaling of plot)

Quick Quiz

What is the **maximum number of empty clusters** with K-Means with a really bad initialization of the centroids and $K \geq 2$?



A 0

B K - 1

C K

D K + 1

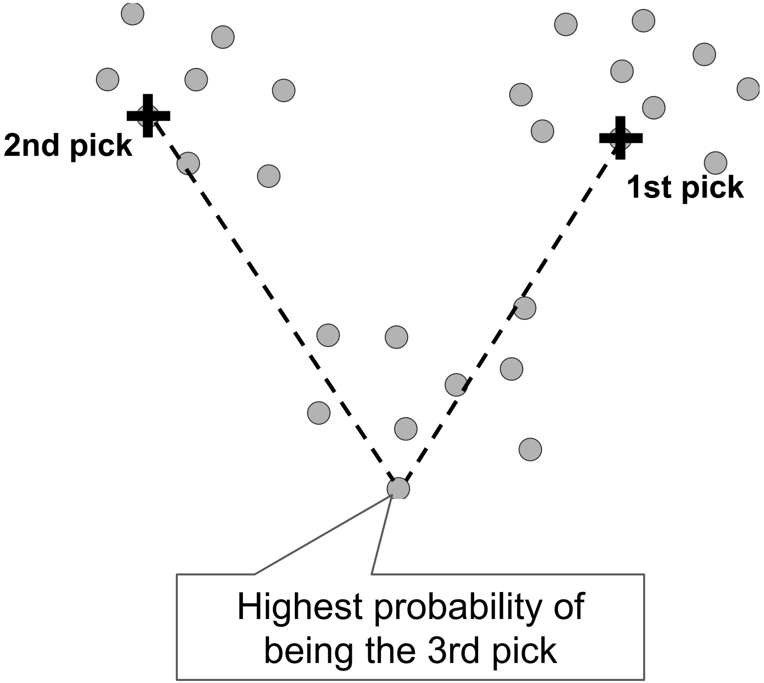
K-Means — Handling Empty Clusters

- Artificially fill empty clusters after assignment step (and continue iterations)
  - Replace empty cluster with point that contributes most to SSE
  - Replace empty cluster with a point from the cluster with the highest SSE
- Post processing
  - Split "loose" clusters = clusters with very high SSE
- Modification of Lloyd's algorithm ➜ K-Means variants
  - Typically aim to address the initial centroids issue

K-Means Variants — K-Means++

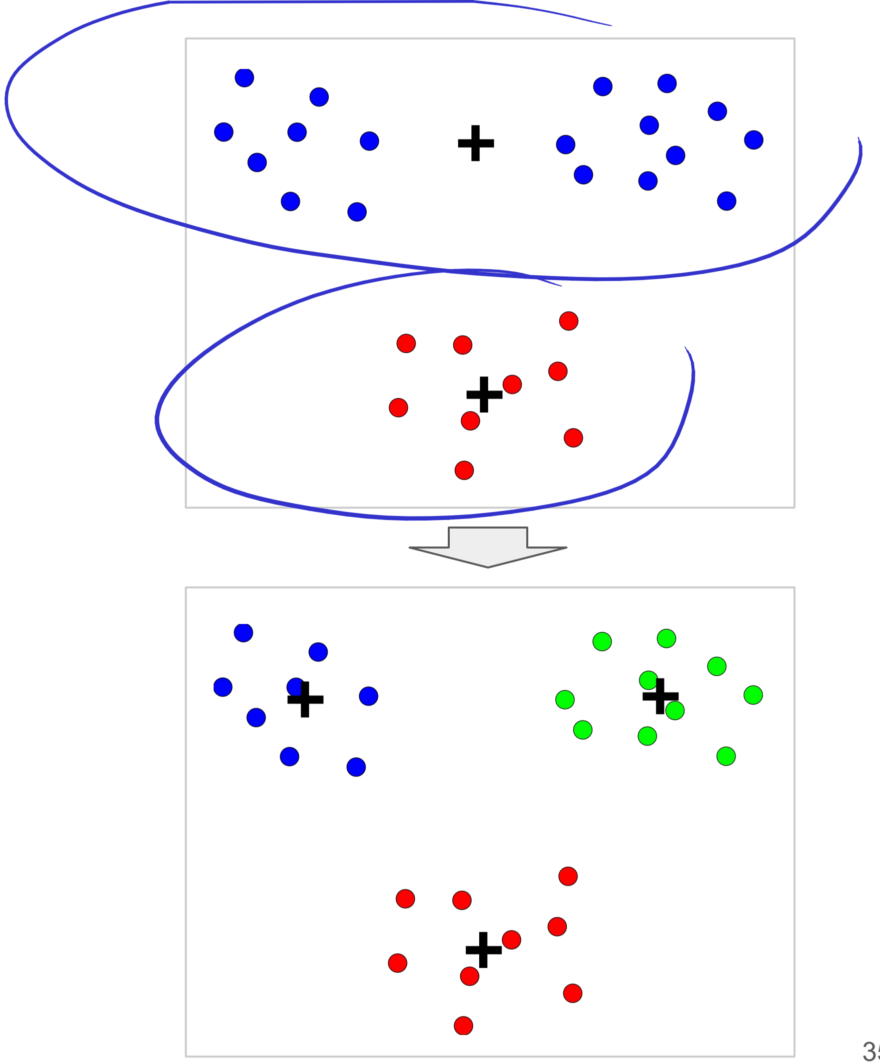
- Only changes initialization of centroids
  (assignment/update steps remain the same)
  - Goal: spread out centroids
  - Better performance in practice
  - Theoretical guarantees
- Initialization process
  1. Pick random point as first centroid c_1
  2. Repeat
     2a) For each point x, calculate distance d_x to nearest existing centroid
     2b) Pick random point for next centroid with probability proportional to d_x^2

  Until K centroids have been picked



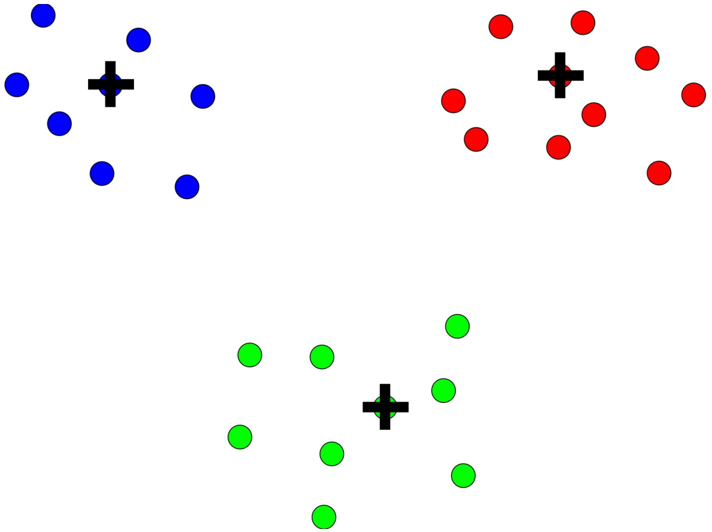
K-Means Variants — X-Means

- Automatic method to choose K
  - Run K-Means with K=2
  - Iteratively, run K-Means with K=2 over each subcluster
  - Split subcluster only if meaningful w.r.t. a scoring function
- Example scoring functions
  - Bayesian Information criterion (BIC)
  - Akaike information criterion (AIC)
  - Minimum Description Length (MDL)



K-Means Variants — K-Medoids

- Restriction: centroids are chosen from the data points
  - Does not require the calculation of the averages
    (no average of sets or more complex objects)
  - Only notion of distance or similarity still needed
    (e.g., Jaccard similarity for sets or custom metrics)
  - More robust to noise and outliers



- Main issue: performance
  - More expensive Update step
  - Swap medoid with each point in cluster and calculate change in cost (e.g., SSE)
  - Choose the point as new medoid that minimizes the cost after swapping

Quick Quiz

Can a theoretically optimal initialization of centroids **guarantee** no empty clusters in any case of running K-Means?

$N =$ # points

$k > N$

A No

B Yes

C Impossible to say

D Unlikely

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- **Clustering Algorithms**
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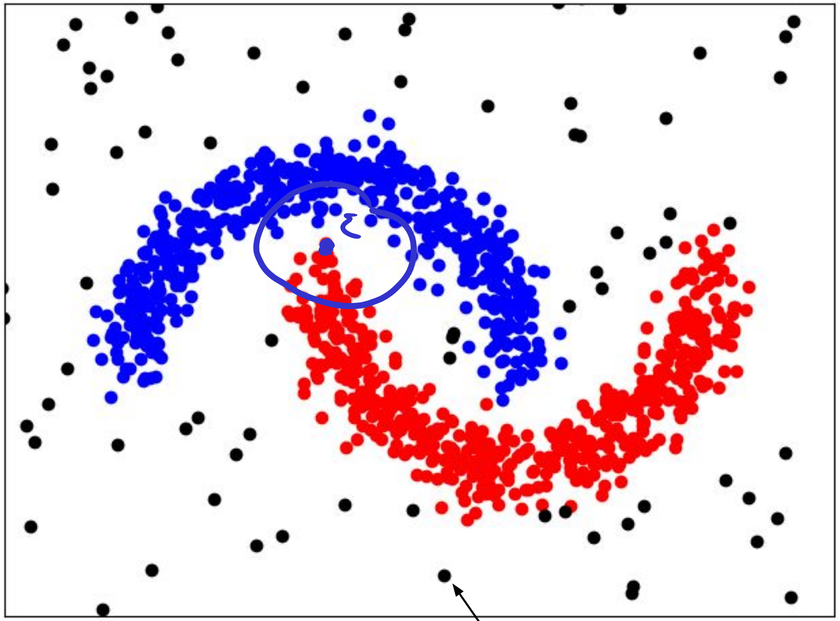
  - **DBSCAN**
  - Hierarchical Clustering
- Cluster Evaluation

DBSCAN (Density-Based Spatial Clustering of Applications with Noise)

- Basic characteristics
  - Clusters: density-based
  - Clustering: partitional, exclusive, partial
- Inputs (for d-dimensional Euclidean space)
  - $(x_1, x_2, ..., x_N), \ x_i \in R^d$
  - ε — radius defining a points neighborhood
  - $MinPts$ — minimum number of points

$$density = \frac{mass}{volume} = \frac{MinPts}{\mathcal{E}}$$

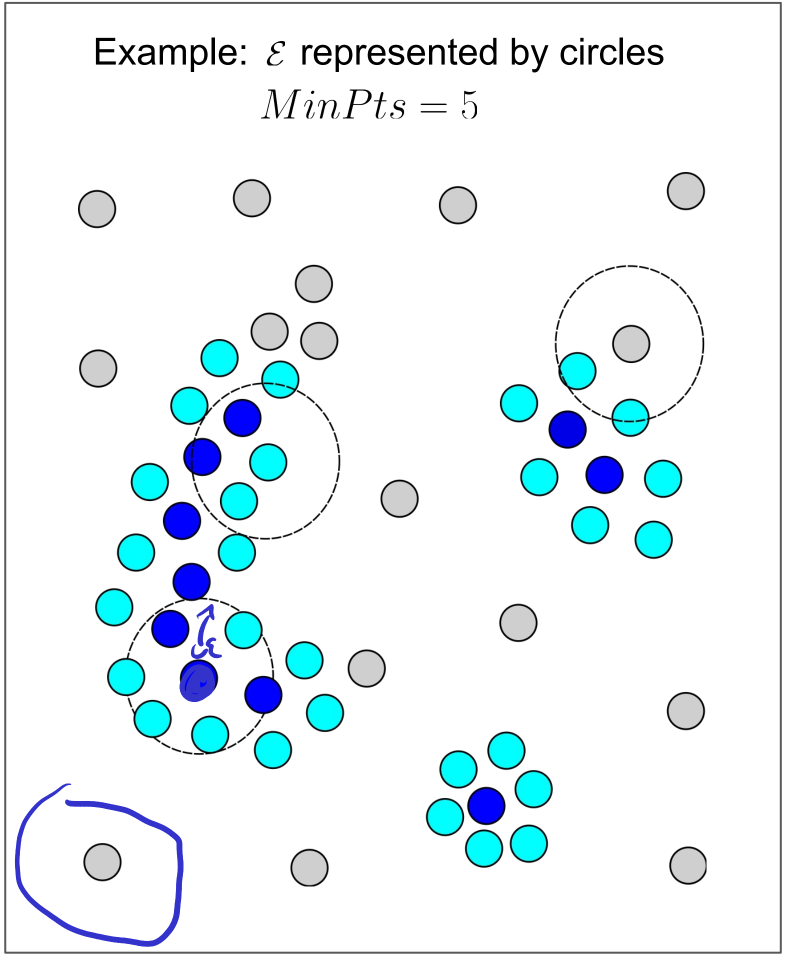


noise: not part of any cluster

DBSCAN — Types of Points

incl. the point itself

- Core points
  - All points with at least $MinPts$ neighbors with radius $\mathcal{E}$ (this includes the point itself!)
  - Form the **interior** of a cluster
- Border Points
  - Non-core points with at least one core point in their neighborhood
  - Form the **border** of a cluster
- Outliers / noise
  - All other points
  - Default node type



DBSCAN — Algorithm (2 Iterative Phases)

1. Find new cluster seed (core point)

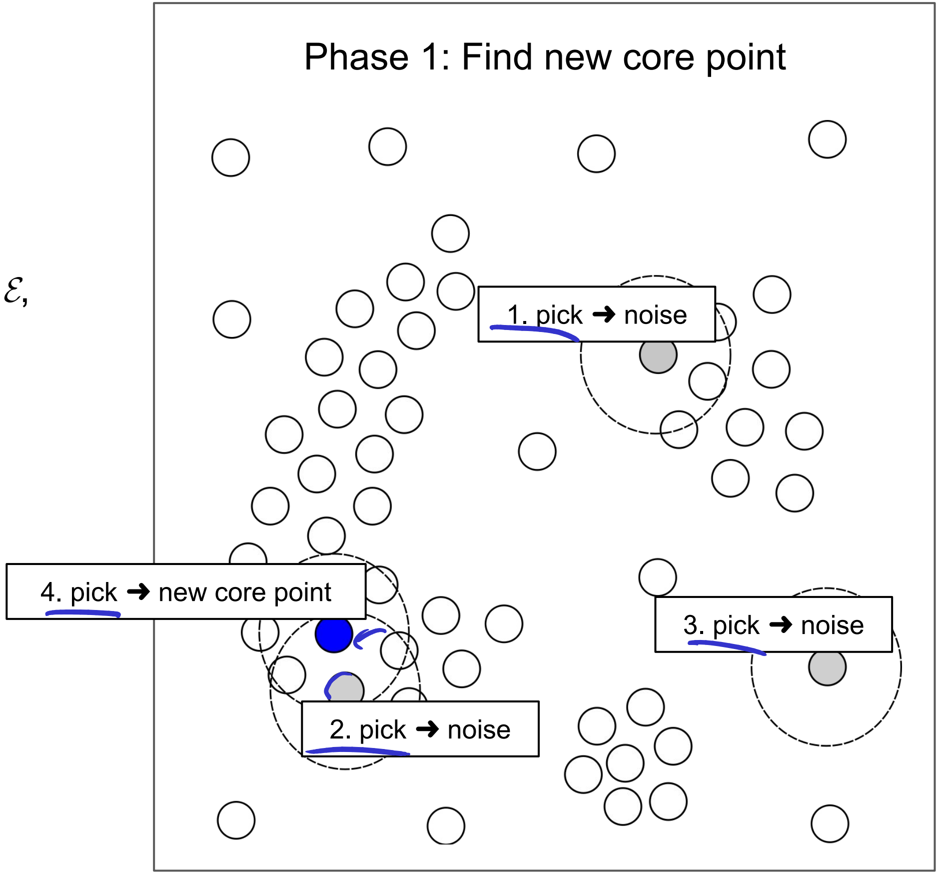
   Repeat

   1a) Pick random unexplored point x

   1b) If x has less than $MinPts$ neighbors within $\mathcal{E}$, label x as noise (might change later)

   Until x is a new core point

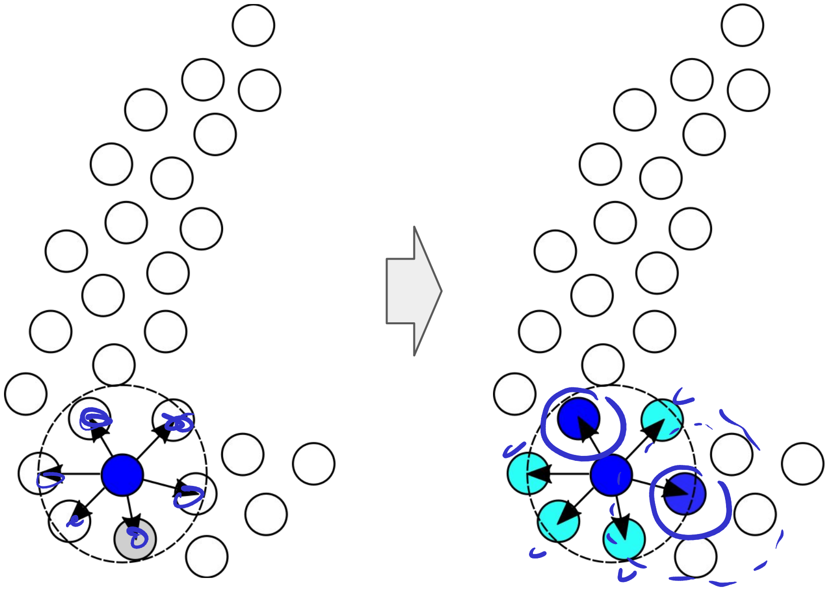
2. Explore new cluster



DBSCAN — Algorithm (Cluster Exploration)

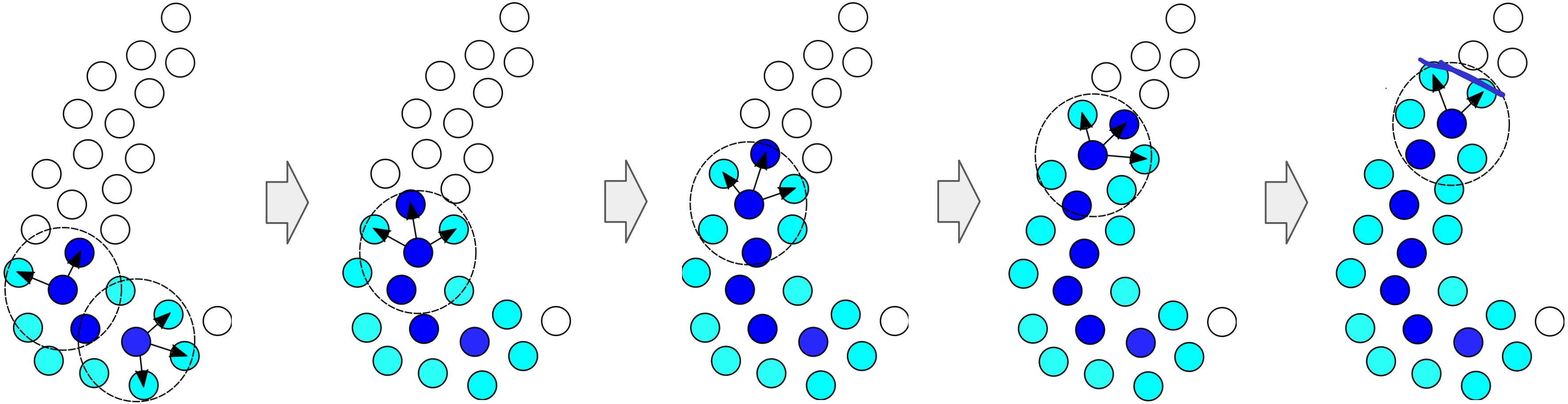
- Explore all neighbors of core point
  - Put all neighbors into the same cluster
  - A neighbor is either a core point or a border point (never noise)
  - New type of neighbor might overwrite previous noise label

- Recursively repeat for each newly found core point



DBSCAN — Algorithm (Cluster Exploration)

- Example: complete exploration of a cluster
  - Further exploration stops at border points
  - Points beyond border points will become noise or part of a new cluster (after Phase 1)

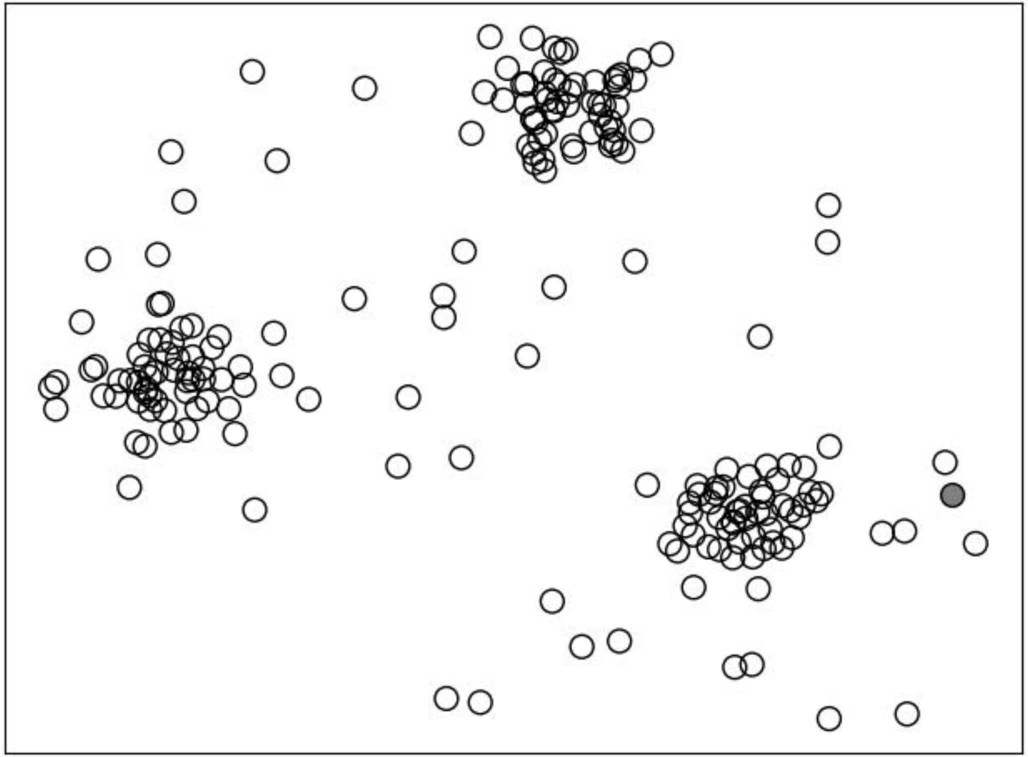


DBSCAN — Algorithm (Cluster Exploration)

- Input: newly found core x_c point signifying a new cluster

$S \leftarrow get\_neighbors(x_c, \mathcal{E})$	Initialize S with the the neighbors of x_c
WHILE $\lvert S \rvert \neq 0$ $\quad s \leftarrow S.pop()$	Pick next point s from S until S is empty
$\quad$ IF $s.label =$ "$noise$" THEN $\quad\quad s.label \leftarrow x_c.cluster\_id$	If point s is (currently) noise, add point to current cluster
$\quad$ IF $s.label \neq$ "$unknown$" THEN $\quad\quad$ CONTINUE	If s has already been explored, continue with next point
$\quad s.label \leftarrow x_c.cluster\_id$	Add s current cluster (s so far unexplored)
$\quad neighbors \leftarrow get\_neighbors(s, \mathcal{E})$	Get all neighbors of s
$\quad$ IF $\lvert neighbors \rvert \geq MinPts$ THEN $\quad\quad S \leftarrow S \cup neighbors$	If s has more than $MinPts$ neighbors, s is also a core point ➜ add neighbors to S (so they will be explored as well)

DBSCAN — Example with Visualization

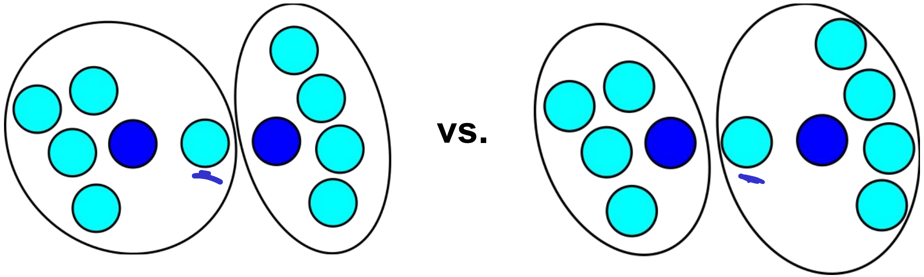


Download at: https://www.comp.nus.edu.sg/~chris/downloads/images/dbscan-visualized.gif

DBSCAN — Characteristics

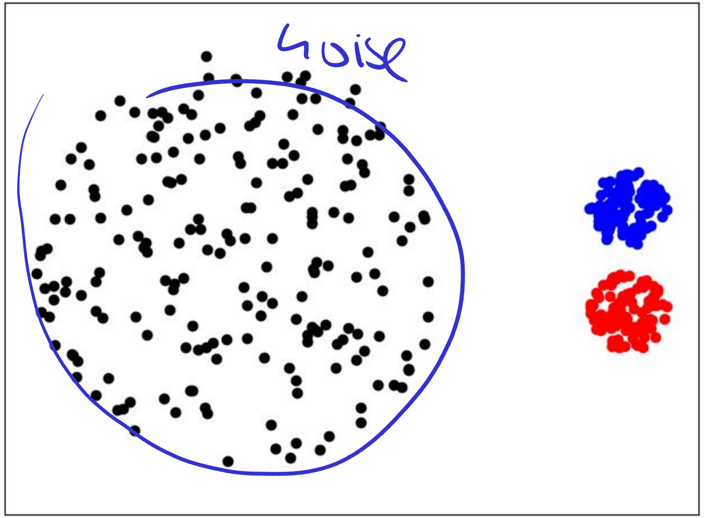
- DBSCAN always converges
  - Each data point gets explored (either in Phase 1 or 2)
  - A data point does not change its type (only exception: noise ➜ border)

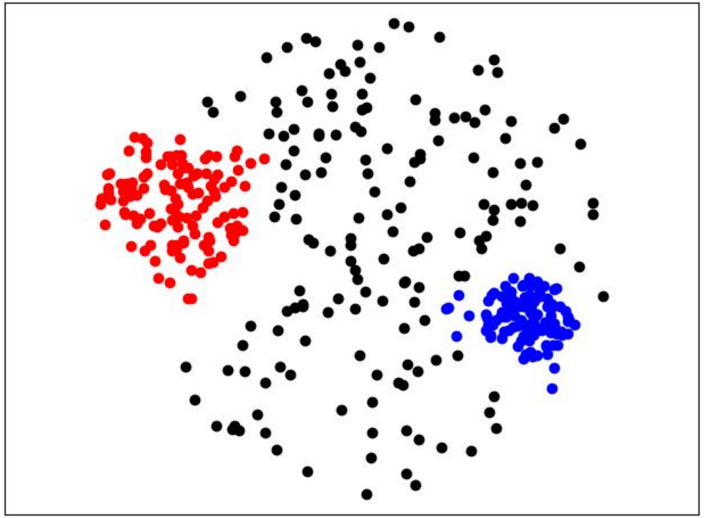
- DBSCAN is not completely deterministic
  - Phase 1 introduces randomness
  - Border points may be reachable from core points of different clusters
  - Noise and core points deterministic



DBSCAN — Limitations

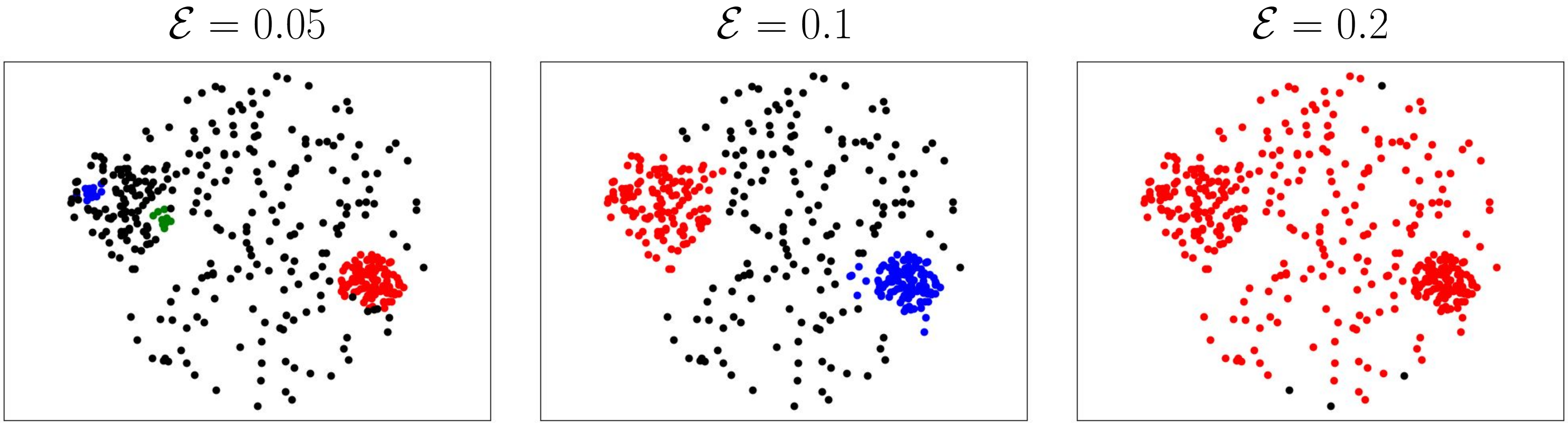
- DBSCAN cannot handle different densities





DBSCAN — Limitations

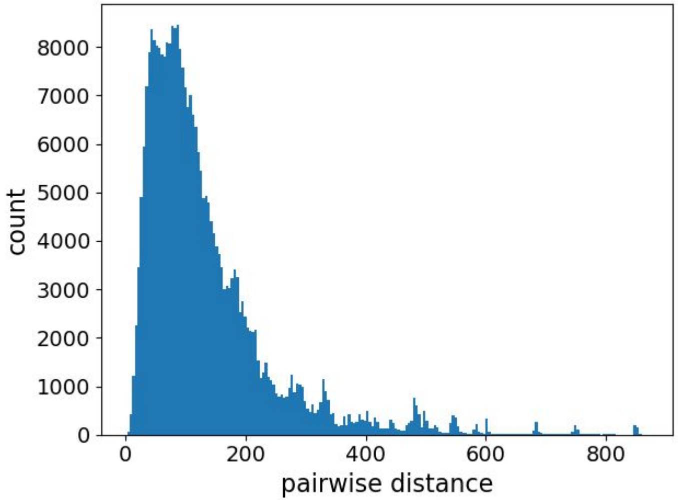
- DBSCAN is generally very sensitive to parameters
  - Choosing $\mathcal{E}$ and $MinPts$ requires good understanding of data and context



($MinPts = 10$ for all three examples)

DBSCAN — How to Choose Parameter Values?

- Informed by results of EDA, e.g.:



Distribution of all pairwise distances

First insights into suitable values for ε

- Density of data points has intuitive semantic meaning, e.g.:
  - Geographic distance between bars in a city
  - Task: Find areas (clusters) with more than 10 bars within 500m

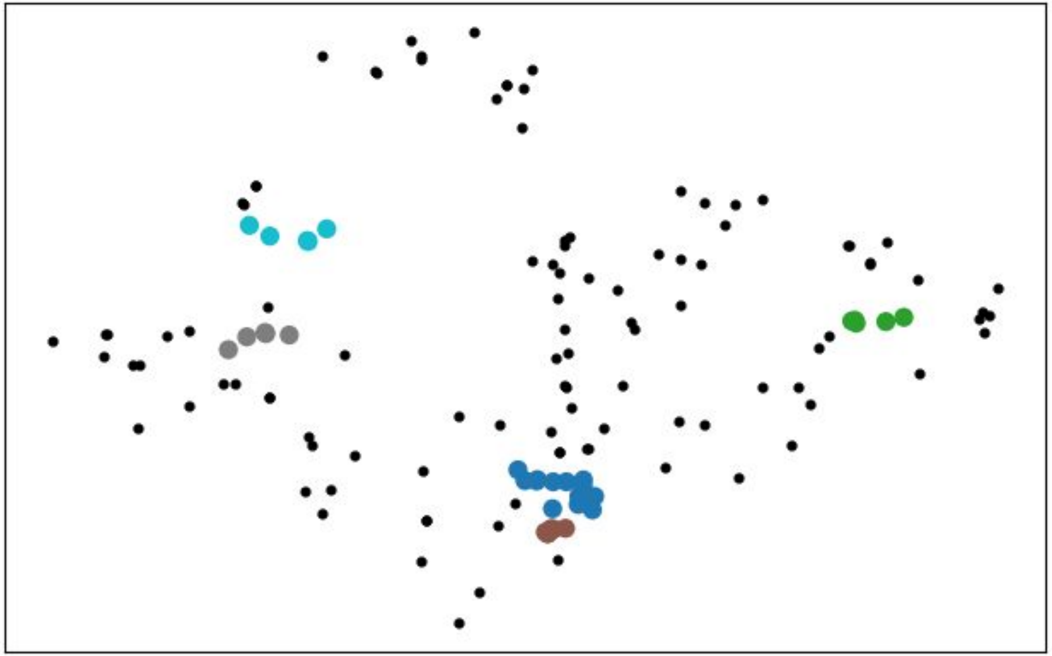
DBSCAN — How to Choose Parameter Values?

- Intuitive interpretations of meaningful parameter values

- Example
  - 141 McDonald's restaurants across Singapore

    min_pts
  - Find areas with more than 5 restaurants within a 500m radius

    ε



Quick Quiz

What is the **smallest cluster size** when using DBSCAN and a given value for *MinPts*?

A 1

B *MinPts* - 1

C *MinPts*

D *MinPts* + 1

Quick Quiz

Given *N*=1,000 data points and using DBSCAN with *MinPts=10*, what is the **minimum** possible number of clusters?

A 0

B 1

C MinPts

D MinPts + 1

Quick Quiz — Side Note

- Slight inconsistencies across different sources
  - Relevant step in algorithm

$$neighbors \leftarrow get\_neighbors(s, \mathcal{E})$$

Does *neighbors* contain *s* itself?

- Original paper: Yes, *s* is part of neighborhood
  - Smallest cluster size: $MinPts$
  - Maximum number of clusters: $\left\lfloor \dfrac{N}{MinPts} \right\rfloor$

N = number of data points

Clustering Algorithms

- K-Means
- DBSCAN
- **Hierarchical Clustering** (next lecture)

Outline

- Clustering
  - Overview
  - Applications
  - Concepts
- **Clustering Algorithms**
  - K-Means
  - DBSCAN
  - **Hierarchical Clustering** (next lecture)
- Cluster Evaluation

Summary — Clustering I

- Clustering as fundamental data mining algorithm
  - Cluster provide a "meso-view" on data
  - Required: well-defined notion of similarity between data points
  - No single definition what a good cluster / clustering is

➜ Wide range of different clustering algorithms

- In this lecture: K-Means & DBSCAN
  - K-Means: split all data points into k clusters based in their **relative similarities**
  - DBSCAN: find clusters based on **absolute similarities** between data points

Solutions to Quick Quizzes

- Slide 18: D
- Slide 32: B
- Slide 37: A
- Slide 51: C
- Slide 52: A