K-Means

Class Algorithmic Methods of Data Mining
Program M. Sc. Data Science
University Sapienza University of Rome
Semester Fall 2015
Lecturer Carlos Castillo http://chato.cl/

Sources:

- Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms, Cambridge University Press, May 2014. Example 13.1. [download]
- Evimaria Terzi: Data Mining course at Boston University http://www.cs.bu.edu/~evimaria/cs565-13.html

The k-means problem

- consider set $X=\{x_1,...,x_n\}$ of n points in R^d
- assume that the number k is given
- problem:
  - find k points $c_1,...,c_k$ (named centers or means)

so that the cost

$$\sum_{i=1}^{n} \min_j \left\{ L_2^2(x_i, c_j) \right\} = \sum_{i=1}^{n} \min_j ||x_i - c_j||_2^2$$

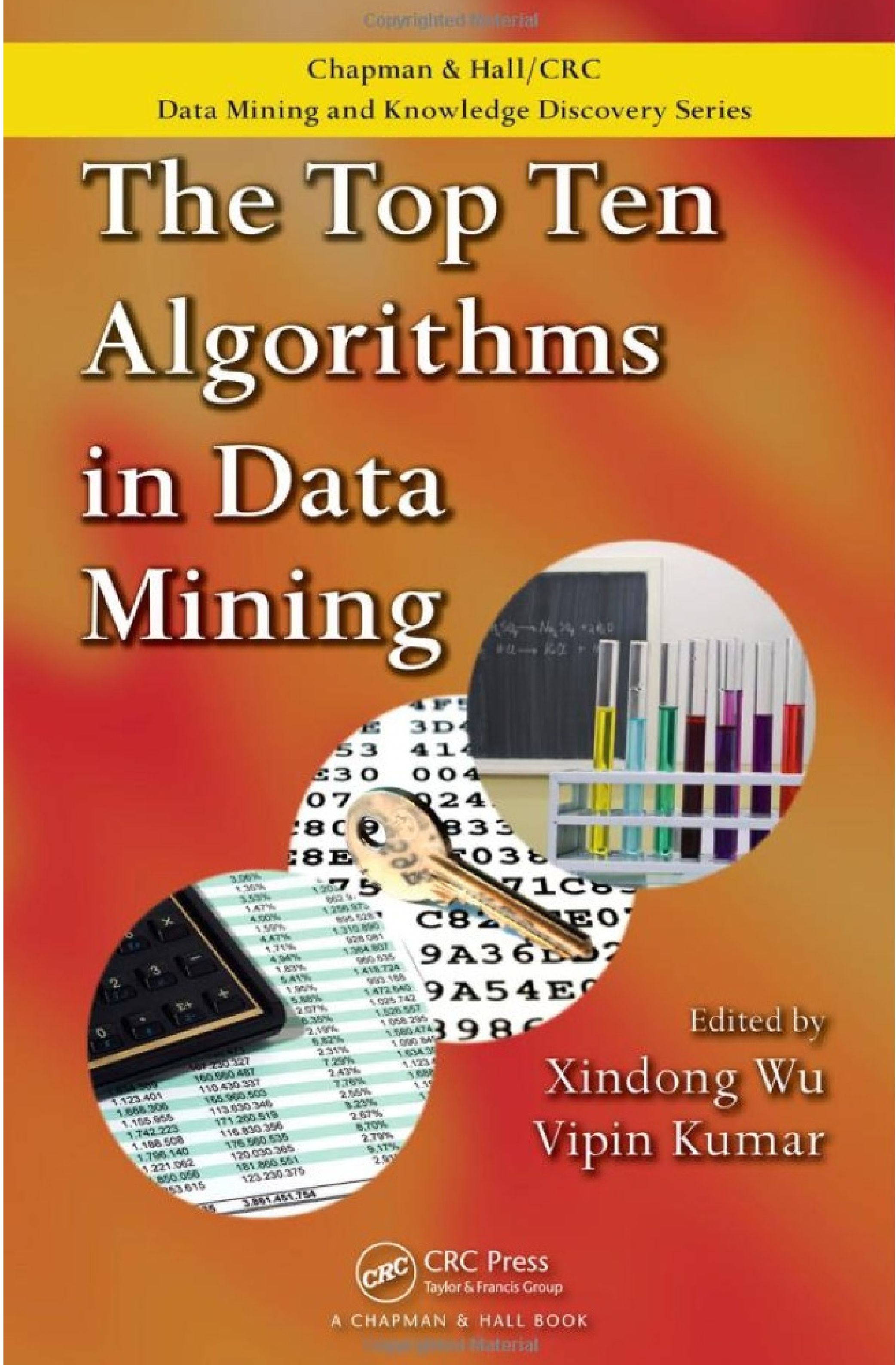
is minimized

The k-means problem

- $k=1$ and $k=n$ are easy special cases (*why?*)
- an NP-hard problem if the dimension of the data is at least 2 ($d \geq 2$)
- in practice, a simple iterative algorithm works quite well

The k-means algorithm

- voted among the top-10 algorithms in data mining
- one way of solving the k-means problem



K-means algorithm

K-MEANS $(\mathbf{D}, k, \epsilon)$:

$t = 0$

Randomly initialize k centroids: $\boldsymbol{\mu}_1^t, \boldsymbol{\mu}_2^t, \ldots, \boldsymbol{\mu}_k^t \in \mathbb{R}^d$

repeat

  $t \leftarrow t + 1$

  $C_j \leftarrow \emptyset$ for all $j = 1, \cdots, k$

  `// Cluster Assignment Step`

  foreach $\mathbf{x}_j \in \mathbf{D}$ **do**

    $j^* \leftarrow \text{argmin}_i \left\{ \left\| \mathbf{x}_j - \boldsymbol{\mu}_i^t \right\|^2 \right\}$ `// Assign` $\mathbf{x}_j$ `to closest centroid`

    $C_{j^*} \leftarrow C_{j^*} \cup \{\mathbf{x}_j\}$

  `// Centroid Update Step`

  foreach $i = 1$ *to* k **do**

    $\boldsymbol{\mu}_i^t \leftarrow \frac{1}{|C_i|} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$

until $\sum_{i=1}^{k} \left\| \boldsymbol{\mu}_i^t - \boldsymbol{\mu}_i^{t-1} \right\|^2 \leq \epsilon$

The k-means algorithm

1. randomly (or with another method) pick k cluster centers $\{c_1,\ldots,c_k\}$

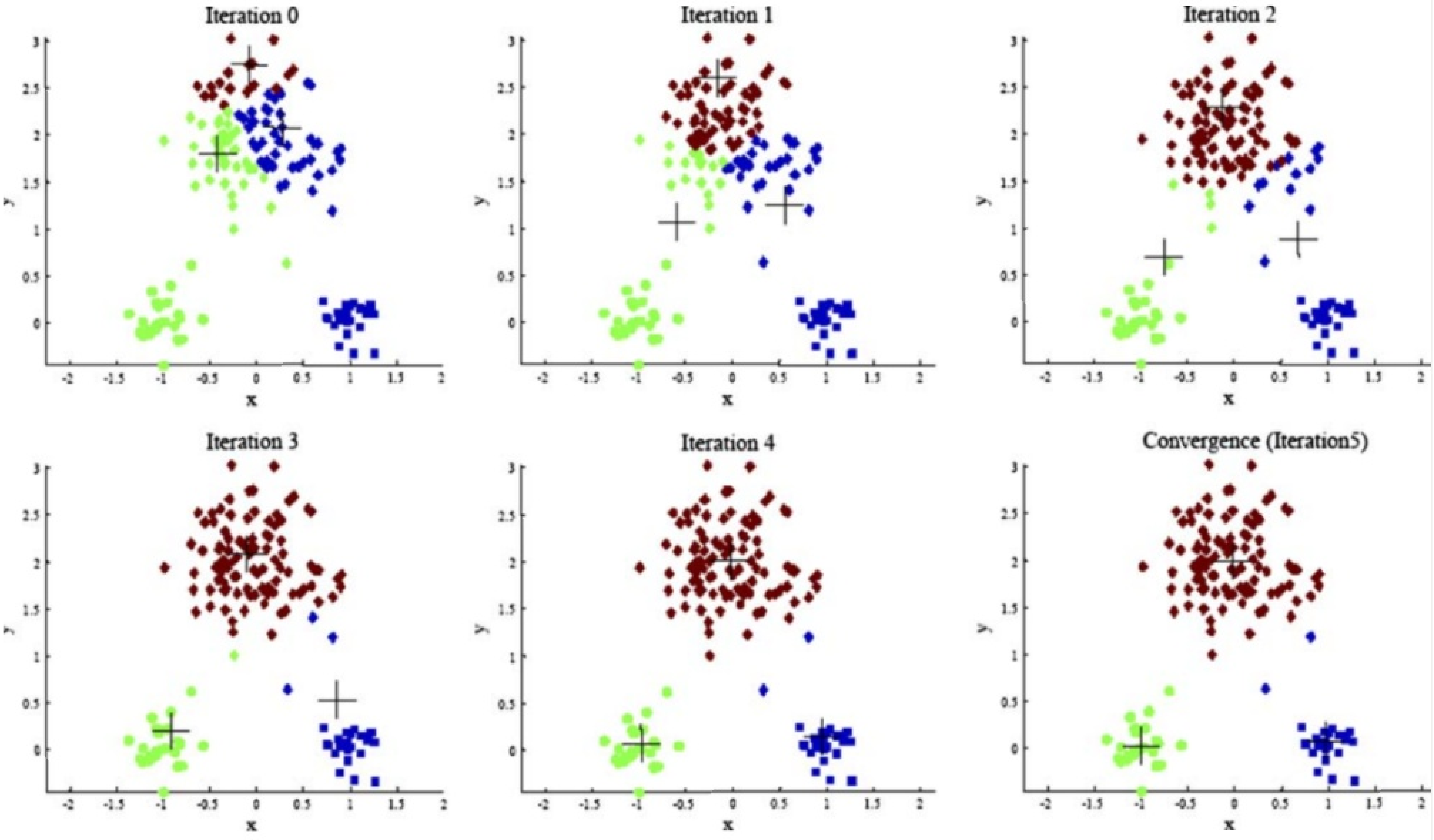
2. for each j, set the cluster X_j to be the set of points in X that are the closest to center c_j

3. for each j let c_j be the center of cluster X_j

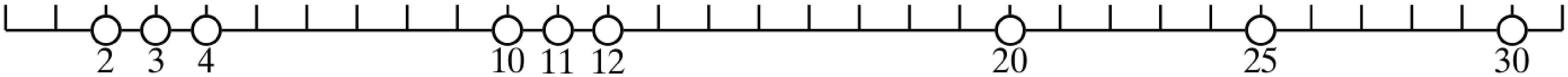
(mean of the vectors in X_j)

1. repeat (go to step 2) until convergence

Sample execution



1-dimensional clustering exercise



Exercise:

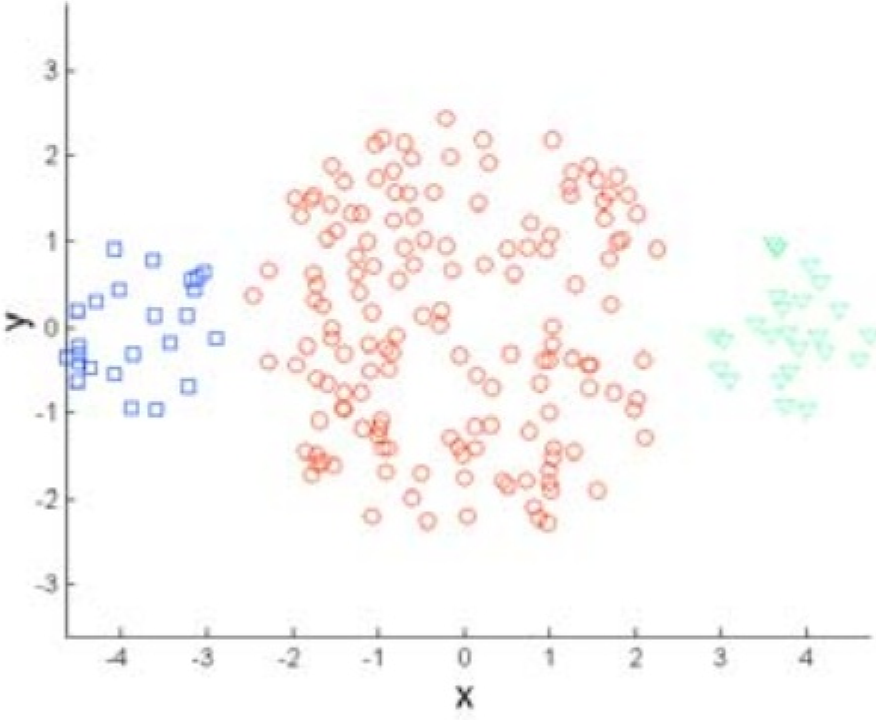
- *For the data in the figure*
  - *Run k-means with k=2 and initial centroids u1=2, u2=4 (Verify: last centroids are 18 units apart)*

- *Try with k=3 and initialization 2,3,30*

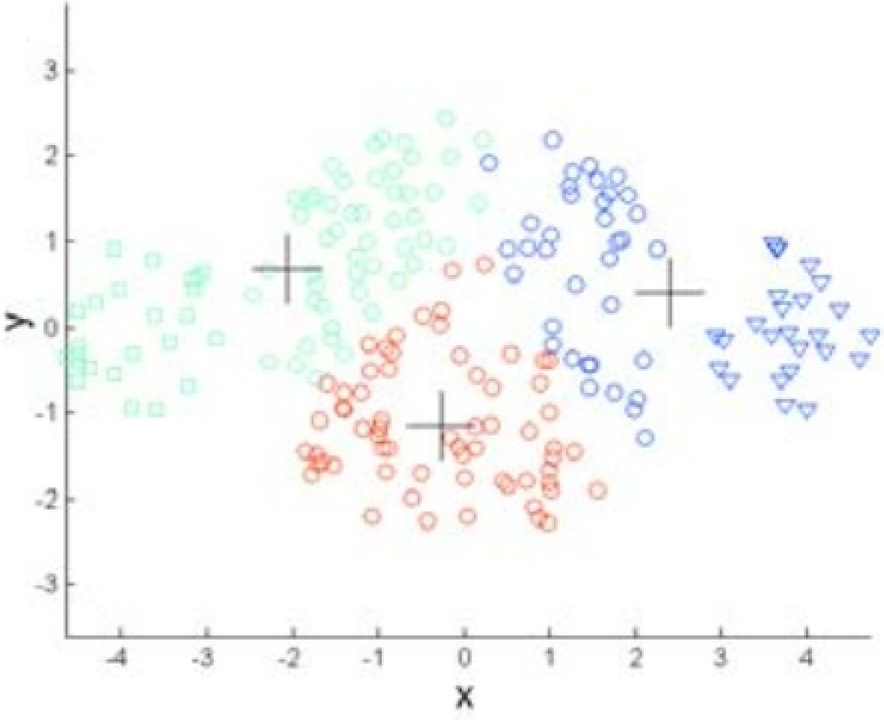
Limitations of k-means

- Clusters of different size
- Clusters of different density
- Clusters of non-globular shape
- Sensitive to initialization

Limitations of k-means: different sizes

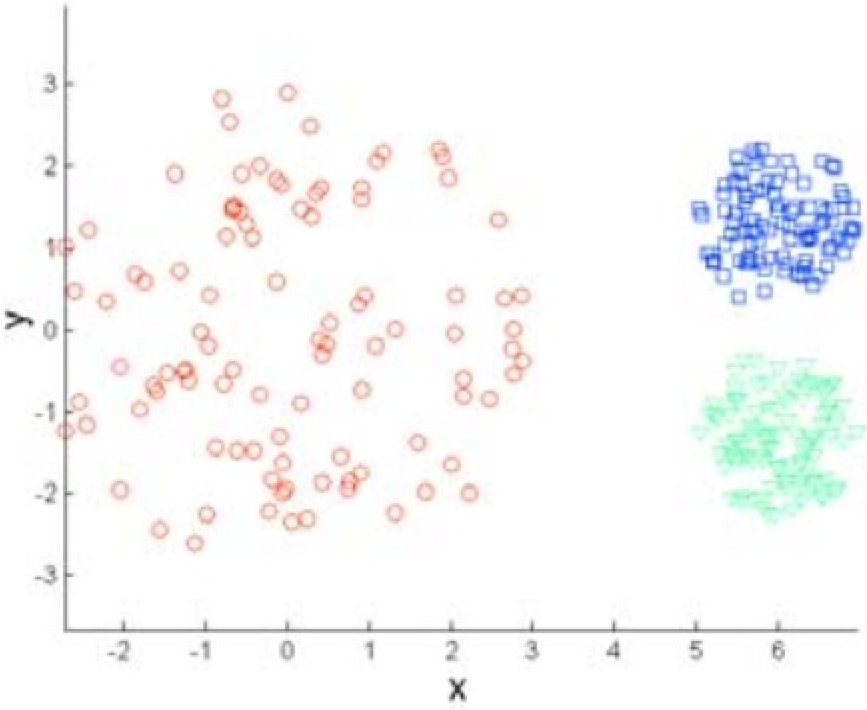


Original Points

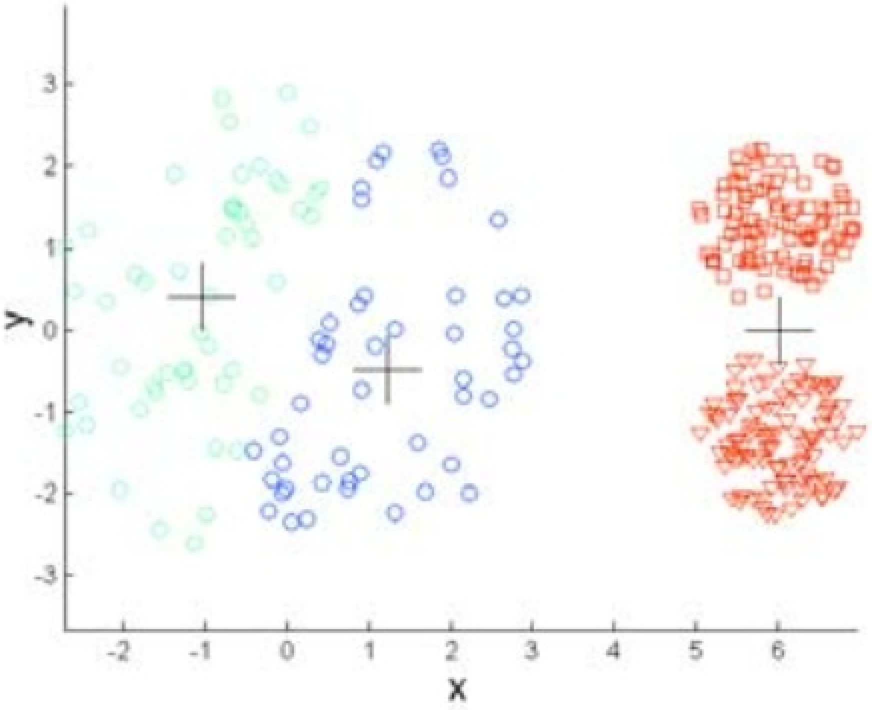


K-means (3 Clusters)

Limitations of k-means: different density

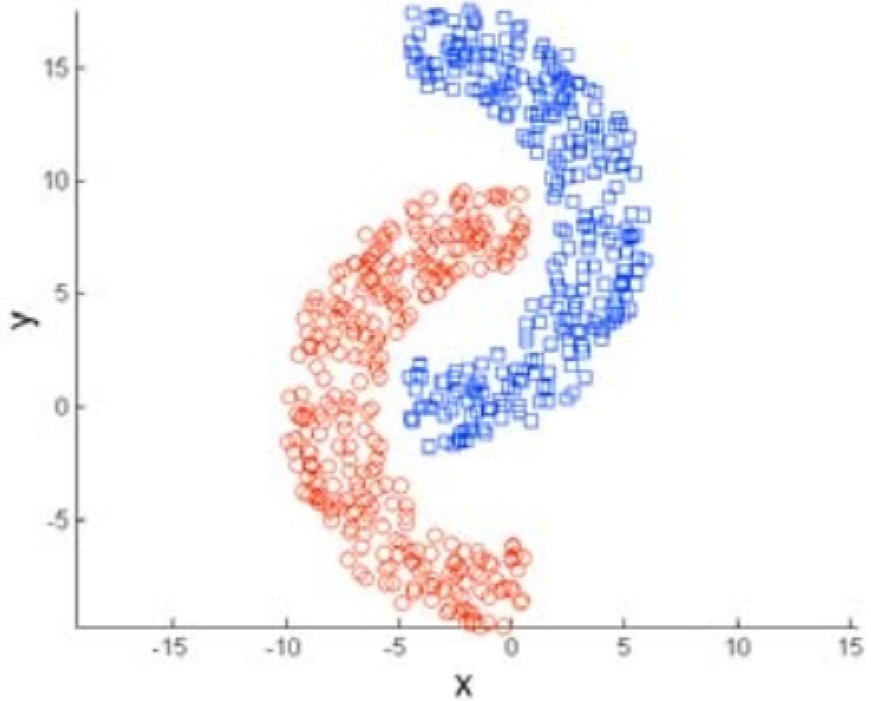


Original Points

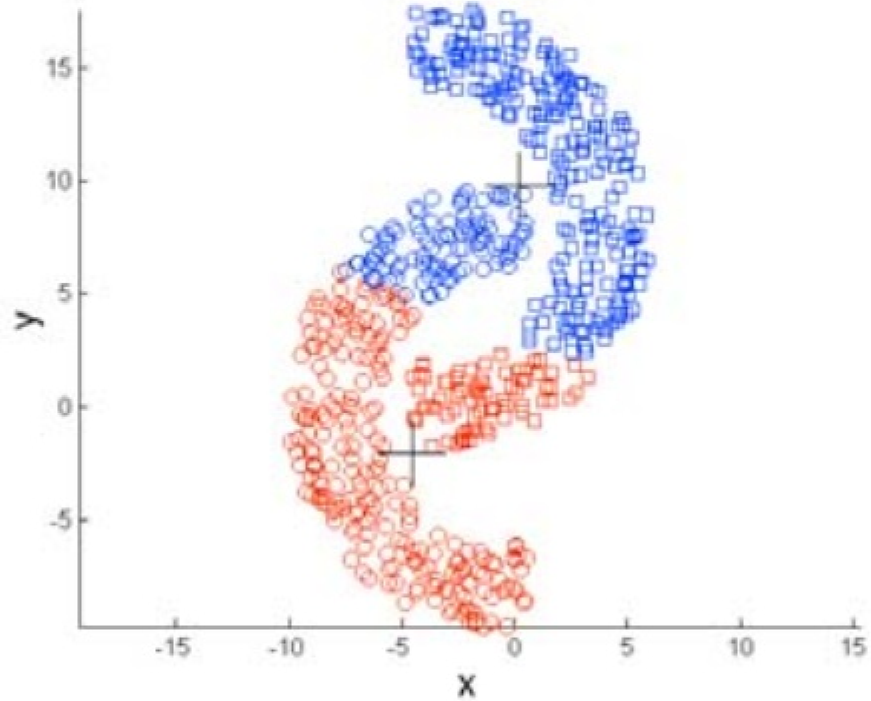


K-means (3 Clusters)

Limitations of k-means: non-spherical shapes

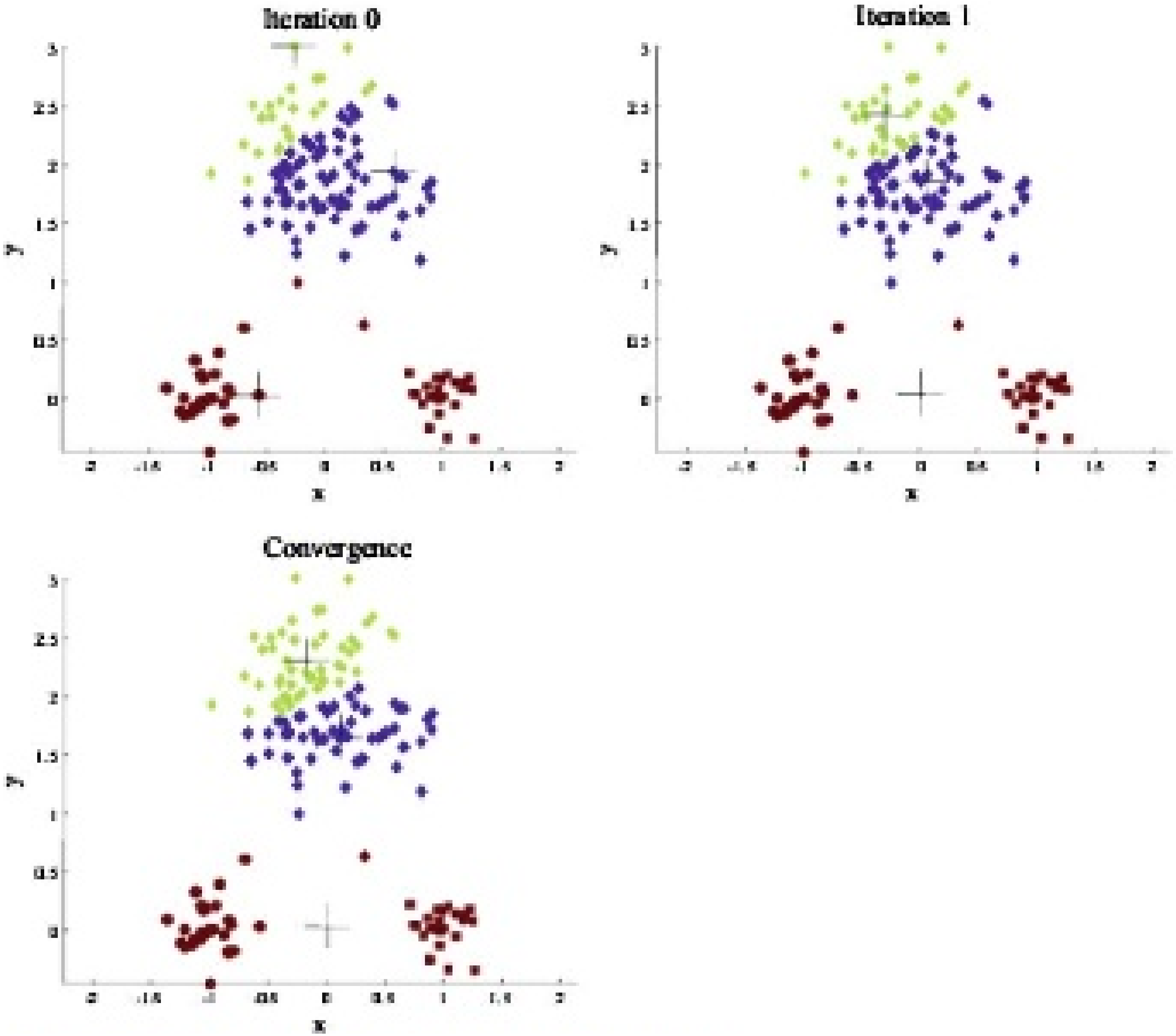


Original Points



K-means (2 Clusters)

Effects of bad initialization



k-means algorithm

- finds a local optimum
- often converges quickly

  but not always
- the choice of initial points can have large influence in the result
- tends to find spherical clusters
- outliers can cause a problem
- different densities may cause a problem

Advanced: k-means initialization

Initialization

- random initialization
- random, but repeat many times and take the best solution
    - helps, but solution can still be bad
- pick points that are distant to each other
    - k-means++
    - provable guarantees

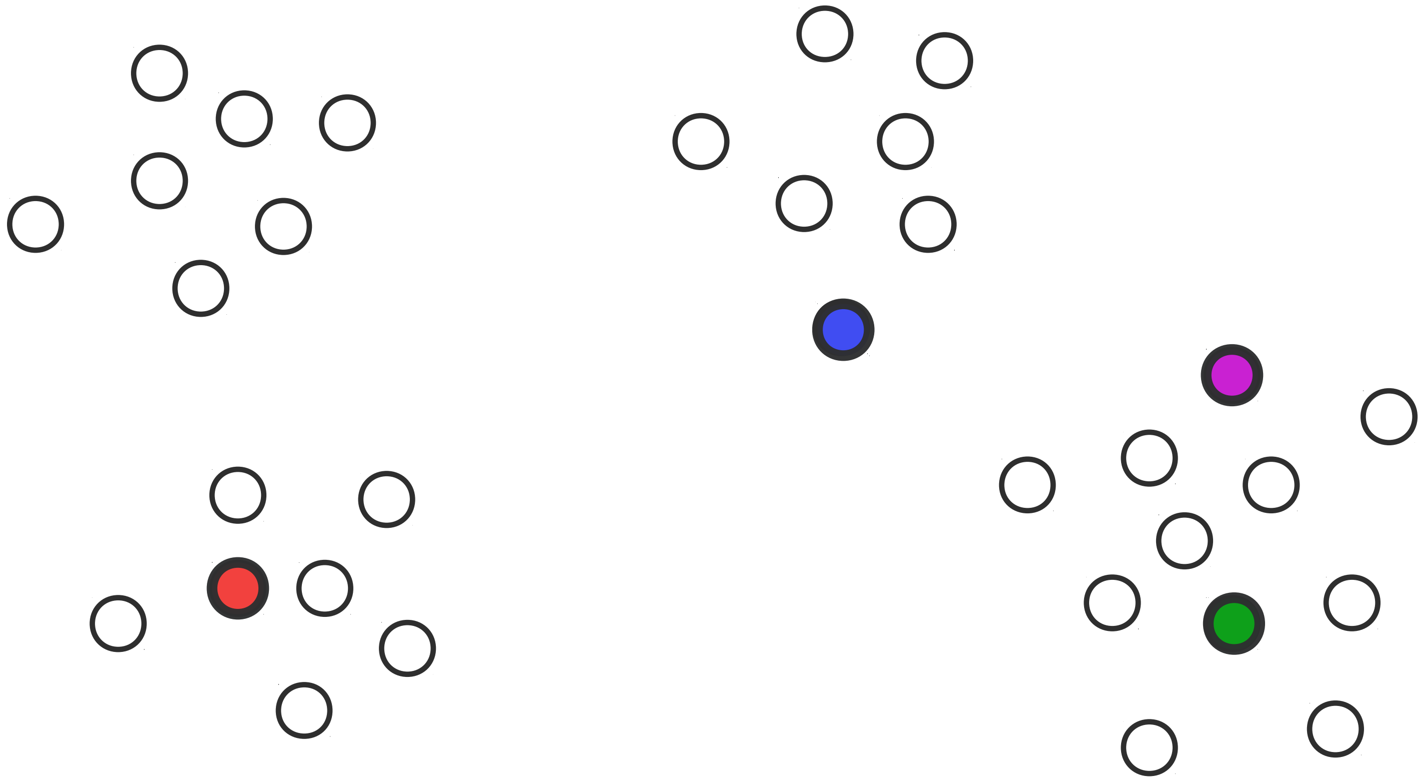
k-means++

David Arthur and Sergei Vassilvitskii

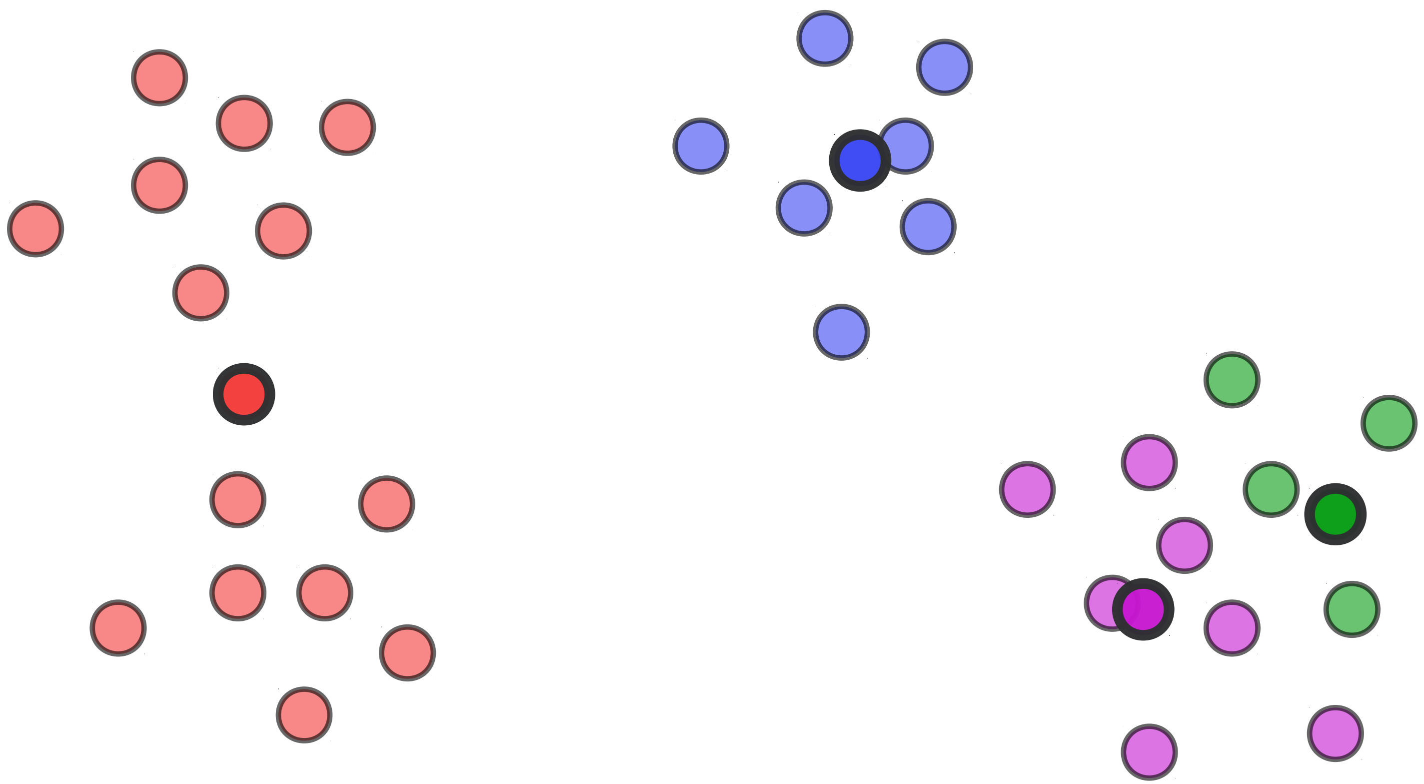
k-means++: The advantages of careful seeding

SODA 2007

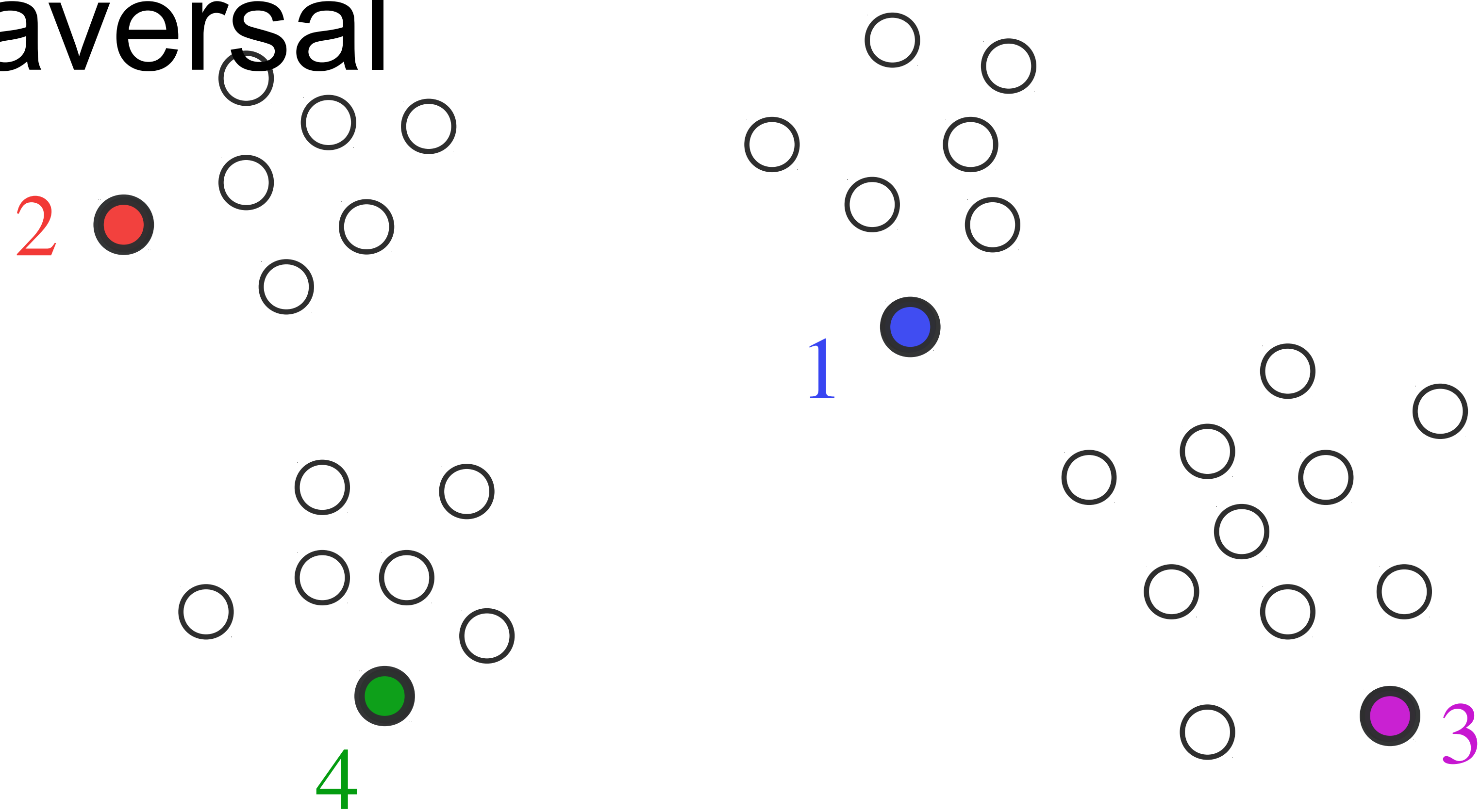
k-means algorithm: random initialization



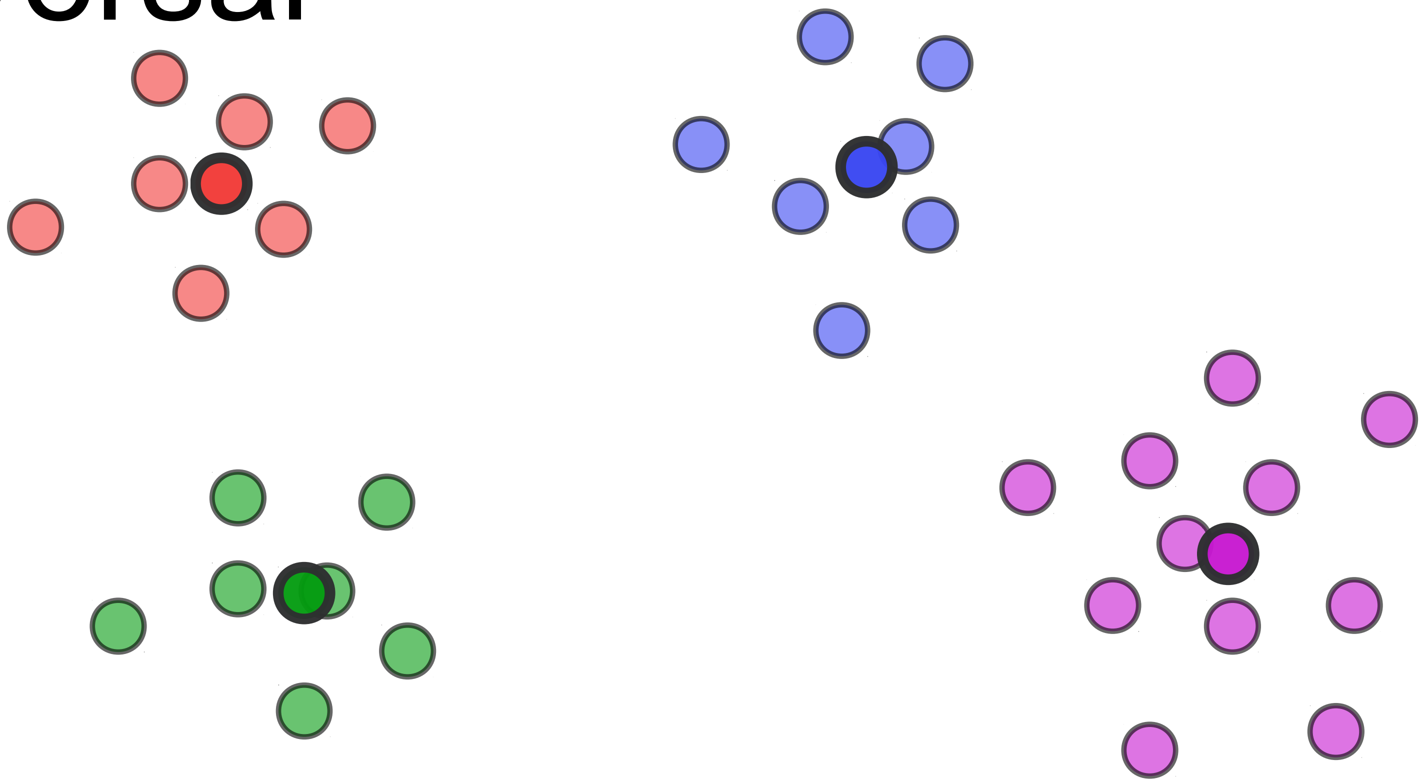
k-means algorithm: random initialization



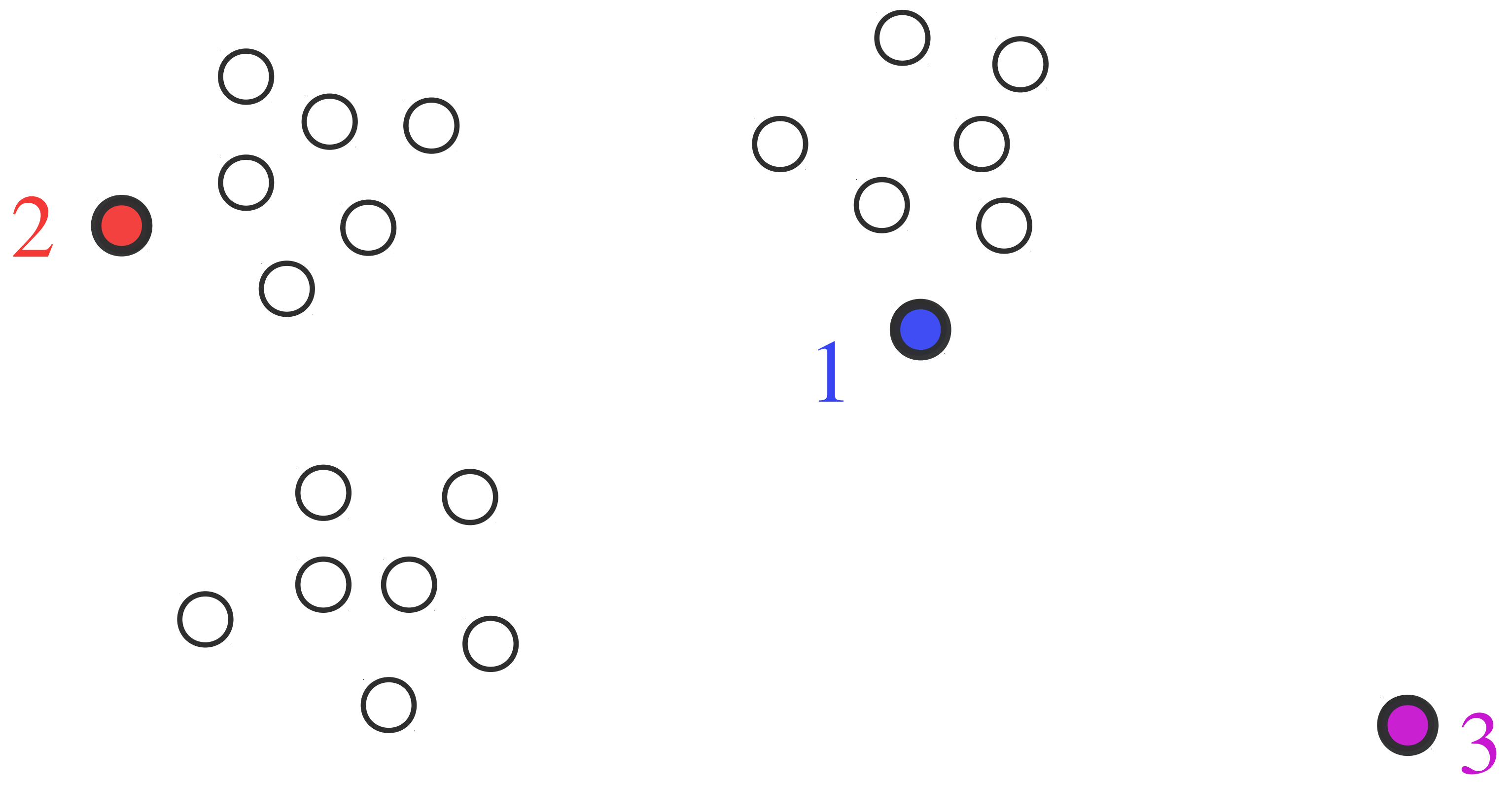
k-means algorithm: initialization with further-first traversal



k-means algorithm: initialization with further-first traversal



but... sensitive to outliers



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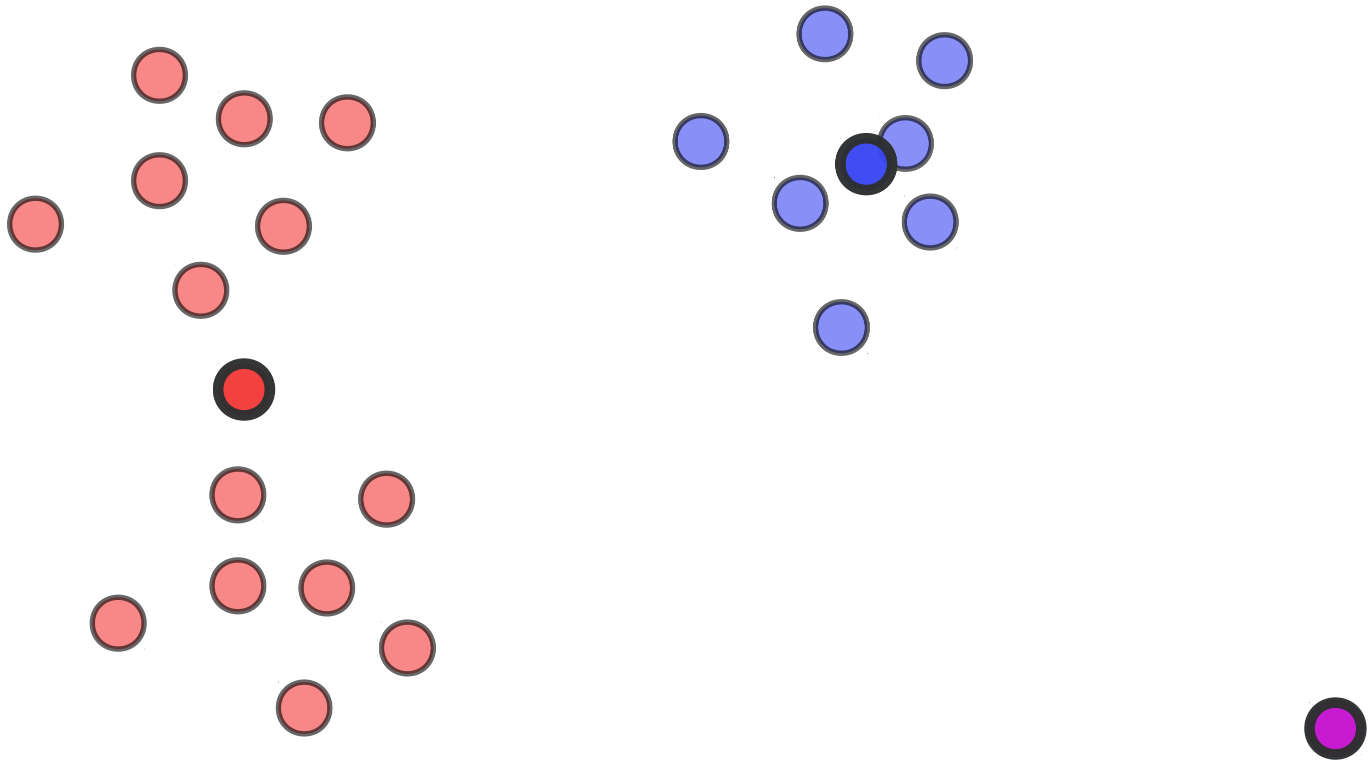
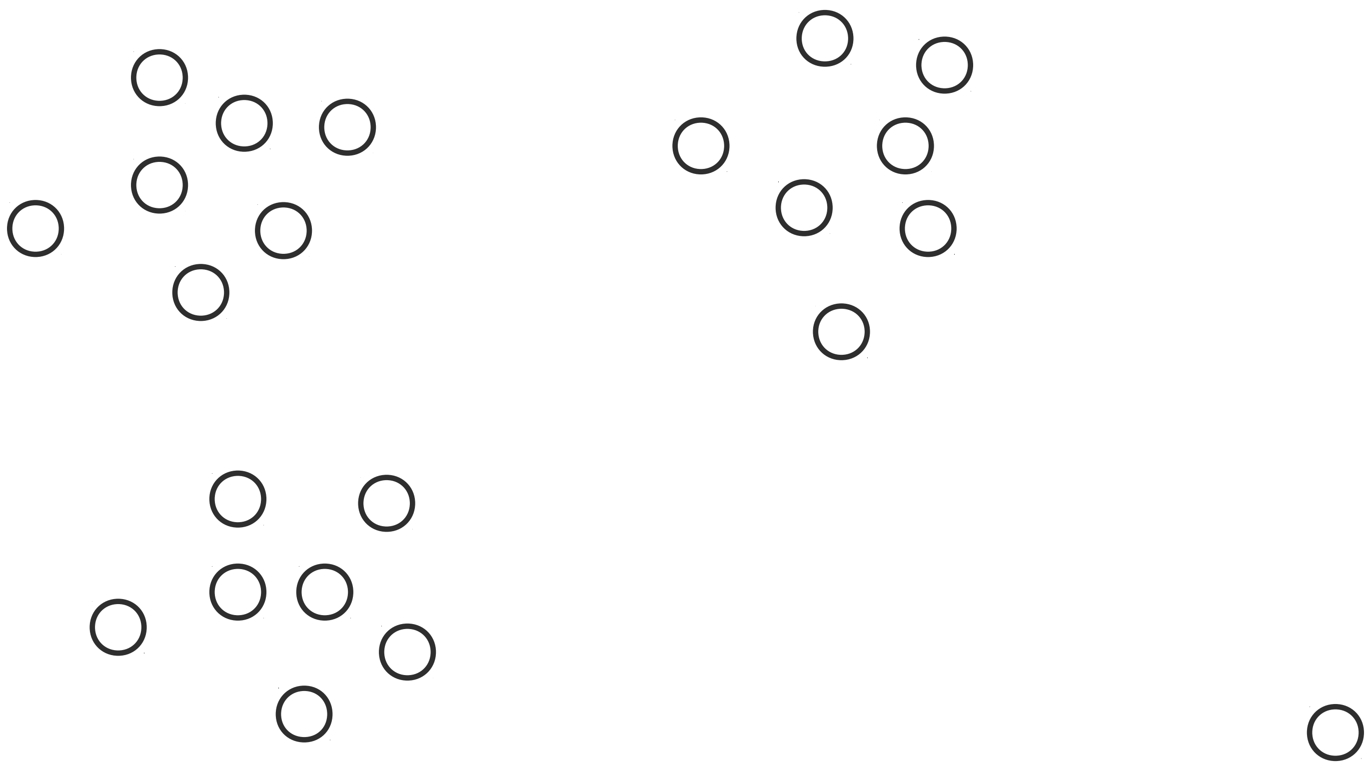


Here random may work well



k-means++ algorithm

- interpolate between the two methods
- let $D(x)$ be the distance between x and the nearest center selected so far
- choose next center with probability proportional to

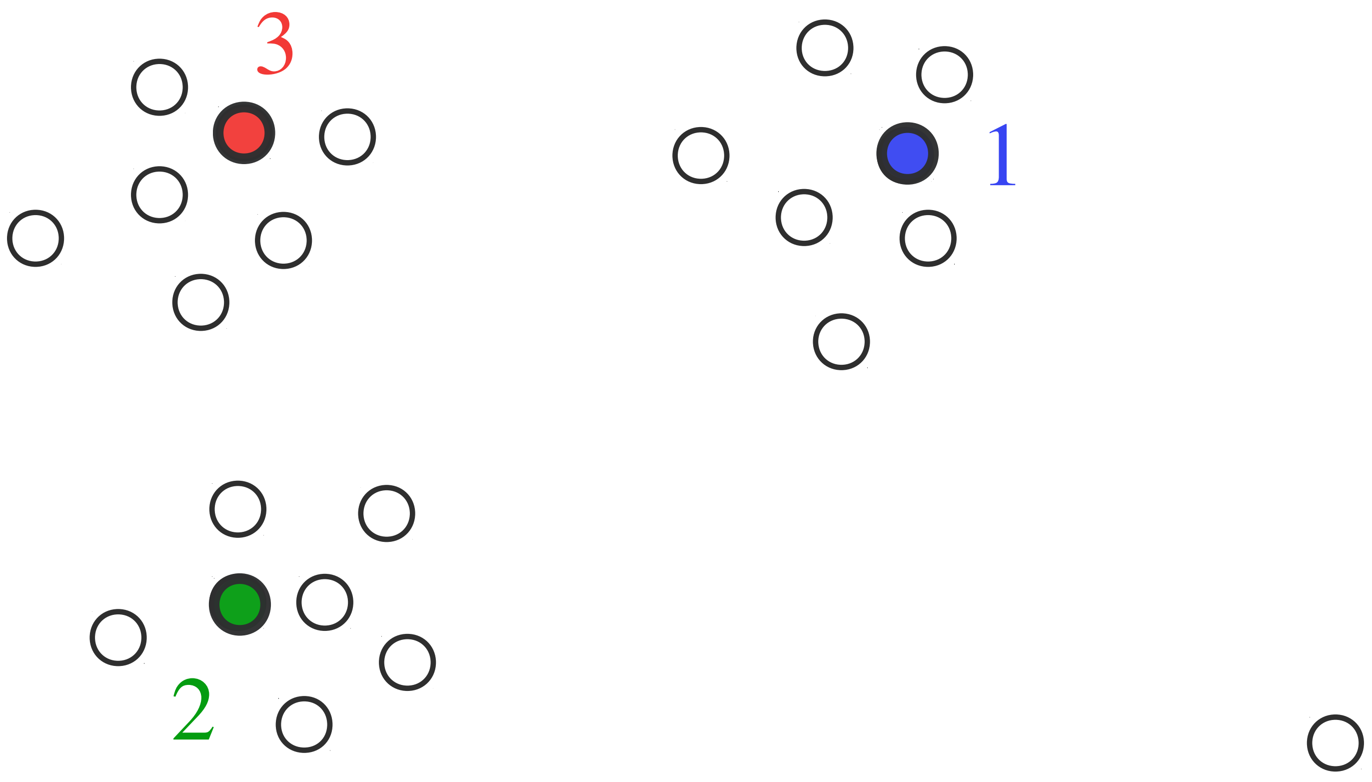
$$(D(x))^a = D^a(x)$$

- $a = 0$ random initialization
- $a = \infty$ furthest-first traversal
- $a = 2$ k-means++

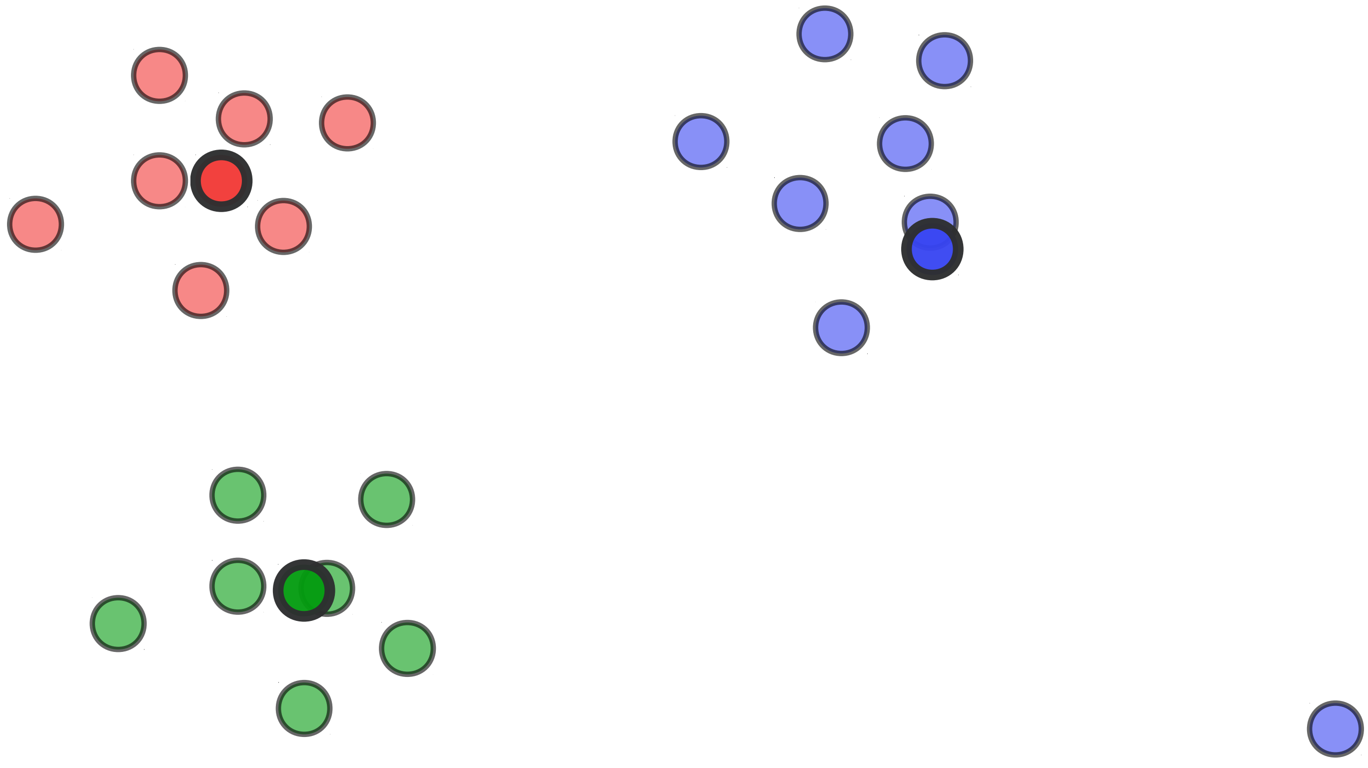
k-means++ algorithm

- initialization phase:
  - choose the first center uniformly at random
  - choose next center with probability proportional to $D^2(x)$
- iteration phase:
  - iterate as in the k-means algorithm until convergence

k-means++ initialization



k-means++ result



k-means++ provable guarantee

- approximation guarantee comes just from the first iteration (initialization)
- subsequent iterations can only improve cost

Lesson learned

- no reason to use k-means and not k-means++

- k-means++ :
  - easy to implement
  - provable guarantee
  - works well in practice

k-means--

- Algorithm 4.1 in [Chawla & Gionis SDM 2013]