K-MEANS CLUSTERING

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Clustering: super quick intro

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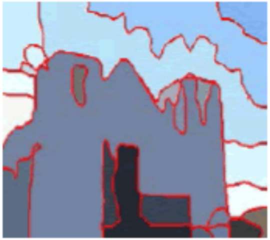
Unlike many basic computational problems (sorting, compression, ...), clustering is very **vague** and **underspecified**:

- how do we represent objects?
- what does "similar" mean?
- how many clusters should we form?
- how to measure the quality of a cluster?

Examples

Examples



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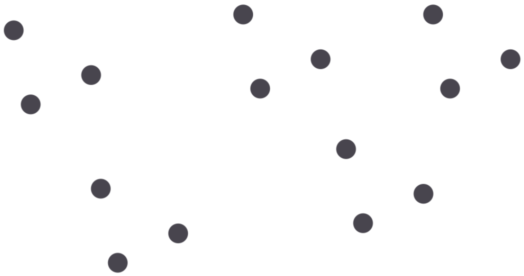
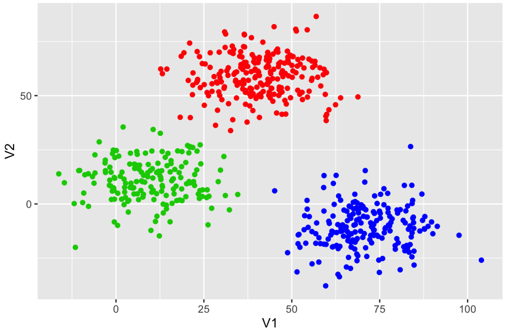


Today we will consider clustering of points in $\mathbb{R}^d$.

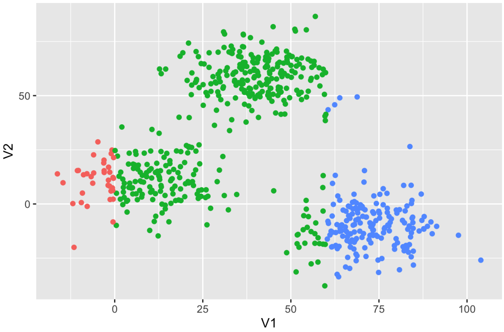
K-means

What does it mean for a clustering to be good?

A "good" clustering



A "bad" clustering



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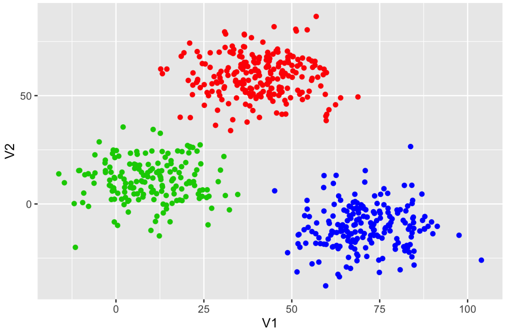

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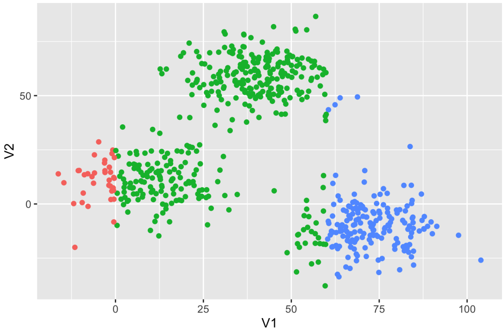


Intuition: a cluster is good if its points are all close to some “central” point.

K-means

Suppose we know k, the number of clusters to be formed.

Given an input set $X \subset \mathbb{R}^d$, we choose k **centers** $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$.
(Note: we are free to choose the centers anywhere — they need not be in X).

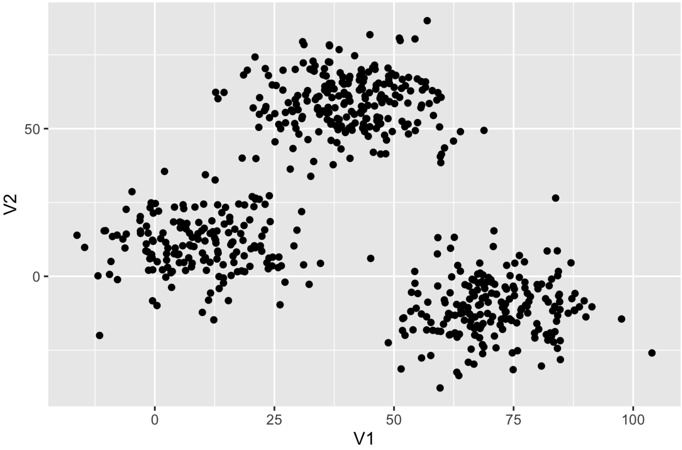
We assign every point $\boldsymbol{x} \in X$ to the closest center among $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$.

We pay the cost:

$$\phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k) = \sum_{\boldsymbol{x} \in X} \min_{j=1}^{k} \|\boldsymbol{x} - \boldsymbol{c}_j\|_2^2$$

That is, each point pays the squared distance to its center.

Example with k=3



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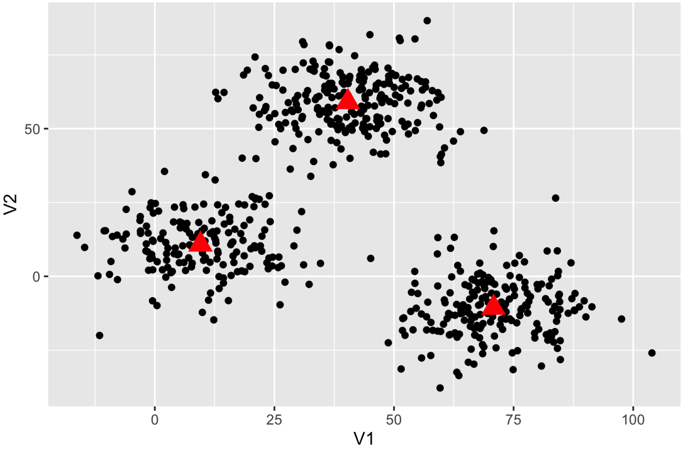

$$c_1 = (40, 59)$$
$$c_2 = (10, 11)$$
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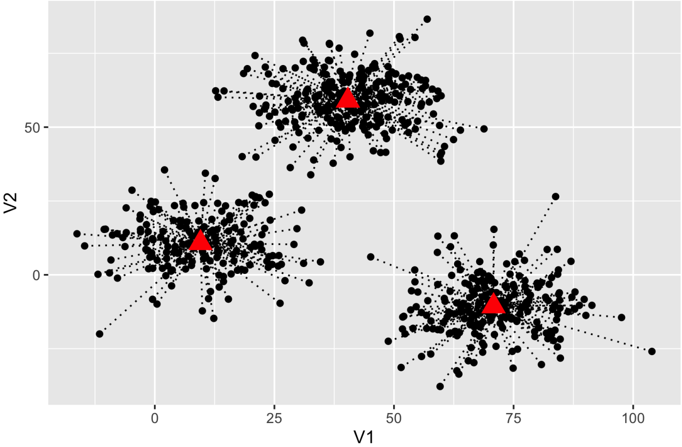

$$c_1 = (40, 59)$$
$$c_2 = (10, 11)$$
$$c_3 = (71, -11)$$

$$\phi(c_1, c_2, c_3) = 121368.6$$

K-means

Each choice of centers $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ identifies a clustering $\mathcal{C} = (C_1, \ldots, C_k)$:

$$C_i = \{x \in X : d(x, c_i) < d(x, c_j) \, \forall j \neq i\}$$

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The **optimal k-means clustering**, denoted by $\mathcal{C}^{OPT}$, is the one given by the centers that minimize ϕ,

$$\boldsymbol{c}_1^{OPT}, \ldots, \boldsymbol{c}_k^{OPT} = \arg \min_{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k} \phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k)$$

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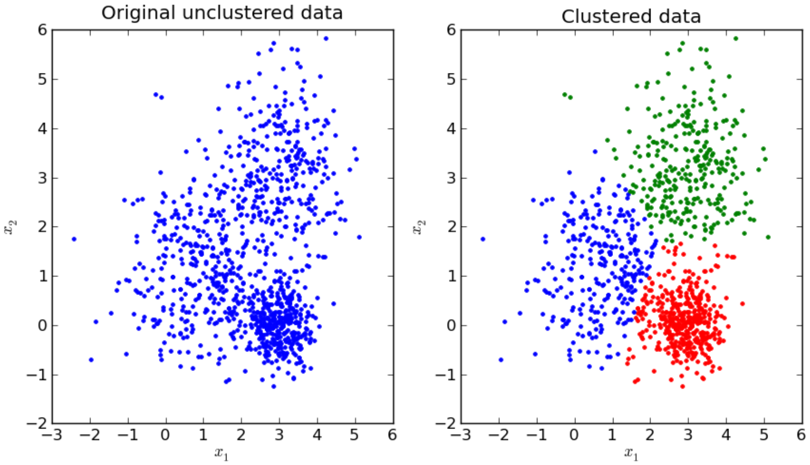
So, the k-means problem is: given X, compute $\mathcal{C}^{OPT}$.

K-means examples



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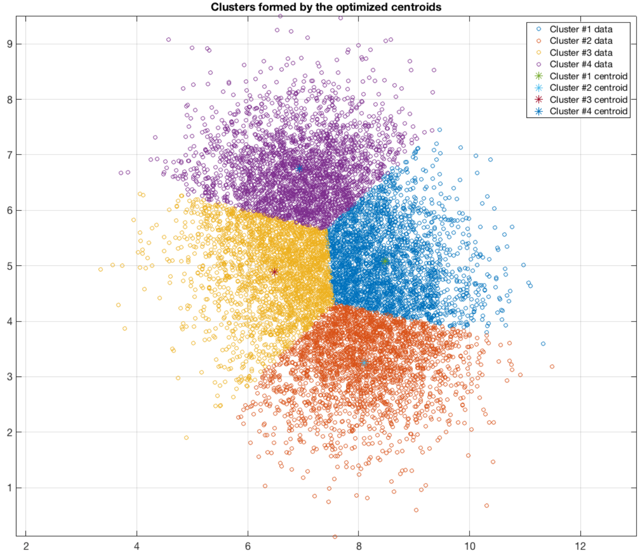
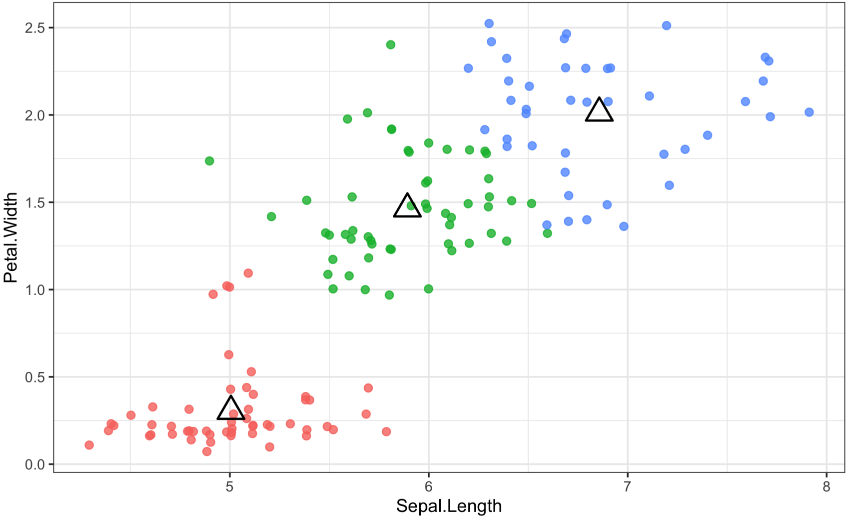


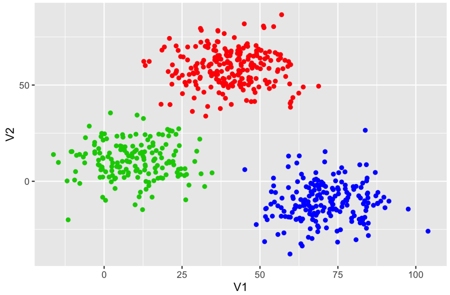
K-means examples



Beware of the dimensionality!

When $d = 2$ or $d = 3$, finding the k-means solution looks easy, because the human eye is good at it. This is not the case when $d \gg 1$.

$d = 2$



$d = 11$

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	0	3	1
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	0	3	4
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	0	4	2
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	0	4	2
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	0	4	4
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	0	4	4
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	0	3	3
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	0	3	3

How to solve k-means?

Dumb approach: exhaustive enumeration.

Running time:

$$T \leq \tag{1}$$

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k-means is NP-hard (Aloise et al., 2009).

Interlude: distances

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Consider 10 points at distance 1 from the center:

$$\phi = 10 \times 1^2 = 10$$

versus 1 point at distance 10 from the center:

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Consider 10 points at distance 1 from the center:

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versus 1 point at distance 10 from the center:

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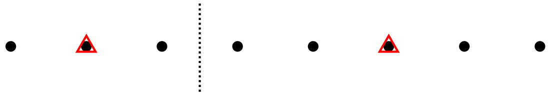
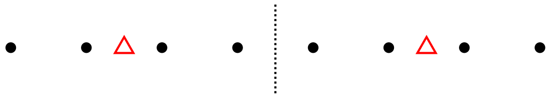
It's like progressive taxes: the farther from the center you are, the more (in proportion) you pay. This tends to give "round" clusters with points roughly equally close to the center.

Example

$X = \{1, \ldots, 8\} \subset \mathbb{R}$, $k = 2$



$\boldsymbol{c}_1 = (2, 0), \quad \boldsymbol{c}_2 = (6, 0)$



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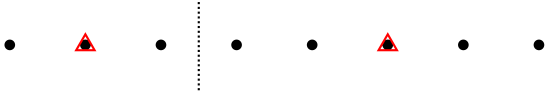
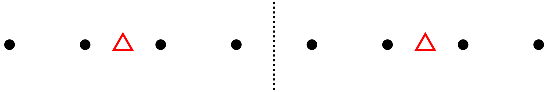


$\boldsymbol{c}_1 = (2, 0)$, $\boldsymbol{c}_2 = (6, 0)$

$\sum_{\boldsymbol{x} \in X} \min_{j=1}^{k} \|\boldsymbol{x} - \boldsymbol{c}_j\|_2 = (1 + 1) + (2 + 1 + 1 + 2) = 8$



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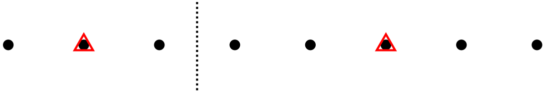

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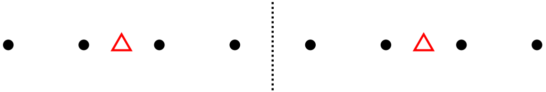
$\sum_{\boldsymbol{x} \in X} \min_{j=1}^{k} \|\boldsymbol{x} - \boldsymbol{c}_j\|_2^2 = (1 + 1) + (4 + 1 + 1 + 4) = 12$



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$\sum_{\boldsymbol{x} \in X} \min_{j=1}^{k} \|\boldsymbol{x} - \boldsymbol{c}_j\|_2^2 = (1.5^2 + 0.5^2 + 0.5^2 + 1.5^2) \cdot 2 = 10 \ \leftarrow$ **k-means**

Lloyd's algorithm

The main and most used k-means algorithm: Lloyd's algorithm.

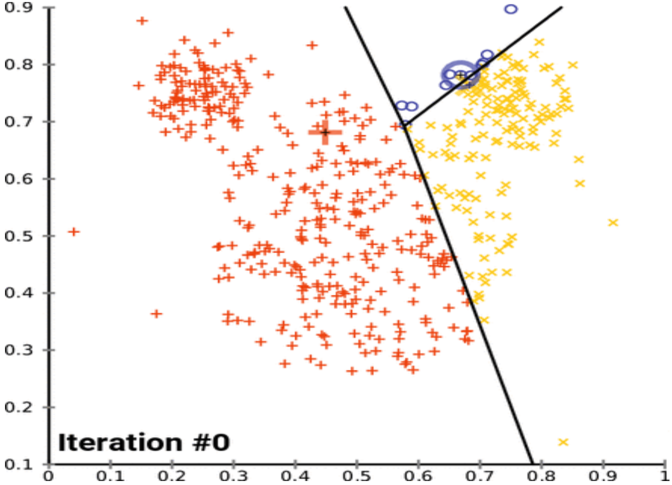
(Very often, by "k-means" people actually mean Lloyd's algorithm.)

Algorithm 1: Lloyd(X, k)

---

choose k distinct points $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ u.a.r. from X;
do
  for $i = 1, \ldots, k$ let $C_i =$ the set of points closest to $\boldsymbol{c}_i$;
  for $i = 1, \ldots, k$ let $\boldsymbol{c}_i =$ the center of mass of C_i;
until $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ *do not change*;
return $C_1, \ldots, C_k$;

Lloyd's algorithm



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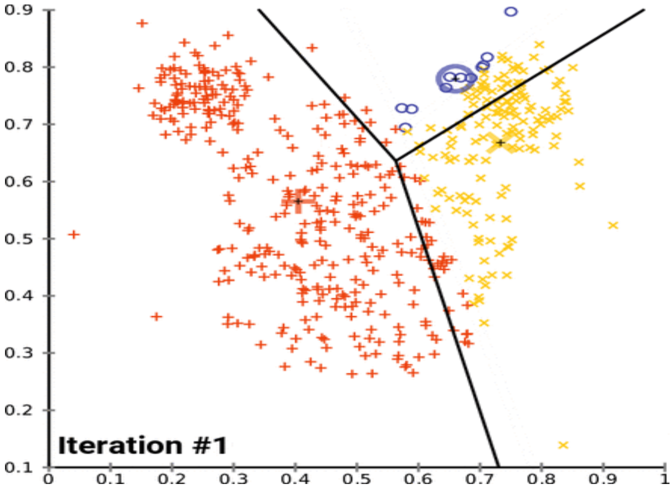

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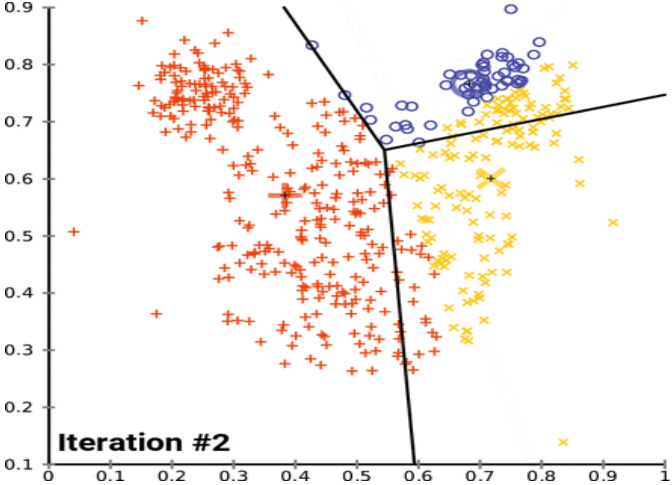

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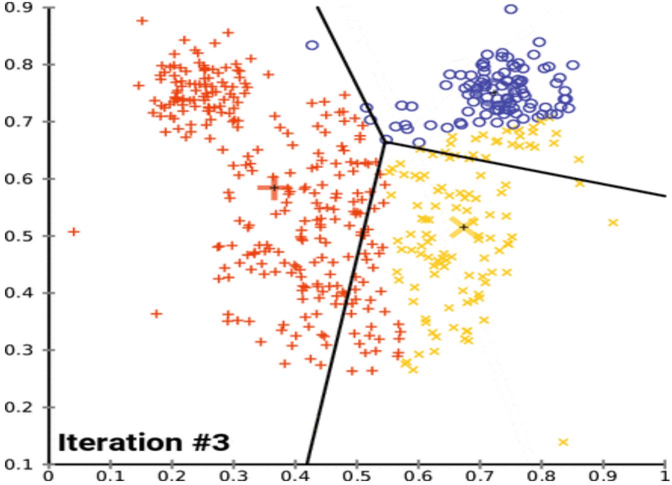

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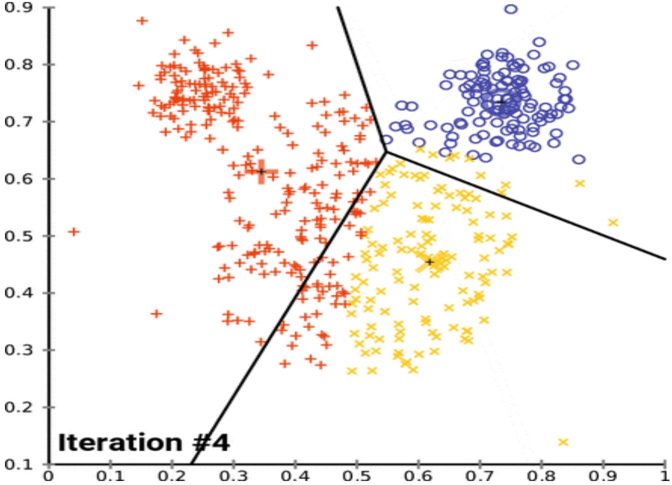

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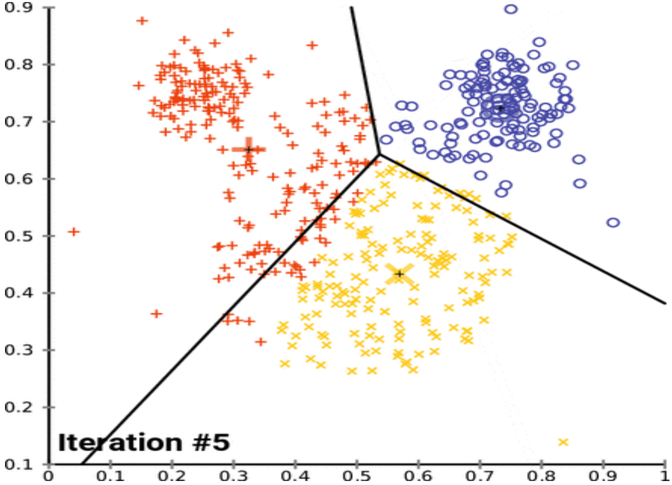

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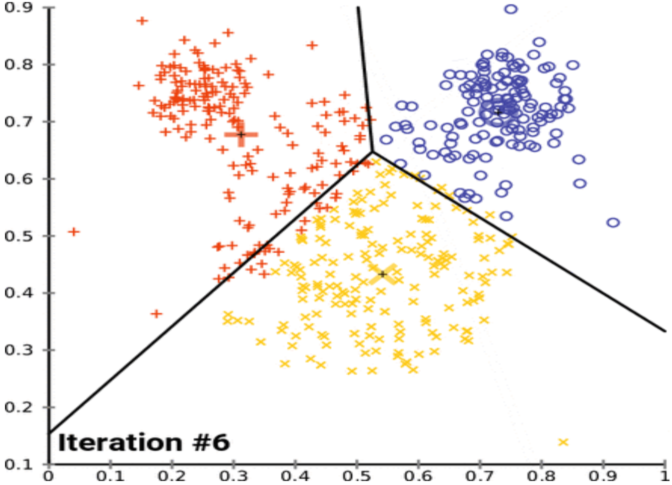

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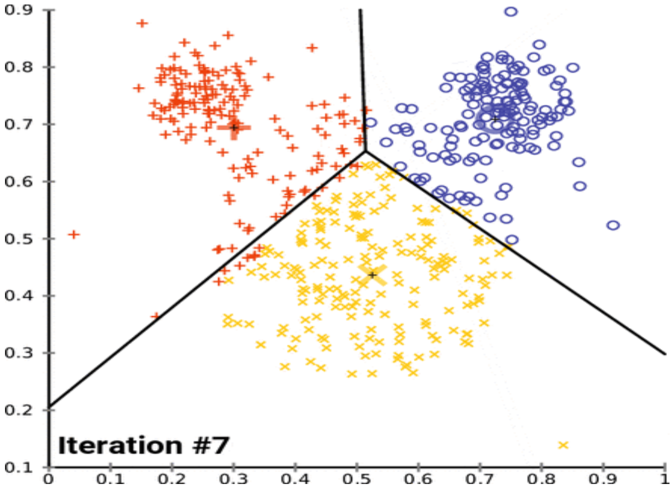

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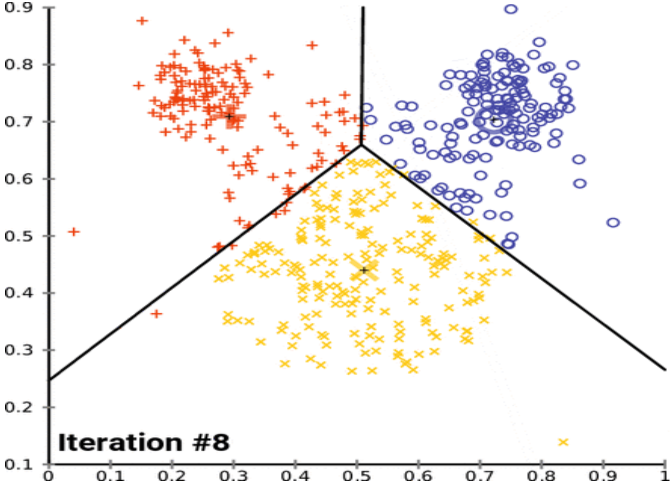

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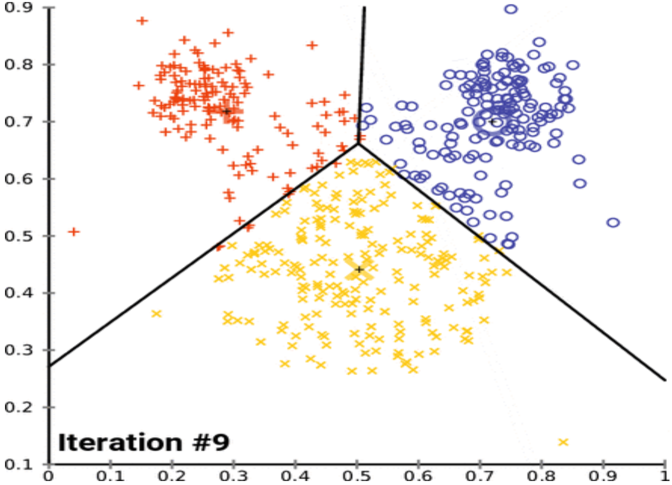

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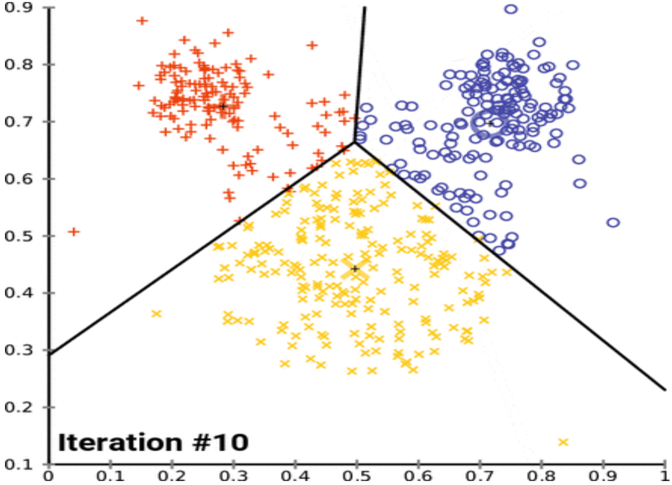

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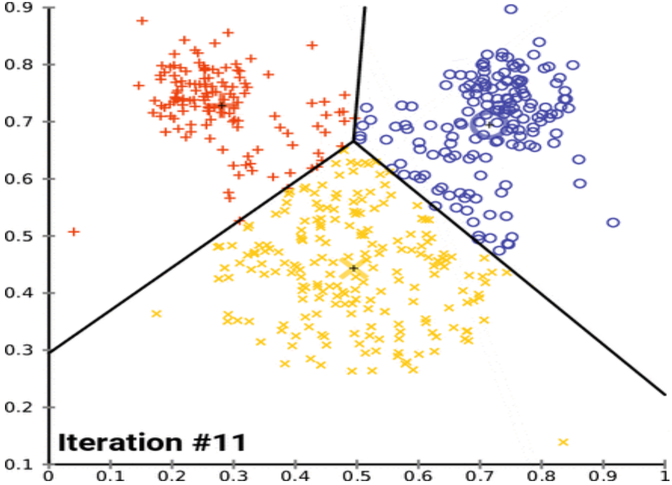

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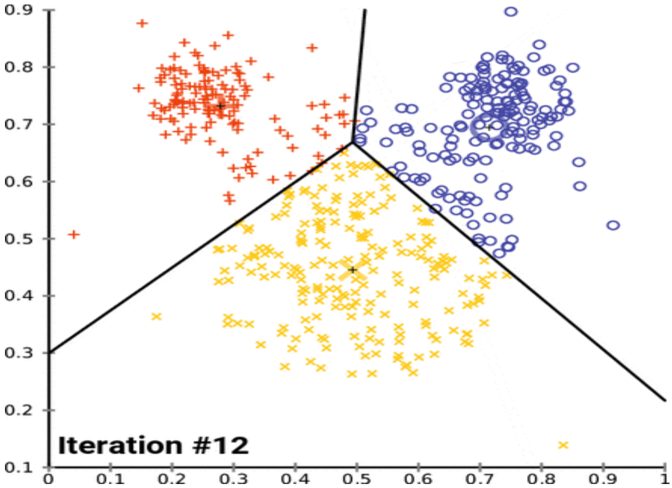

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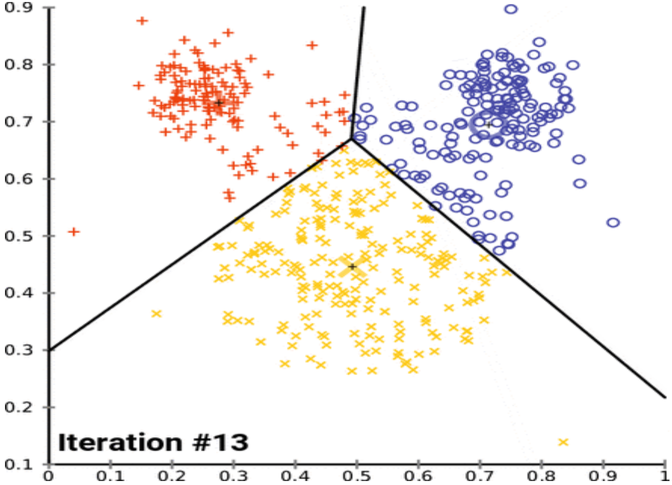

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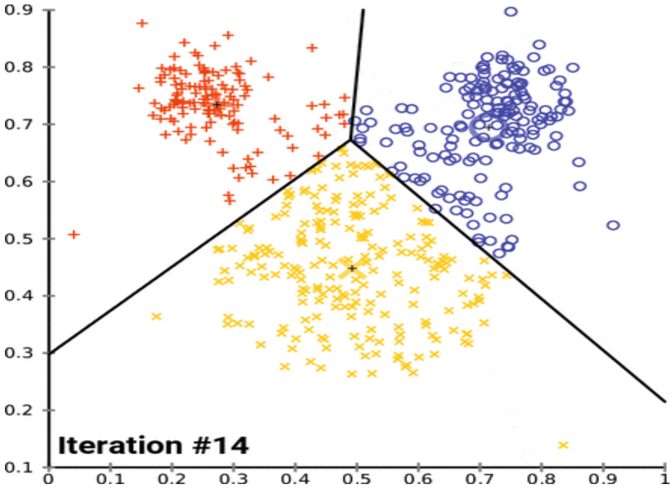

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- Does it have good running time? **NO**
- Why is it so used? It works well in practice

Lloyd's algorithm

Claim: for any constant $a \geq 1$ (say, $a = 1000000$) there are instances on which Lloyd's algorithm, with probability $1 - O(n^{-1})$, returns a clustering $\mathcal{C}$ such that

$$\phi(\mathcal{C}) \geq a \cdot \phi(\mathcal{C}_{OPT}) \tag{2}$$

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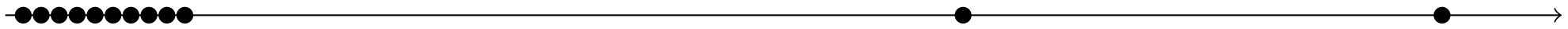
Proof: consider this instance on the real line, with $k = 3$, and X formed by $n - 2$ points in $[0, 1]$ and two "outliers" at $x = 2\sqrt{an}$ and $x = 3\sqrt{an}$:



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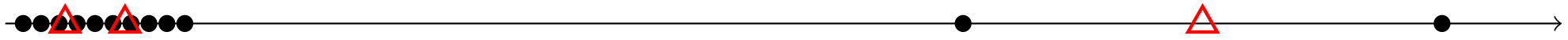

With probability $1 - O(\frac{1}{n})$, Lloyd's draws at most 1 center among the outliers, in which case it ends up $\phi(\mathcal{C}) \geq 2 \cdot (\frac{1}{2}\sqrt{an})^2 > a \cdot \frac{n}{4}$.

However, $\phi(\mathcal{C}_{OPT}) \leq (\frac{1}{2})^2 \cdot n = \frac{n}{4}$ (check it!).

Lloyd's algorithm

Claim: the worst-case running time of Lloyd's algorithm is $2^{\Omega(\sqrt{n})}$.

Proof: see Arthur and Vassilvitskii, *How slow is the k-means method?* , Symposium on Computational Geometry, 2006. `https://doi.org/10.1145/1137856.1137880`.

Lloyd's algorithm

Does it even converge?

Back to k-means

Fundamental fact.

Let $C \subset \mathbb{R}^d$ be a finite set of points, and let $\boldsymbol{\mu}$ be its center of mass:

$$\boldsymbol{\mu} = \frac{1}{|C|} \sum_{\boldsymbol{x} \in C} \boldsymbol{x}$$

Then, for any point $\boldsymbol{c} \in \mathbb{R}^d$, we have the identity:

$$\sum_{\boldsymbol{x} \in C} \|\boldsymbol{x} - \boldsymbol{c}\|_2^2 = \sum_{\boldsymbol{x} \in C} \|\boldsymbol{x} - \boldsymbol{\mu}\|_2^2 \ + \ |C| \cdot \|\boldsymbol{c} - \boldsymbol{\mu}\|_2^2$$

Lloyd's algorithm always terminates

Theorem. Lloyd's algorithm always terminates.

Proof stategy: We show that, if the centers are moved, then ϕ decreases *strictly*, and it can do so at most k^n times (the number of possible clusterings).

Lloyd's algorithm always terminates

Claim. In any given iteration, if some center is moved, then ϕ decreases strictly.

Proof. Recall the two steps of the iteration:

for $i = 1, \ldots, k$ *let* $C_i =$ *the set of points closest to* $\boldsymbol{c}_i$
for $i = 1, \ldots, k$ *let* $\boldsymbol{c}_i =$ *the center of mass of* C_i

Denote the state of the algorithm by:

$\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$	$C_1, \ldots, C_k$	at the beginning of the iteration
$\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$	$C'_1, \ldots, C'_k$	after the first step
$\boldsymbol{c}'_1, \ldots, \boldsymbol{c}'_k$	$C'_1, \ldots, C'_k$	after the second step

We denote

$$\phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C_1, \ldots, C_k) = \sum_{i=1}^{k} \sum_{\boldsymbol{x} \in C_i} \|\boldsymbol{x} - \boldsymbol{c}_i\|_2^2 \tag{3}$$

Lloyd's algorithm always terminates

First, we prove:

$$\phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C_1, \ldots, C_k) \geq \phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C'_1, \ldots, C'_k)$$

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This holds since, for a fixed choice of $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$, the partition $C'_1, \ldots, C_k$ minimizes ϕ, since it assigns every point to the nearest center.

Lloyd's algorithm always terminates

Second, we prove that, if $\boldsymbol{c}'_i \neq \boldsymbol{c}_i$ for some i, then:

$$\phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C'_1, \ldots, C'_k) > \phi(\boldsymbol{c}'_1, \ldots, \boldsymbol{c}'_k, C'_1, \ldots, C'_k)$$

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Consider indeed any such i and recall that $\boldsymbol{c}'_i$ is the *center of mass* of C'_i. By the fundamental observation above,

$$\begin{aligned}\sum_{\boldsymbol{x} \in C'_i} \|\boldsymbol{x} - \boldsymbol{c}_i\|_2^2 &= \sum_{\boldsymbol{x} \in C'_i} \|\boldsymbol{x} - \boldsymbol{c}'_i\|_2^2 + |C'_i| \cdot \|\boldsymbol{c}_i - \boldsymbol{c}'_i\|_2^2 \\ &> \sum_{\boldsymbol{x} \in C'_i} \|\boldsymbol{x} - \boldsymbol{c}'_i\|_2^2\end{aligned}$$

Summing over all clusters yields the claim.

Lloyd's algorithm always terminates

So, if some center is moved, we have:

$$\phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C_1, \ldots, C_k) \geq \phi(\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k, C'_1, \ldots, C'_k) > \phi(\boldsymbol{c}'_1, \ldots, \boldsymbol{c}'_k, C'_1, \ldots, C'_k)$$

which means that ϕ decreases strictly.

Lloyd's algorithm always terminates

Finally, we note that ϕ can decrease only a finite number of times.

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First, ϕ is a function of the current clustering $C_1, \ldots, C_k$, which can take on at most k^n distinct values. Thus, if the algorithm did more than k^n iterations, it would go twice over the same clustering. This implies that ϕ takes the same value in two distinct iterations (ignoring the last one). This is absurd since ϕ always decreases.

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This completes the proof of the theorem.

Lloyd's algorithm

How much does one iteration of Lloyd's algorithm take?

Algorithm 2: Lloyd(X, k)

---

choose k distinct points $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ u.a.r. from X;

do

  for $i = 1, \ldots, k$ let C_i = the set of points closest to $\boldsymbol{c}_i$;

  for $i = 1, \ldots, k$ let $\boldsymbol{c}_i$ = the center of mass of C_i;

until $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ *do not change*;

return $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$;

Lloyd's algorithm

How much does one iteration of Lloyd's algorithm take?

Algorithm 3: Lloyd(X, k)

---

choose k distinct points $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ u.a.r. from X;
do

    ~~for $i = 1, \ldots, k$ let C_i = the set of points closest to $\boldsymbol{c}_i$~~;
    for $\boldsymbol{x} \in X$ let $i_x = \arg\min_{i \in [k]} \|\boldsymbol{x} - \boldsymbol{c}_i\|_2^2$;
    for $i = 1, \ldots, k$ let $\boldsymbol{c}_i$ = the center of mass of C_i;

until $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$ *do not change*;
return $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_k$;

$\Rightarrow O(n \cdot k \cdot d)$ per iteration

Recap

k-means

- probably the most popular idea of “clustering”
- formalizes clustering as an optimization problem
- NP-hardness

Lloyd’s algorithm

- unbounded approximation ratio
- worst-case running time $2^{\Omega(n)}$
- but, in practice, it works well