Computational Data Analysis

Machine Learning

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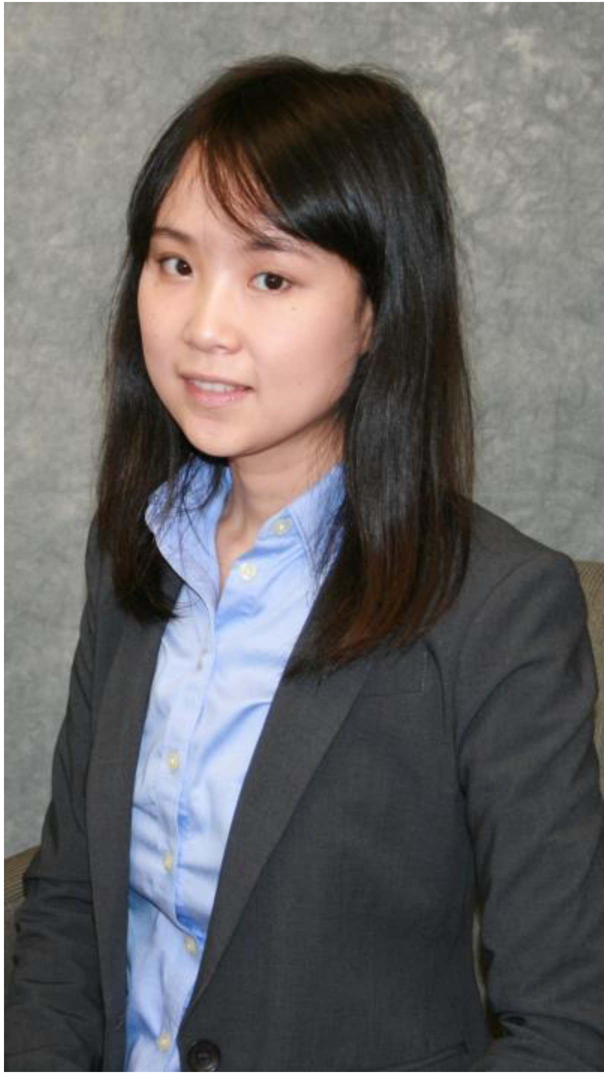
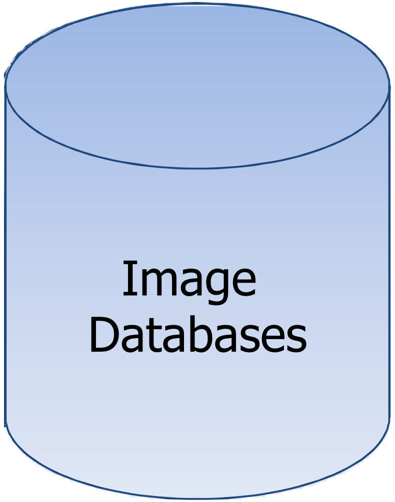
Clustering



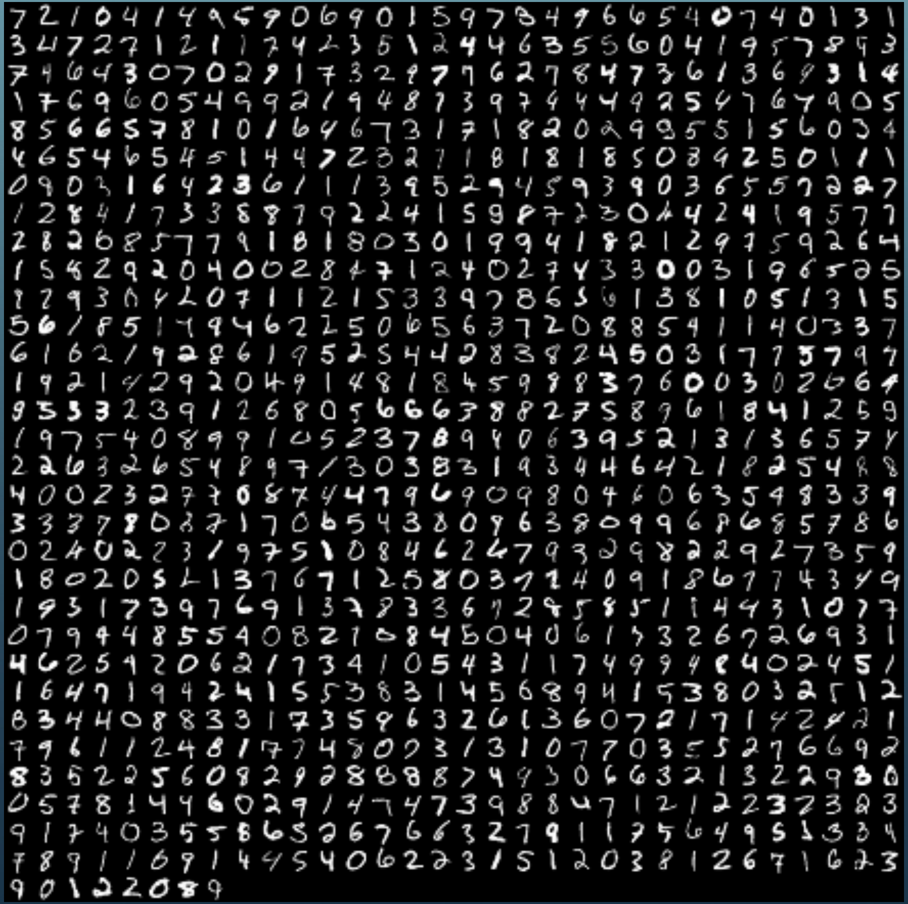
Cluster images



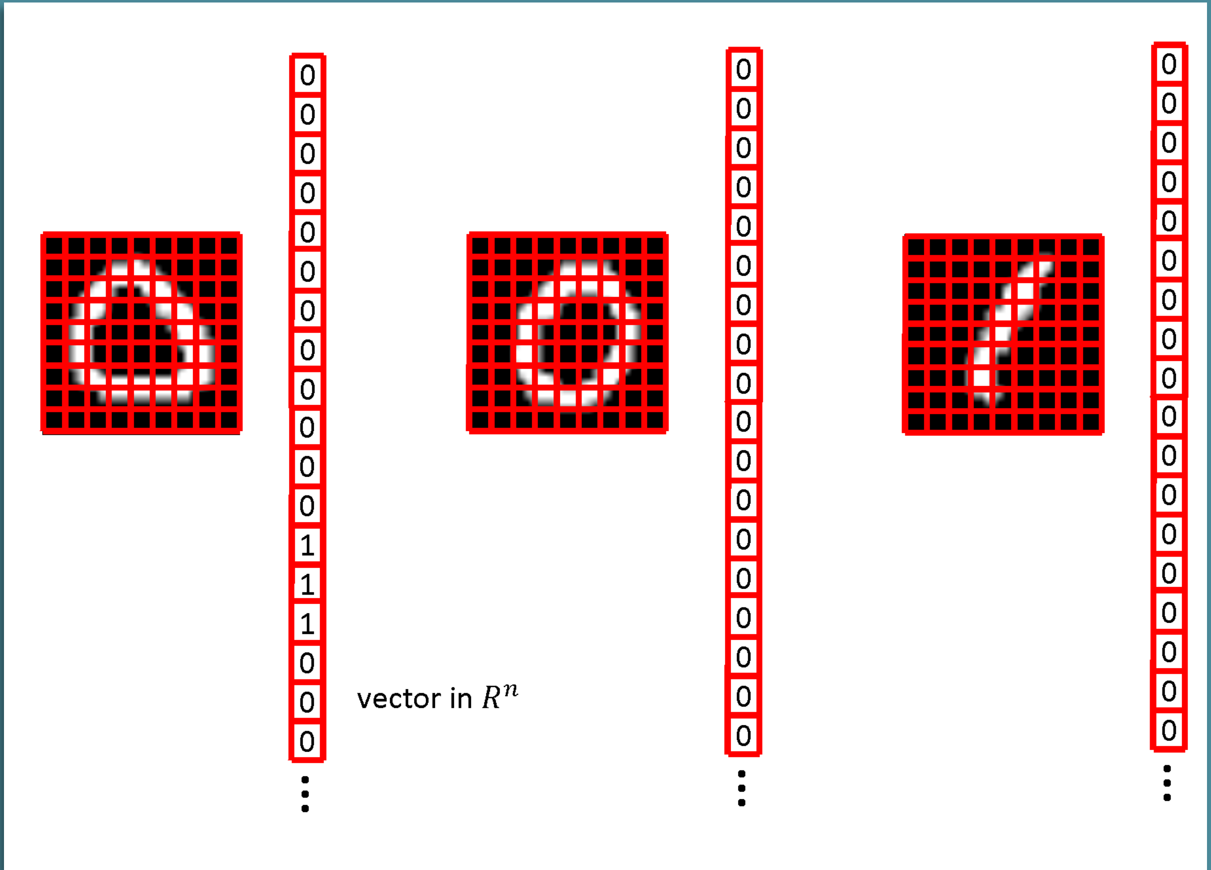
Goal of clustering:

Divide object into groups, and objects within a group are more similar than those outside the group

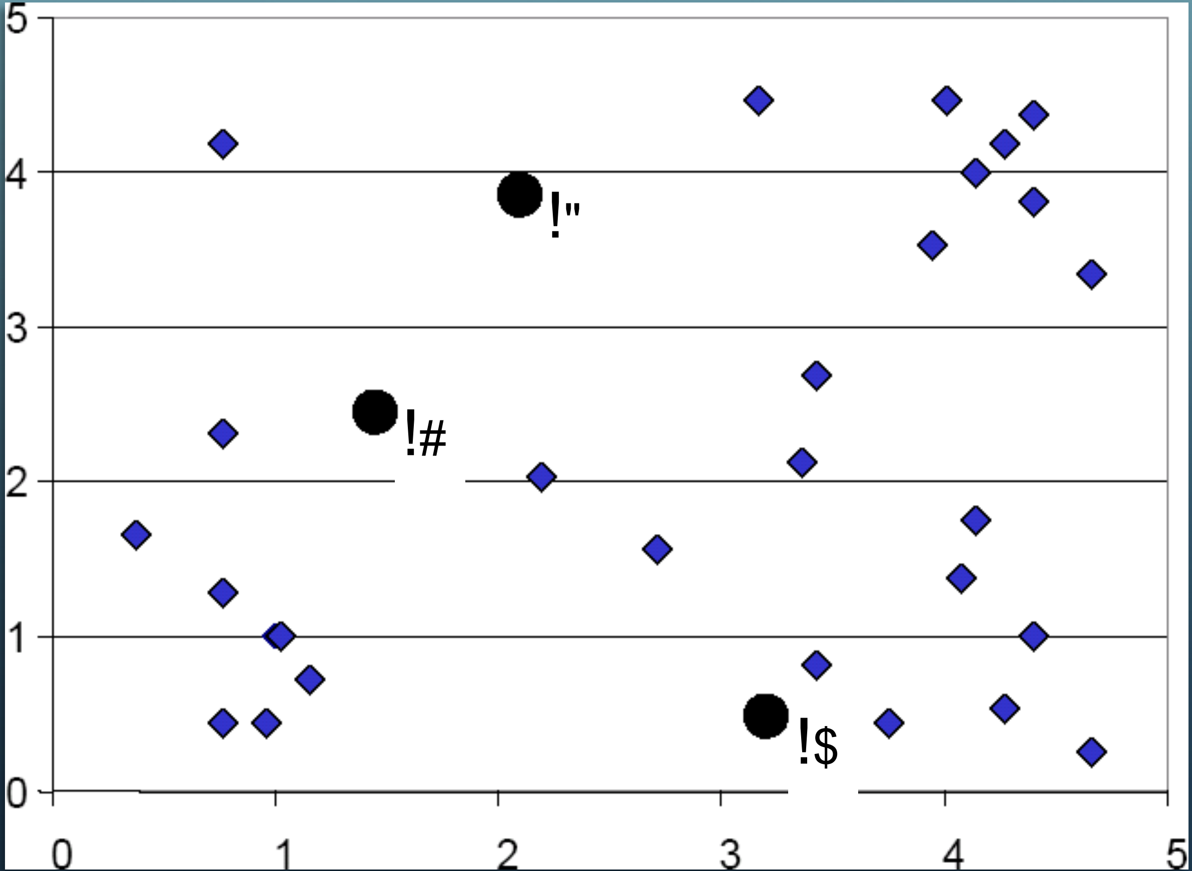
Cluster handwritten digits



How to represent objects?



Before clustering, a bunch of vectors



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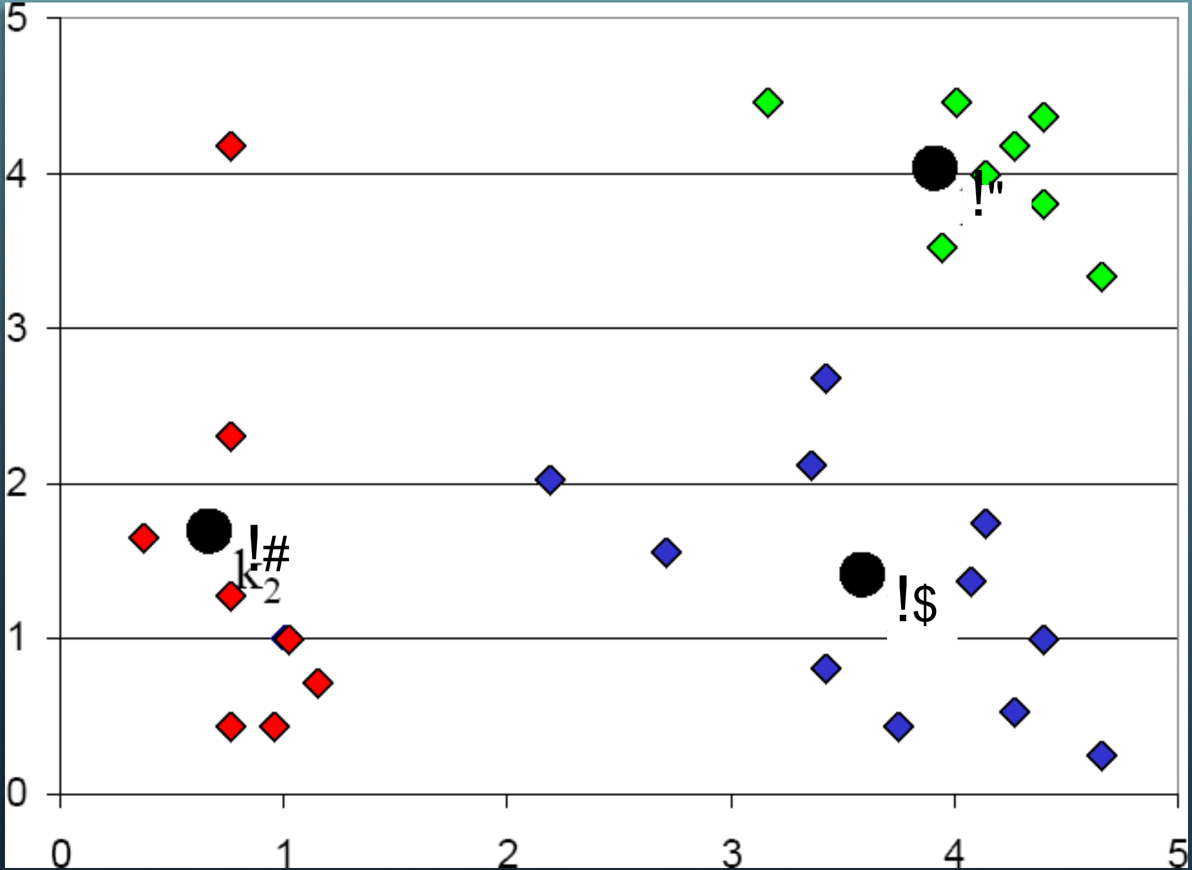
After clustering, group assigned



Formal statement and goal of k-means

- Given m data points, $\{x^1, x^2, \dots x^m\} \in R^n$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^n$
- And assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$

Superscript: index for variables (e.g., sample, cluster index)

Sample size: m number of clusters: k
Dimension of each sample: n

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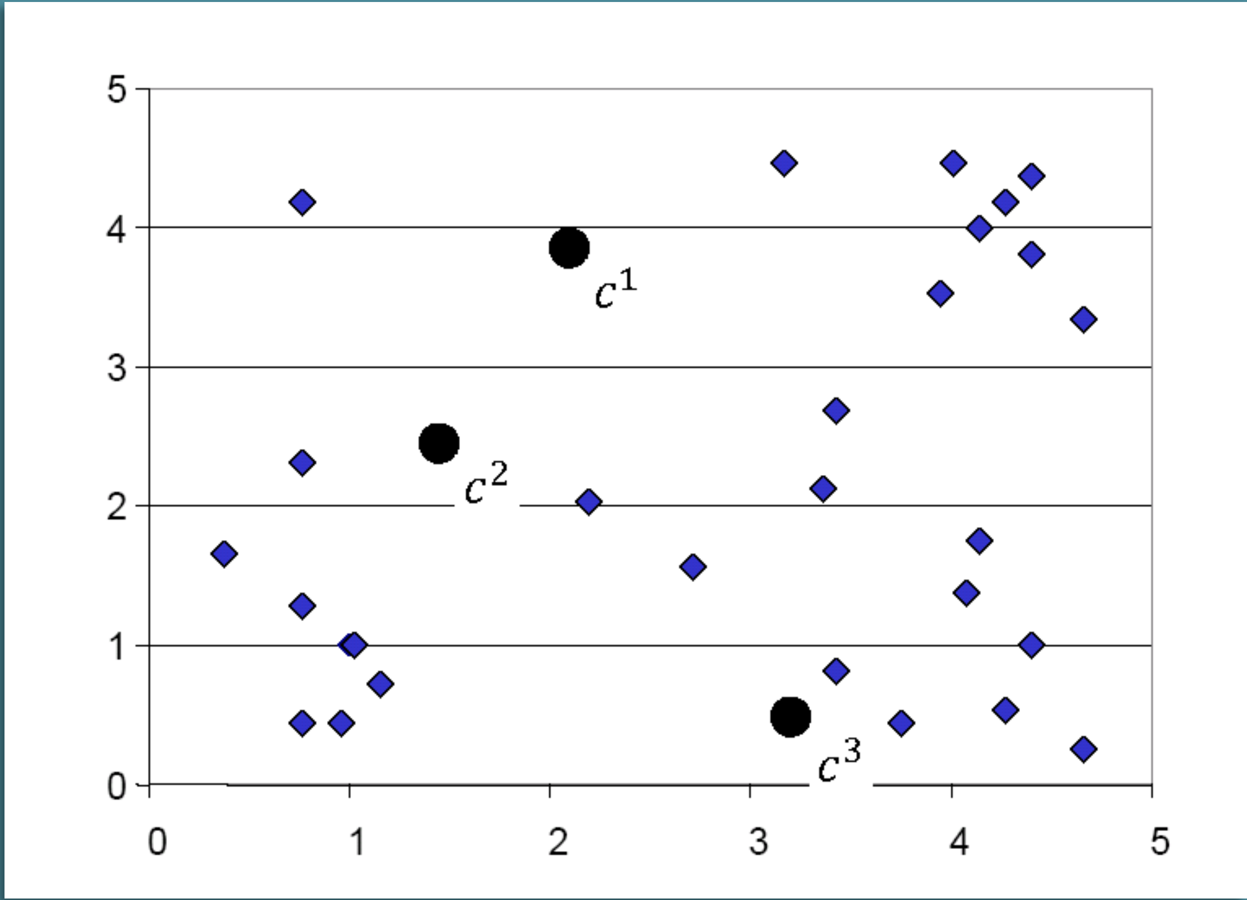
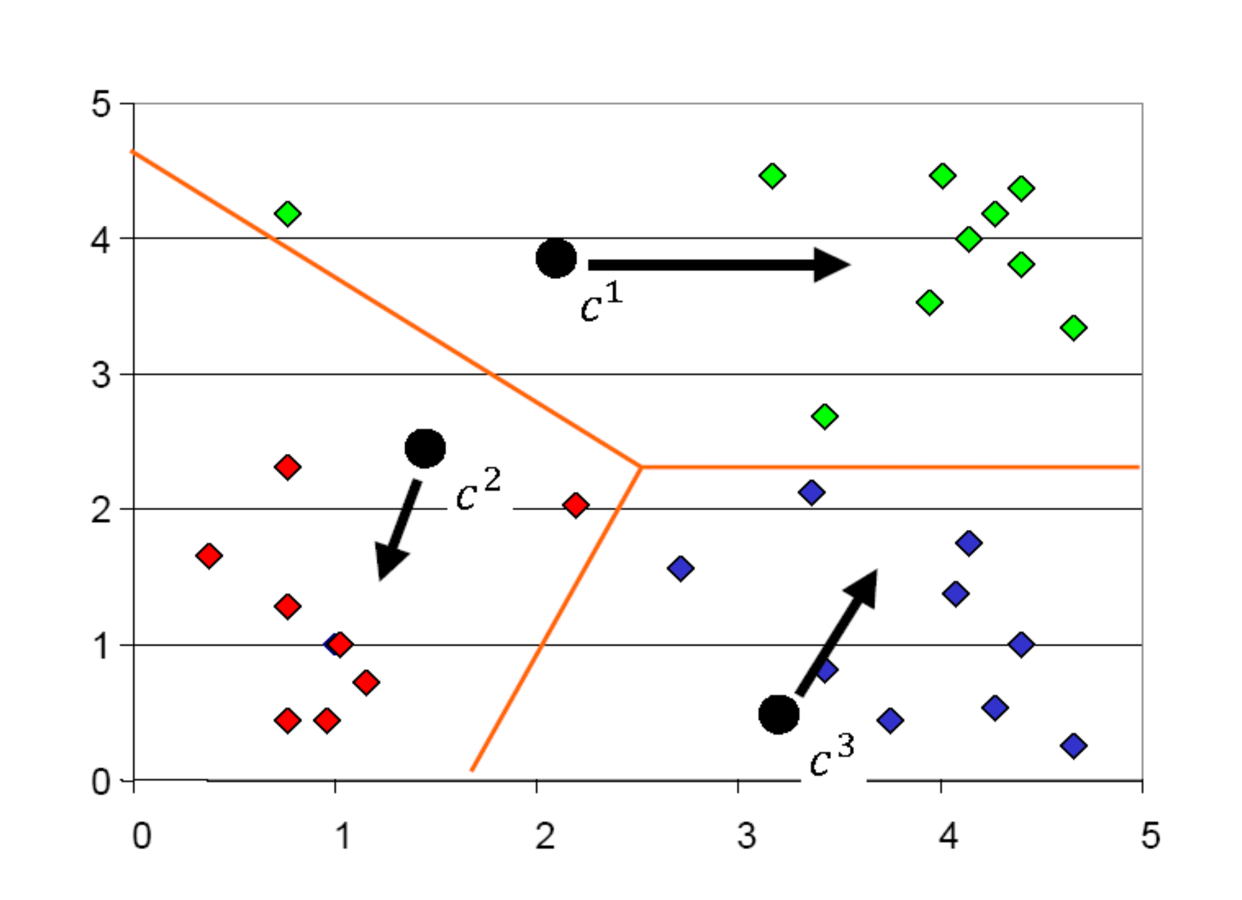
K-means algorithm

- Initialize k cluster centers, $\{c^1, c^2, \ldots, c^k\}$, randomly
- Do
  - Decide the cluster memberships of each data point, x^i, by assigning it to the nearest cluster center (cluster assignment)
  $$\pi(i) = argmin_{j=1,\ldots,k} \left\|x^i - c^j\right\|^2$$
  - Adjust the cluster centers (center adjustment)
  $$c^j = \frac{1}{|\{i : \pi(i) = j\}|} \sum_{i:\pi(i)=j} x^i$$
- While any cluster center has been changed

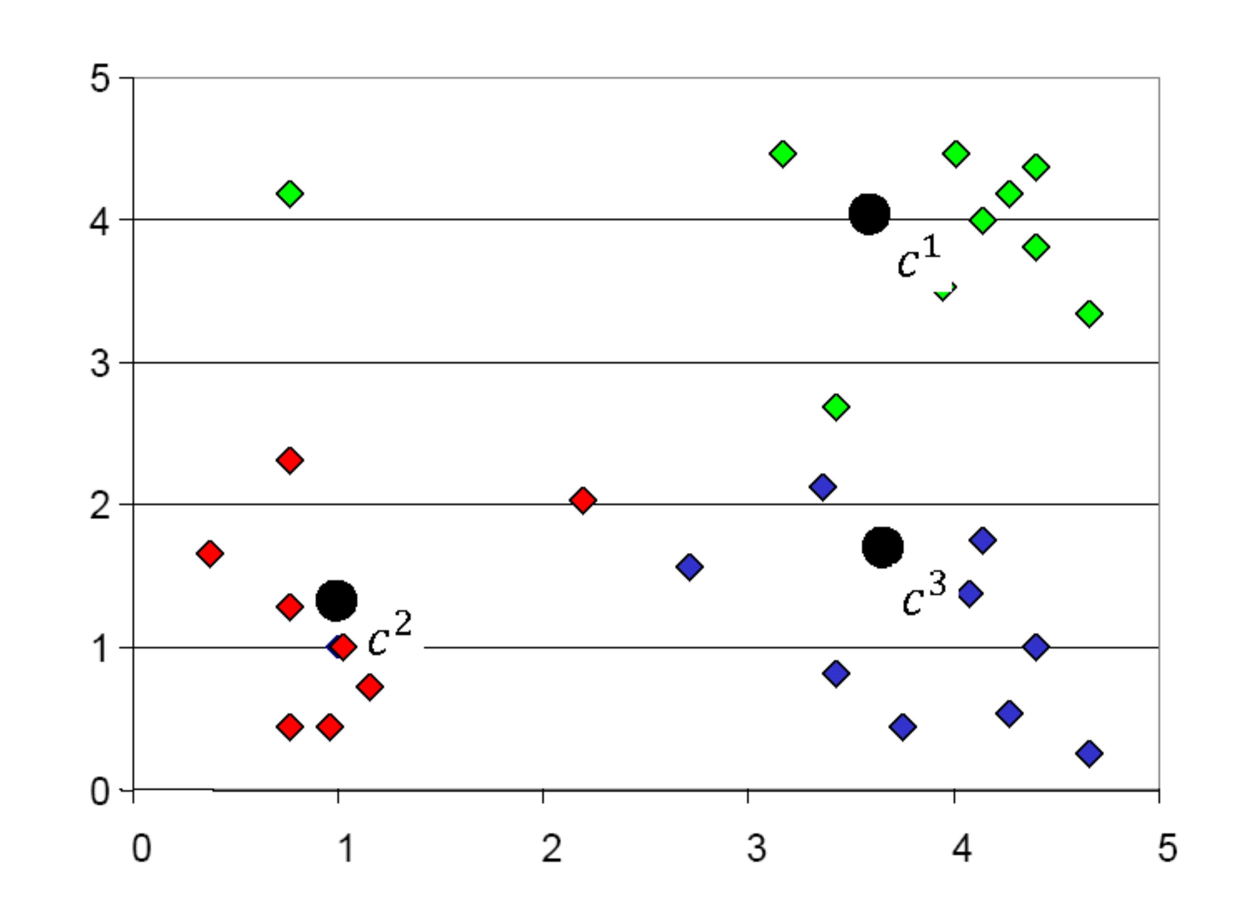
K-means: step 1



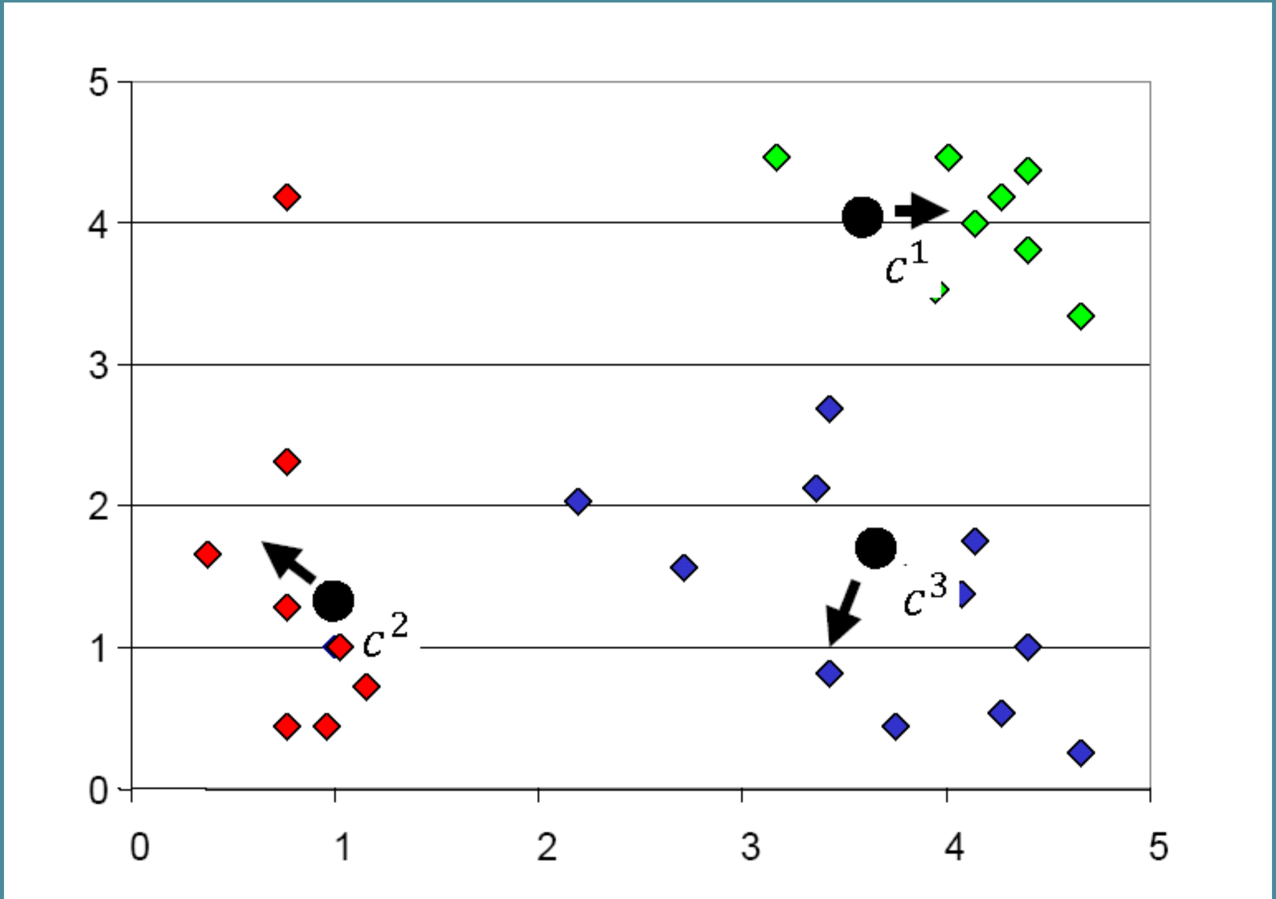
K-means: step 2



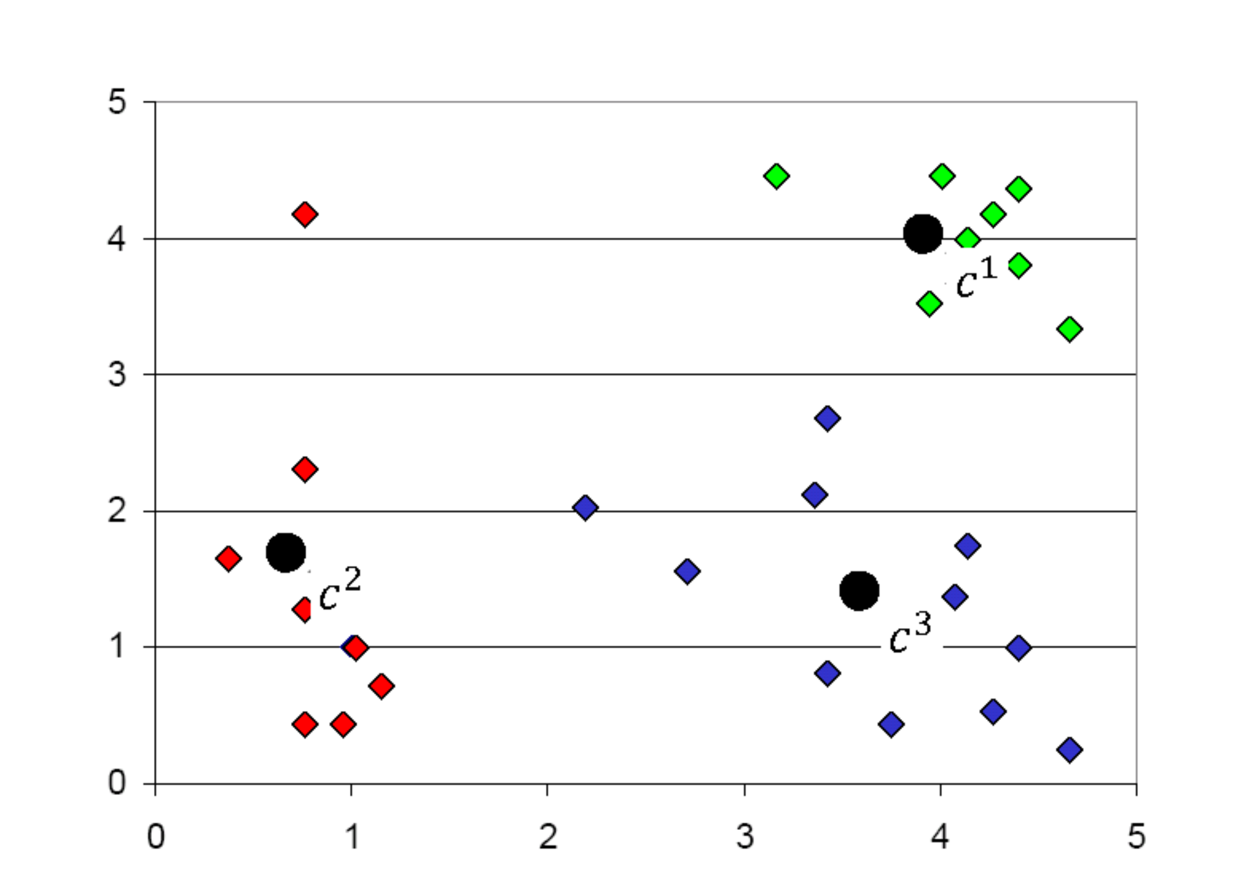
K-means: step 3



K-means: step 4



K-means: step 5



Questions

- Will different initialization lead to different results?
  - Yes
  - No
  - Sometimes

- Will the algorithm always stop after some iteration?
  - Yes
  - No (we have to set a maximum number of iterations)
  - Sometimes

Formal statement of k-means objective

- Given m data points, $\{x^1, x^2, \dots x^m\} \in R^n$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^n$
- And assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$
- Such that the averaged square distances from each data point to its respective cluster center is small

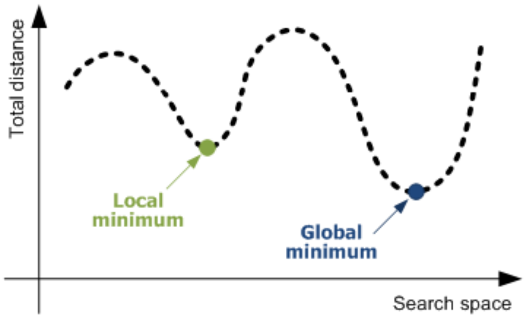
$$\min_{c,\pi} \frac{1}{m} \sum_{i=1}^{m} \left\| x^i - c^{\pi(i)} \right\|^2$$

Clustering is NP-hard in general

- Find k cluster centers, $\{c^1, c^2, \ldots, c^k\} \in R^n$, and assign each data point i to one cluster, $\pi(i) \in \{1, \ldots, k\}$, to minimize

$$\min_{c,\pi} \frac{1}{m} \sum_{i=1}^{m} \left\| x^i - c^{\pi(i)} \right\|^2$$

- A search problem over the space of discrete assignments
  - For all m data point together, there are k^m possibility
  - The cluster assignment determines cluster centers, and vice versa



Convergence of kmeans algorithm

- Will kmeans objective oscillate?

$$\frac{1}{m}\sum_{i=1}^{m}\left\|x^i - c^{\pi(i)}\right\|^2$$

- The minimum value of the objective is finite

- Each iteration of kmeans algorithm decrease the objective
  - Cluster assignment step decreases objective
    - $\pi(i) = argmin_{j=1,\ldots,k}\left\|x^i - c^j\right\|^2$ for each data point i
  - Center adjustment step decreases objective
    - $c^j = \frac{1}{|\{i:\pi(i)=j\}|}\sum_{i:\pi(i)=j} x^i = argmin_c \sum_{i:\pi(i)=j}\left\|x^i - c\right\|^2$

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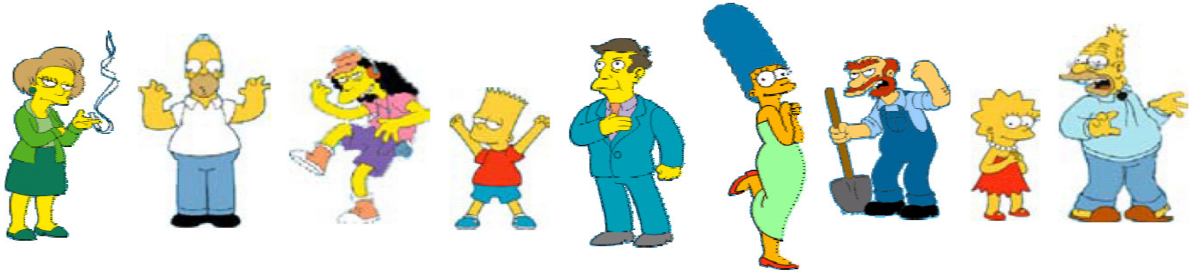
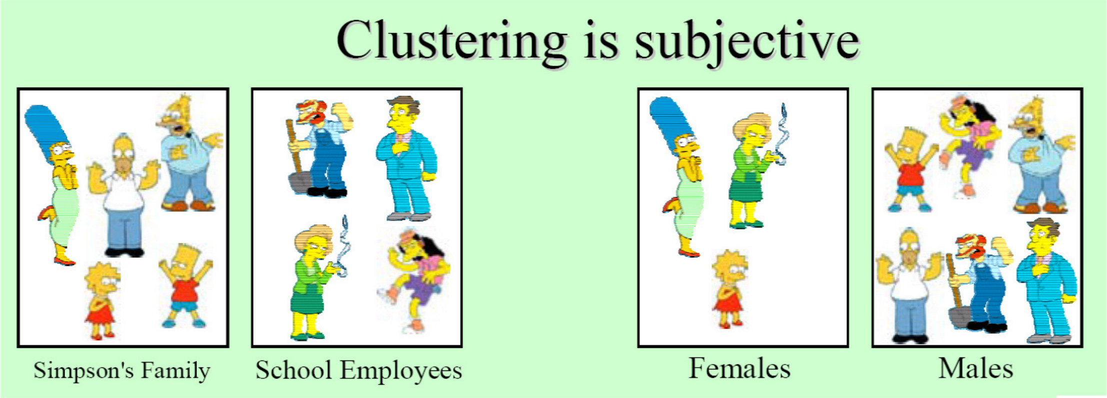
What else needs to be considered?



What is consider similar/dissimilar?



https://www.cs.us.es/~fran/curso_unia/clustering.html

You pick your similarity/dissimilarity

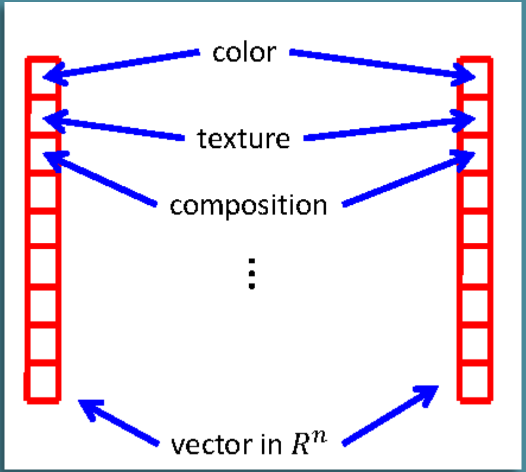
https://www.paddingtonpups.com.au/tag/similarities-between-owners-and-dogs

So what is clustering in general?

- You pick your similarity/dissimilarity function

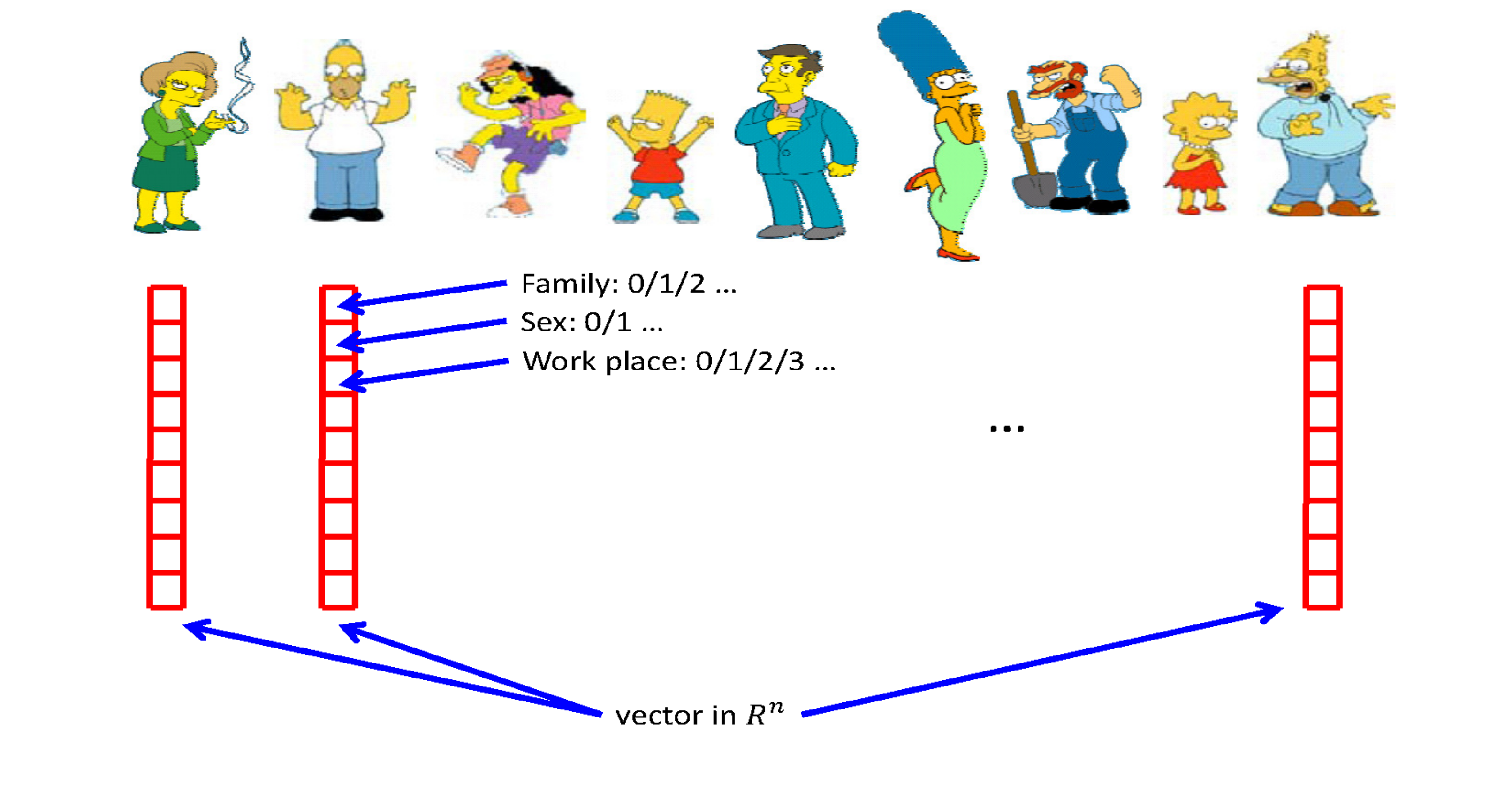
- The algorithm figures out the grouping of objects based on the chosen similarity/dissimilarity function
  - Points within a cluster is similar
  - Points across clusters are not so similar

Images of different sizes



http://www.wildnatureimages.com/search/index.php?module=media&pId=102&id=11413

Objects in real life



What similarity/dissimilarity function?

- Desired properties of dissimilarity function
  - Symmetry: $d(x, y) = d(y, x)$
    - *Otherwise you could claim "Alex looks like Bob, but Bob looks nothing like Alex"*
  - Positive separability: $d(x, y) = 0$, if and only if $x = y$
    - *Otherwise there are objects that are different, but you cannot tell apart*
  - Triangular inequality: $d(x, y) \leq d(x, z) + d(z, y)$
    - *Otherwise you could claim "Alex is very like Bob, and Alex is very like Carl, but Bob is very unlike Carl"*

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Distance functions for vectors

- Suppose two data points, both in R^n
  - $x = (x_1, x_2, \dots, x_n)^\top$
  - $y = (y_1, y_2, \dots, y_n)^\top$

- Euclidian distance: $d(x, y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$

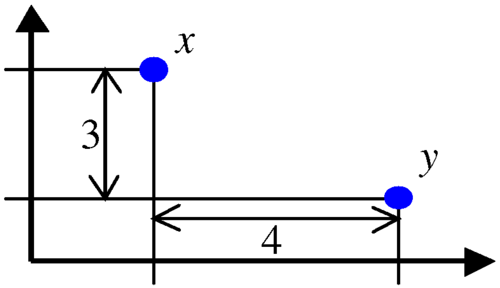
- Minkowski distance: $d(x, y) = \sqrt[p]{\sum_{i=1}^{n}(x_i - y_i)^p}$

  - Euclidian distance: $p = 2$

  - Manhattan distance: $p = 1, d(x, y) = \sum_{i=1}^{n}|x_i - y_i|$

  - "inf"-distance: $p = \infty, d(x, y) = \max_{i=1}^{n}|x_i - y_i|$

Distance example



- Euclidian distance: $\sqrt{4^2 + 3^2} = 5$
- Manhattan distance: $4 + 3 = 7$
- "inf"-distance: $max\{4,3\} = 4$

Hamming distance

- Manhattan distance is also called *Hamming distance* when all features are binary
  - Count the number of difference between two binary vectors
  - Example, $x, y \in \{0,1\}^{17}$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
x	0	1	1	0	0	1	0	0	1	0	0	1	1	1	0	0	1
y	0	1	1	1	0	0	0	0	1	1	1	1	1	1	0	1	1

$$d(x, y) = 5$$

Edit distance

- Transform one of the objects into the other, and measure how much effort it takes

x	I	N	T	E	*	N	T	I	O	N
	|	|	|	|	|	|	|	|	|	|
y	*	E	X	E	C	U	T	I	O	N
	d	s	s		i	s				

d: deletion (cost 5)
s: substitution (cost 1)
i: insertion (cost 2)

$$d(x, y) = 5 \times 1 + 3 \times 1 + 1 \times 2 = 10$$

Generalization of K-means

- Given m data points, $\{x^1, x^2, \dots x^m\} \in R^n$
- Find k cluster centers, $\{c^1, c^2, \dots, c^k\} \in R^n$
- And assign each data point i to one cluster, $\pi(i) \in \{1, \dots, k\}$
- Such that the sum of the squared distances from each data point to its respective cluster center is minimized

$$\min_{c,\pi} \sum_{i=1}^{m} d\left(x^i, c^{\pi(i)}\right)^2$$

NP-hard!

Generalized K-means algorithm

Initialize k cluster centers, $\{c^1, c^2, \ldots, c^k\}$, randomly

Do

Decide the cluster memberships of each data point, x^i, by assigning it to the nearest cluster center

$$\pi(i) = argmin_{j=1,\ldots,k}\ d(x^i, c^j)$$

Adjust the cluster centers

$$c^j = argmin_{v \in R^n} \sum_{i:\pi(i)=j} \boxed{d(x^i, v)}$$

Main difference from k-means

[A convex optimization problem in many cases.]

While any cluster center has been changed.


SUMMARY