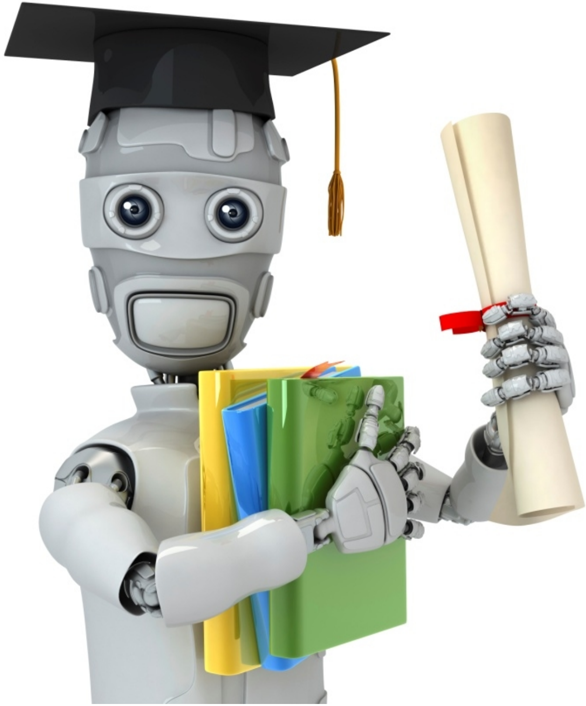
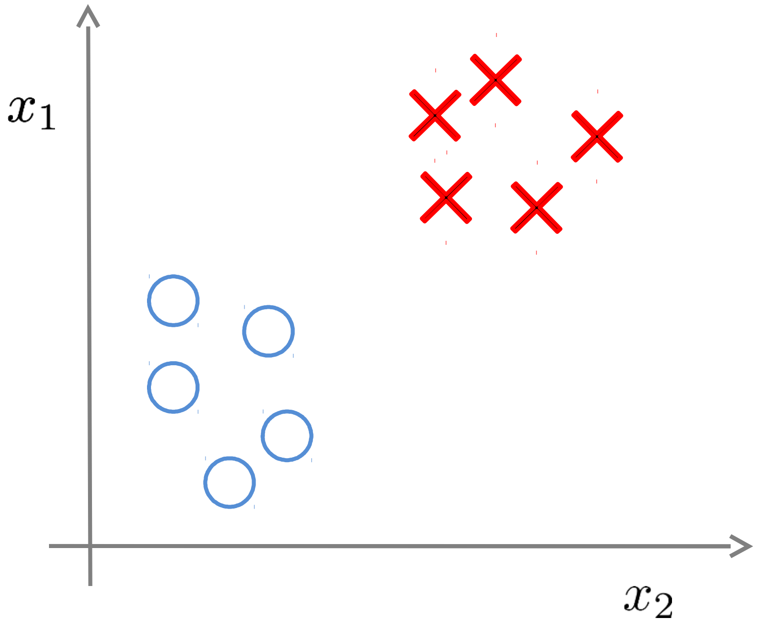


Clustering

Unsupervised learning introduction

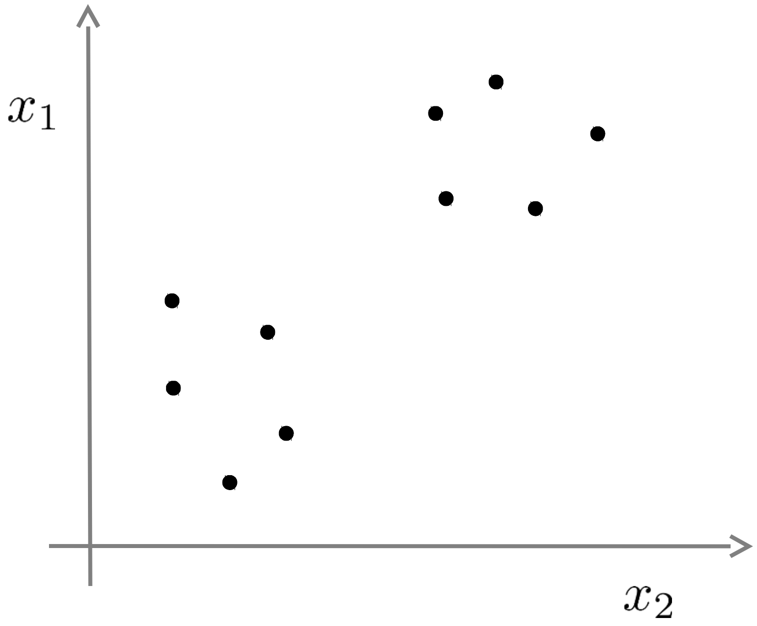
Machine Learning

Supervised learning



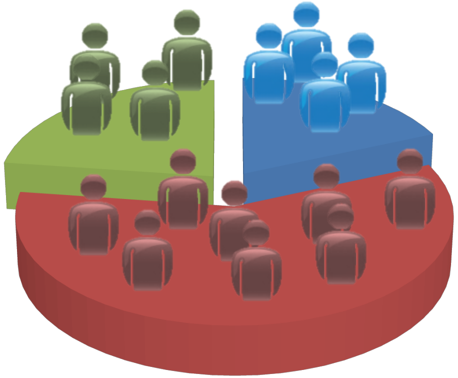
Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), (x^{(3)}, y^{(3)}), \ldots, (x^{(m)}, y^{(m)})\}$

Unsupervised learning

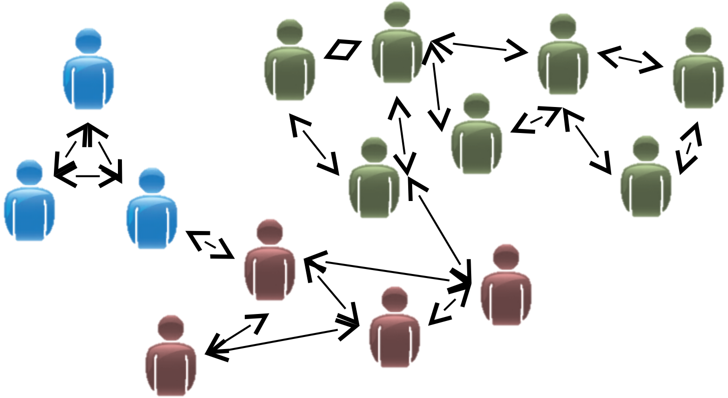


Training set: $\{x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(m)}\}$

Applications of clustering



Market segmentation



Social network

Organize computing

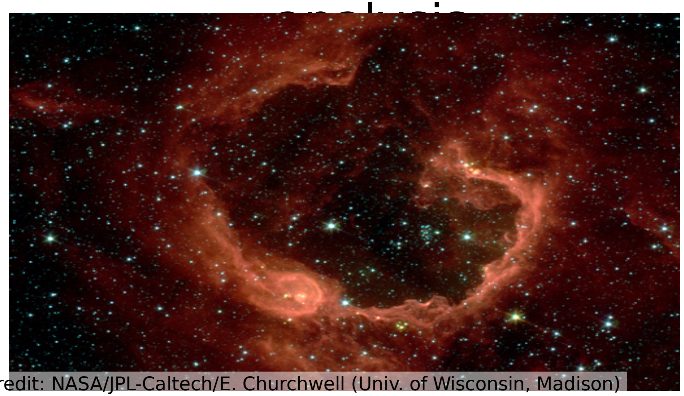


Image credit: NASA/JPL-Caltech/E. Churchwell (Univ. of Wisconsin, Madison)

Astronomical data

Which of the following statements are true? Check all that apply.

- [x] In unsupervised learning, the training set is of the form $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ without labels $y^{(i)}$.

Correct Response

- [x] Clustering is an example of unsupervised learning.

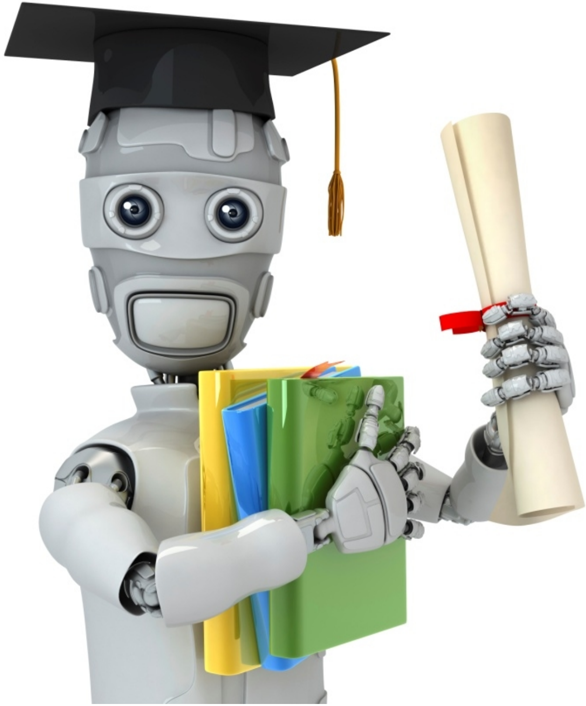
Correct Response

- [x] In unsupervised learning, you are given an unlabeled dataset and are asked to find "structure" in the data.

Correct Response

- [ ] Clustering is the only unsupervised learning algorithm.

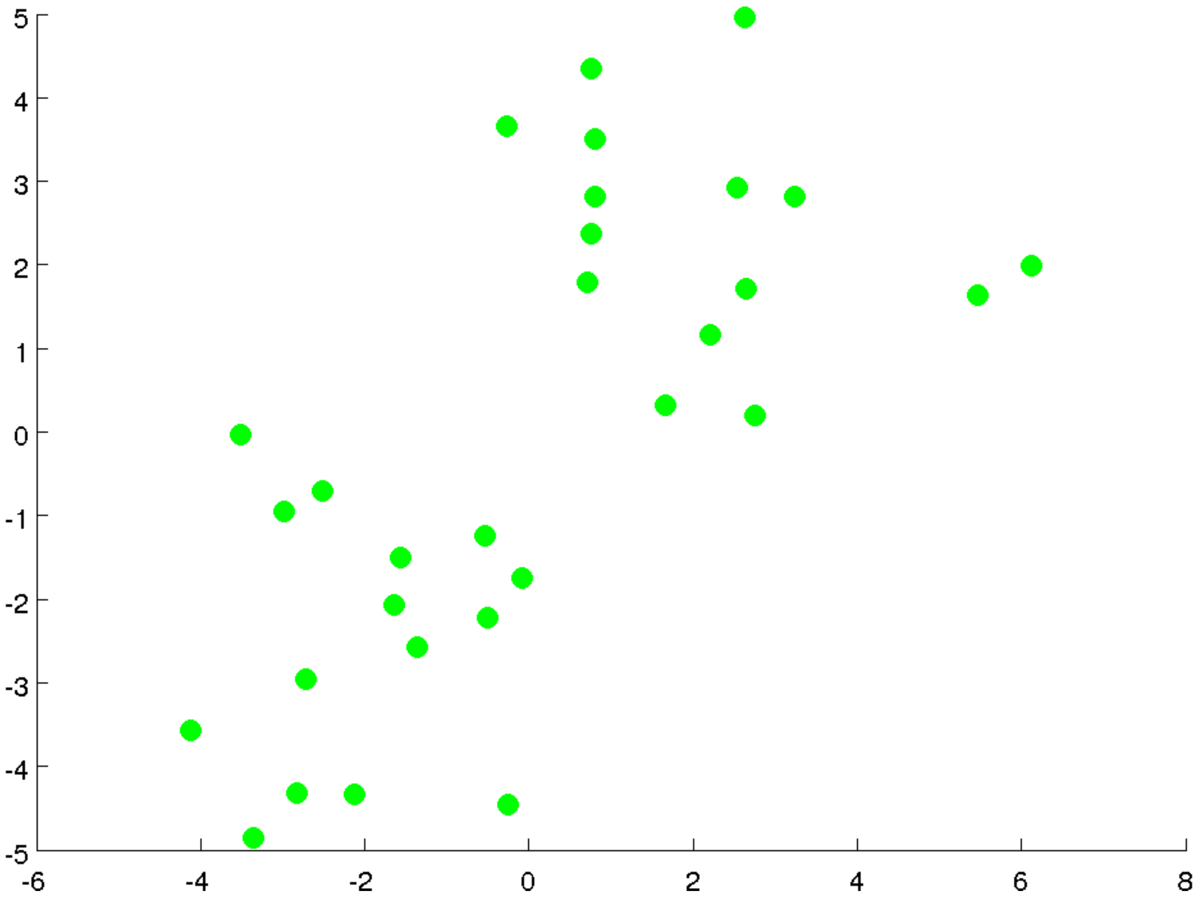
Correct Response



Machine Learning

Clustering

K-means algorithm



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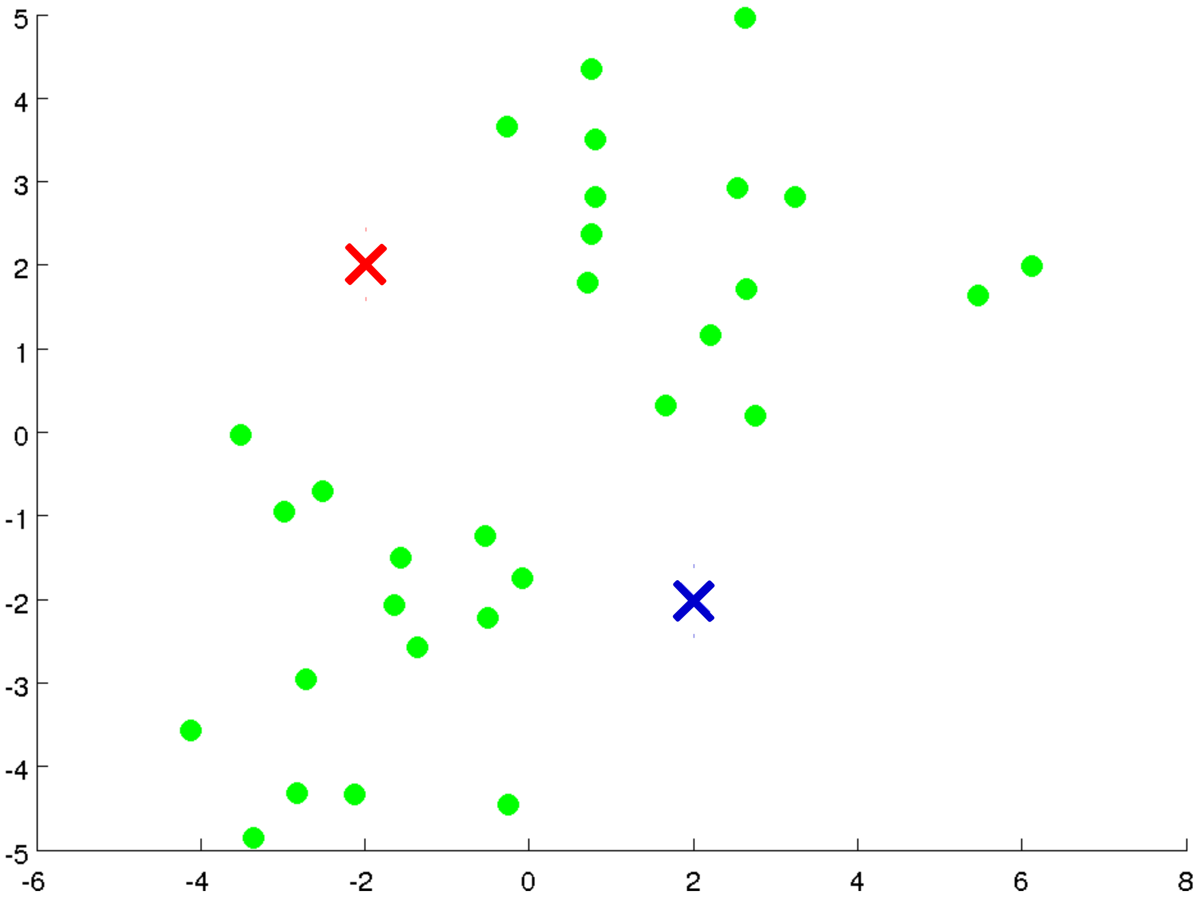

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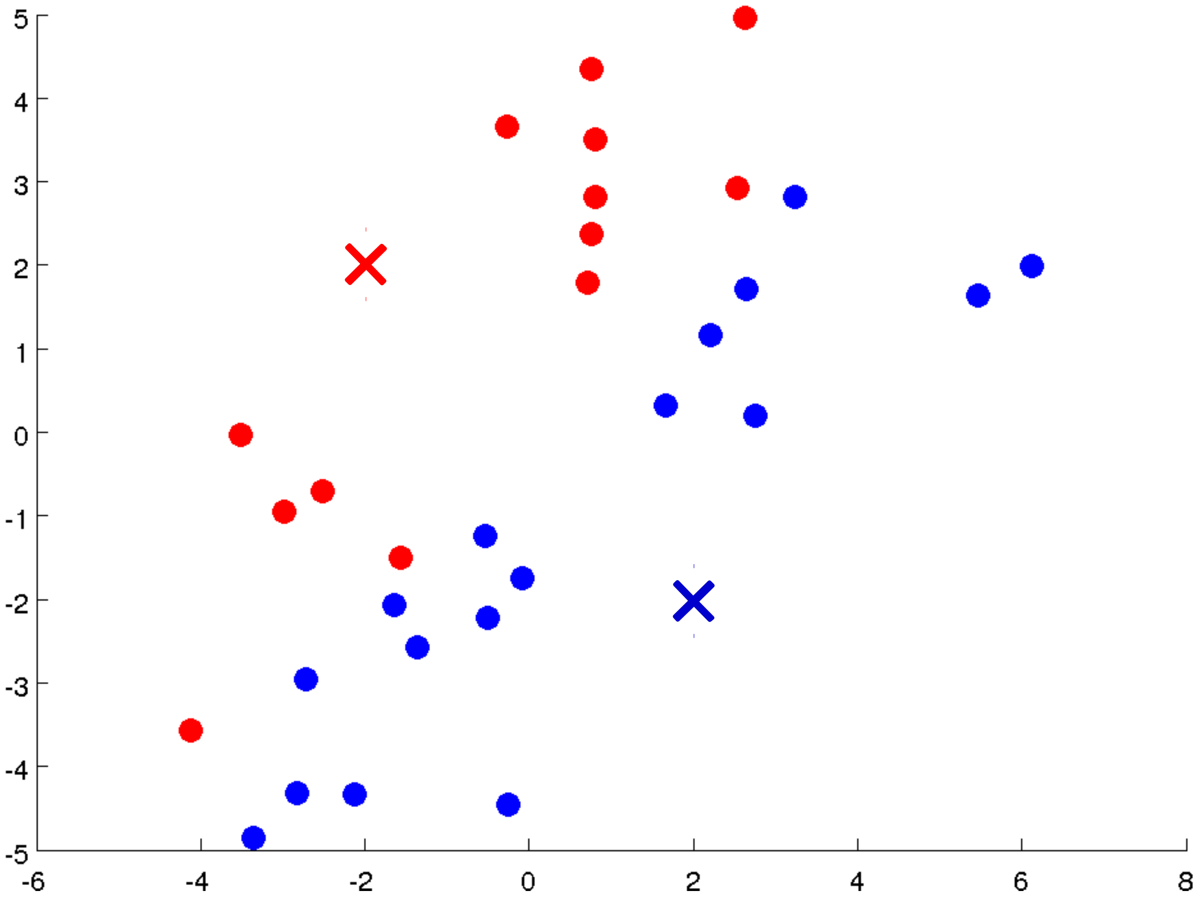
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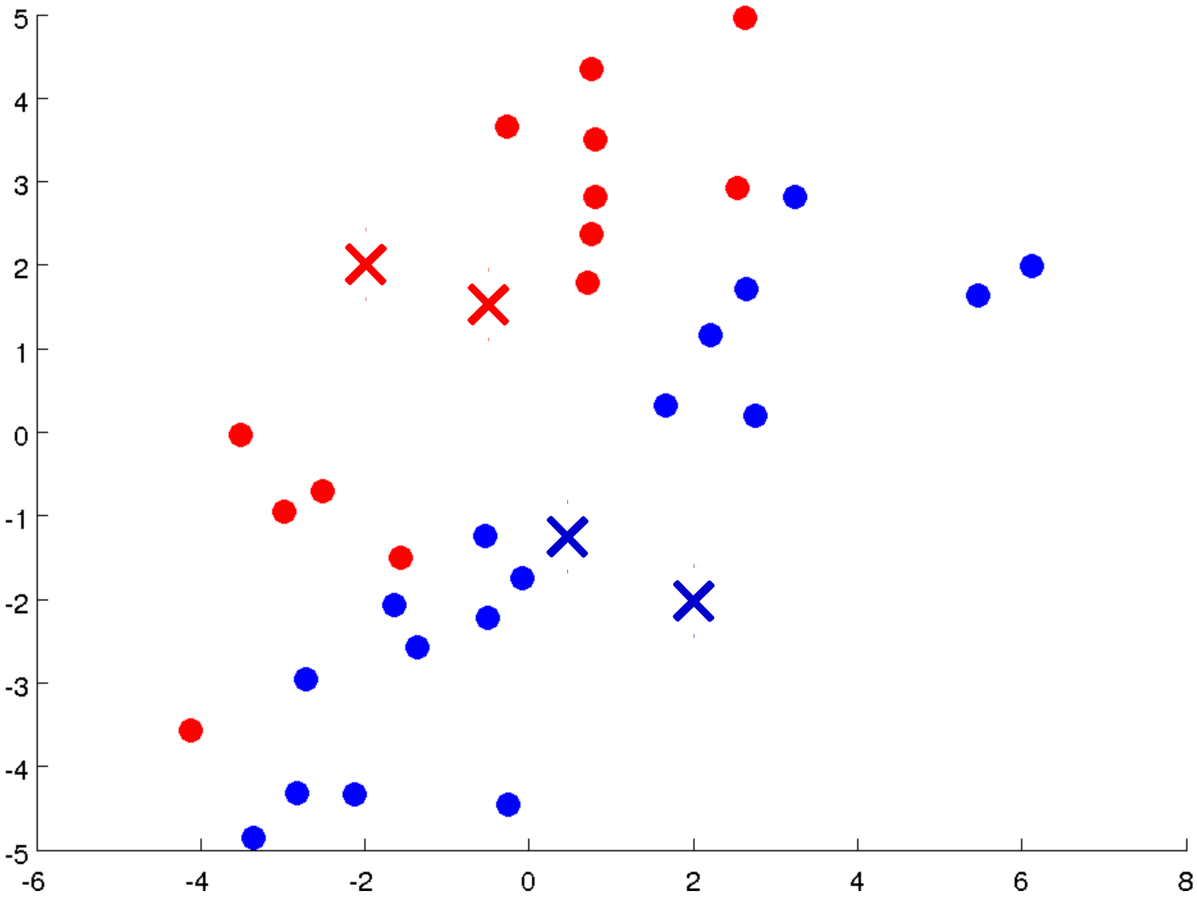

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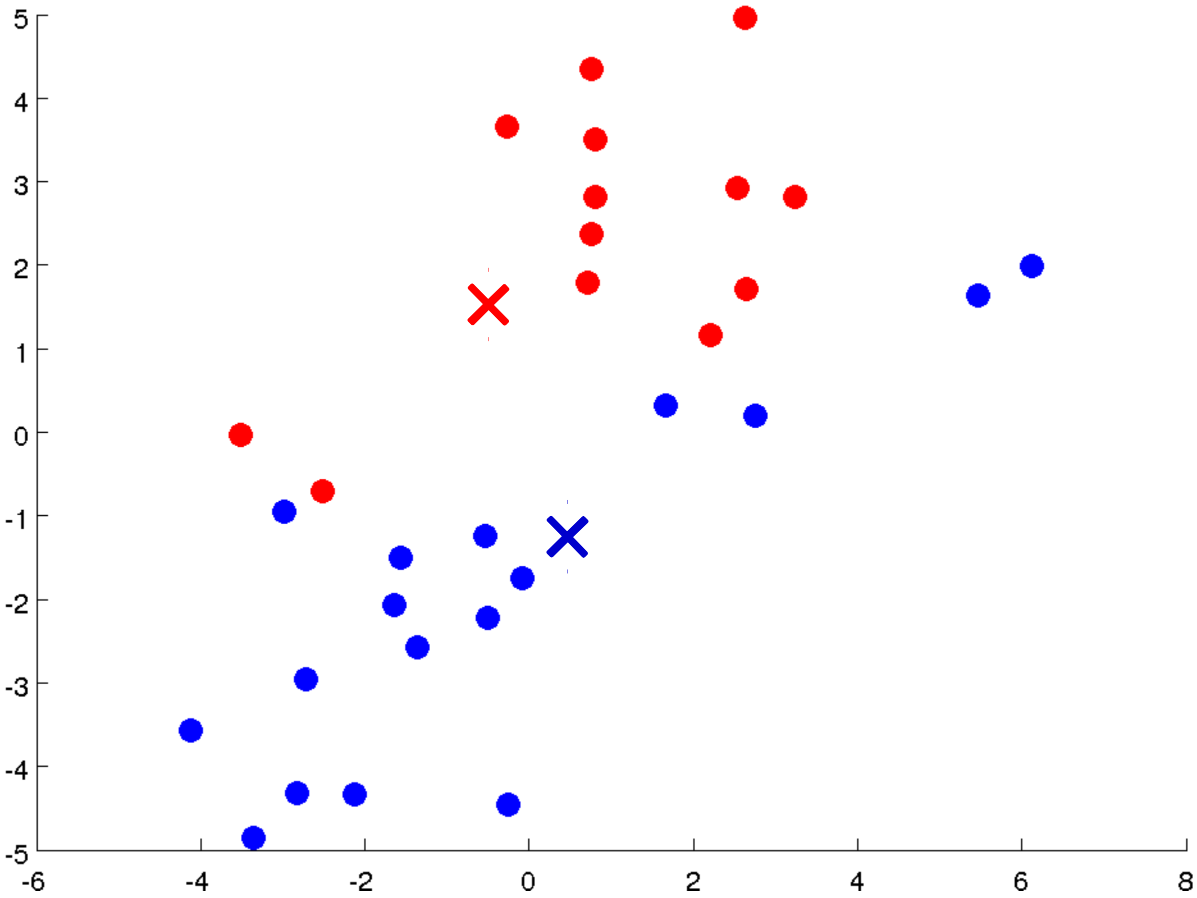
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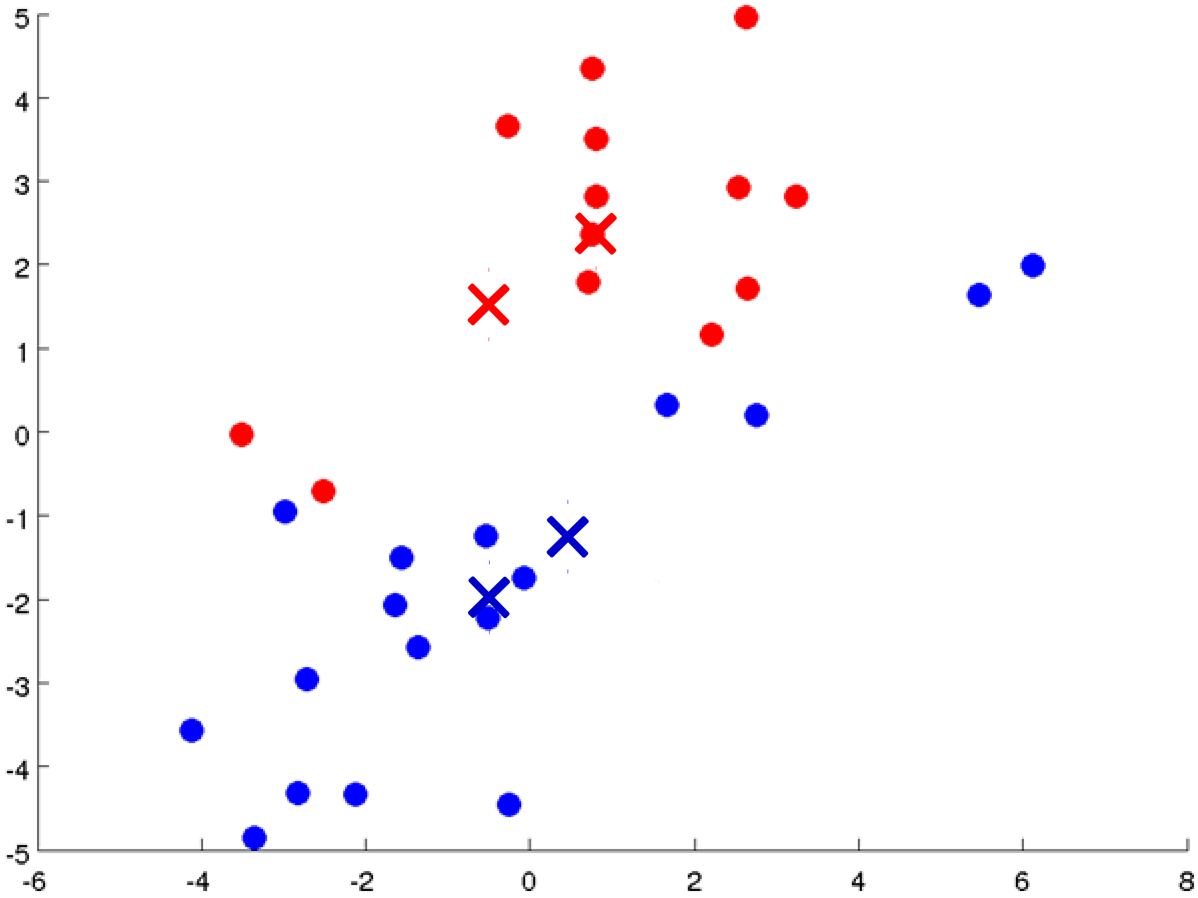

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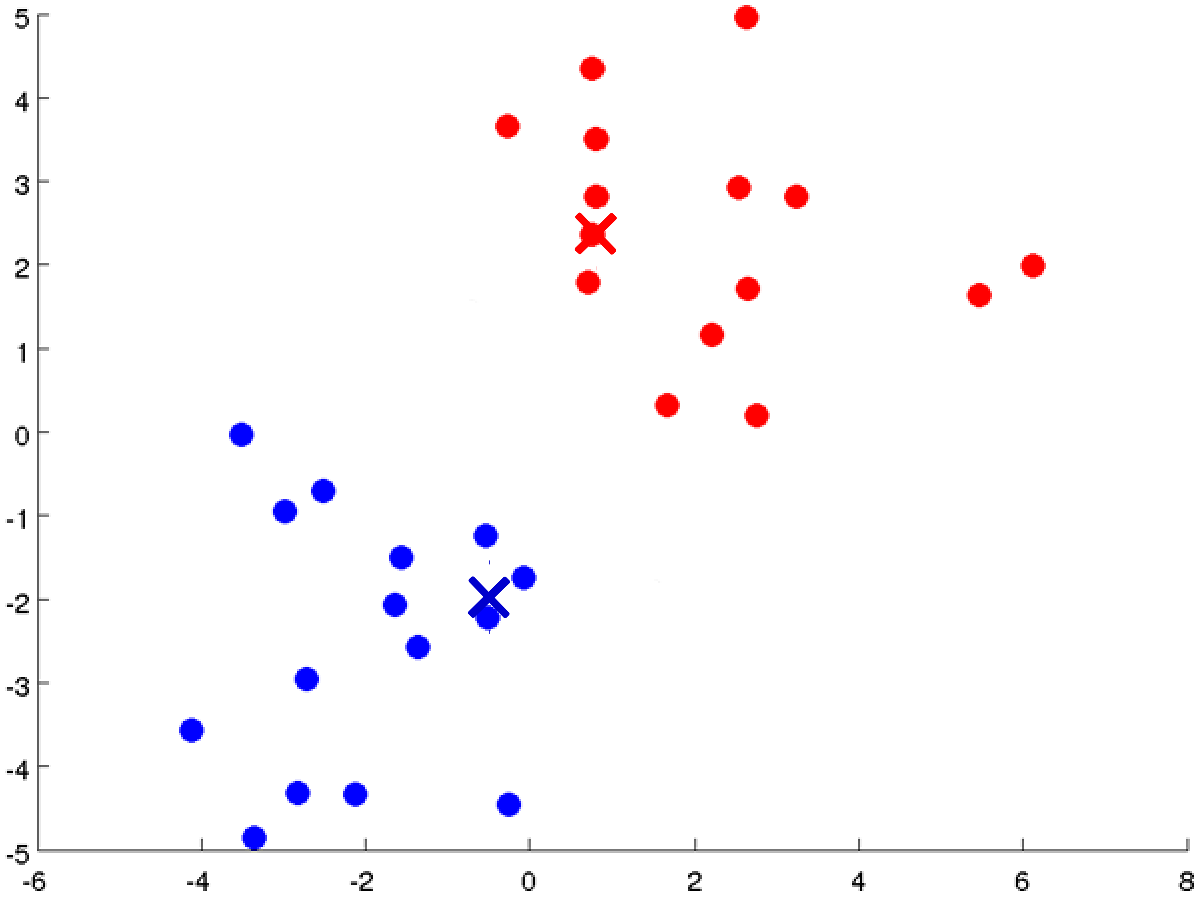

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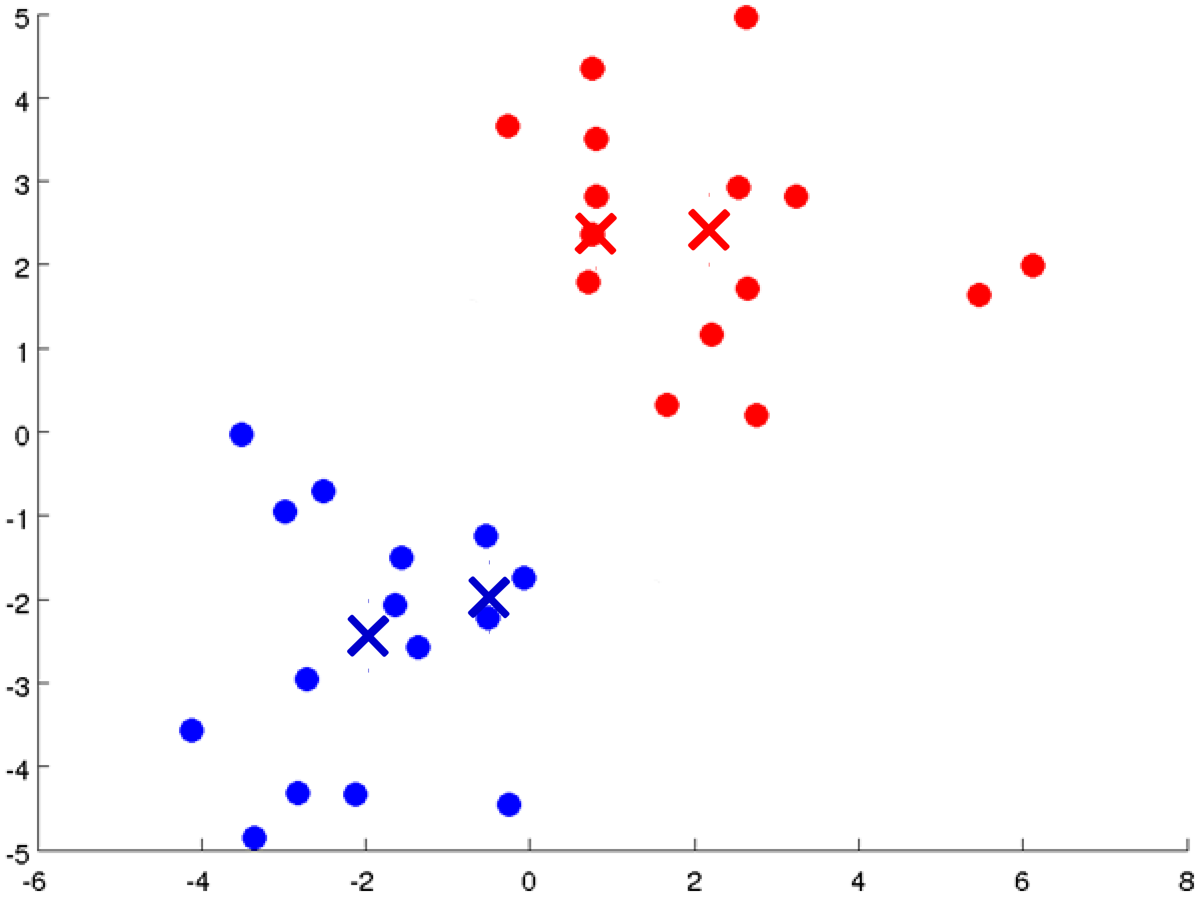
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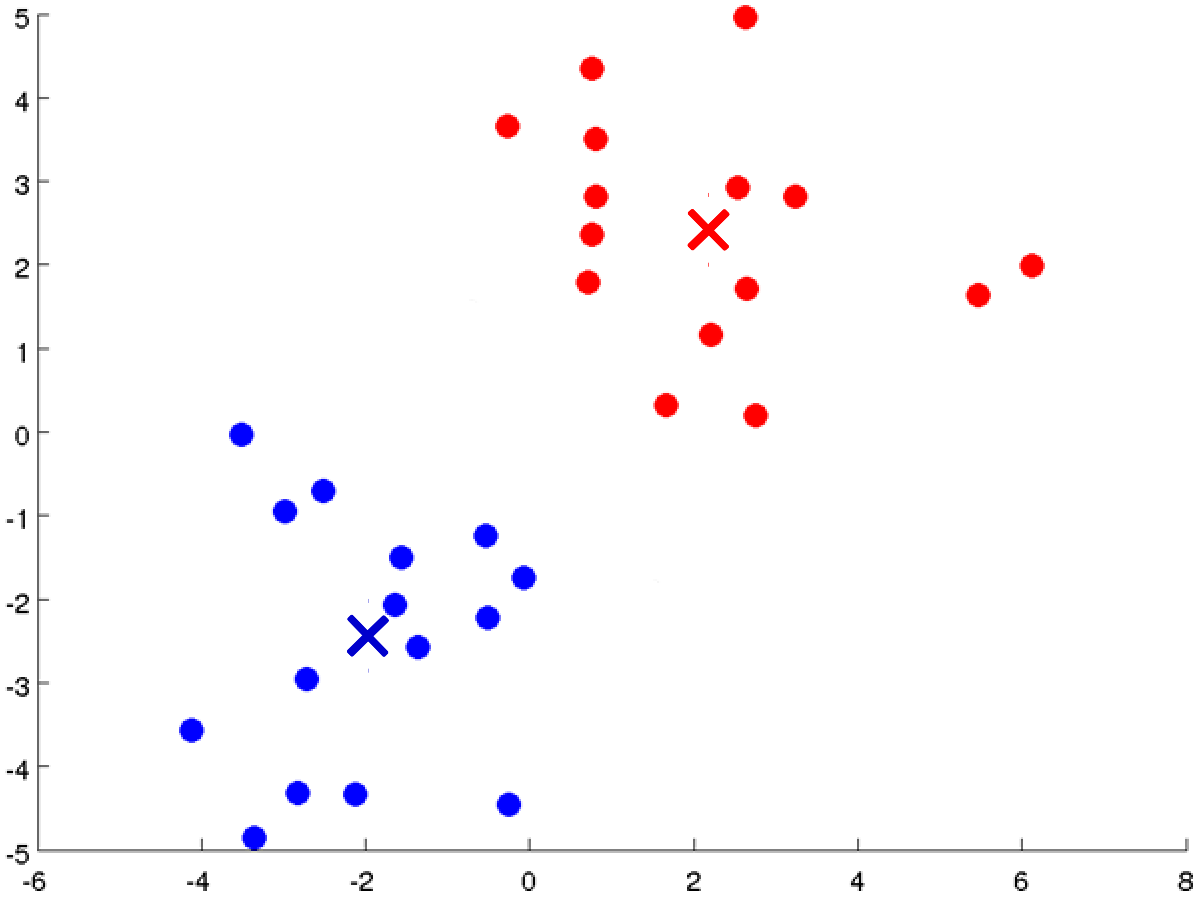
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K-means algorithm

assumption

Input:

- K (number of clusters)
- Training set $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$

$x^{(i)} \in \mathbb{R}^n$ (drop $x_0 = 1$ convention)

K-means algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to cluster k

}

Suppose you run k-means and after the algorithm converges, you have:
$c^{(1)} = 3, c^{(2)} = 3, c^{(3)} = 5, \ldots$

Which of the following statements are true? Check all that apply.

- [x] The third example $x^{(3)}$ has been assigned to cluster 5.

Correct Response

- [x] The first and second training examples $x^{(1)}$ and $x^{(2)}$ have been assigned to the same cluster.

Correct Response

- [ ] The second and third training examples have been assigned to the same cluster.

Correct Response

- [x] Out of all the possible values of $k \in \{1, 2, \ldots, K\}$ the value $k = 3$ minimizes $\|x^{(2)} - \mu_k\|^2$.

Correct Response

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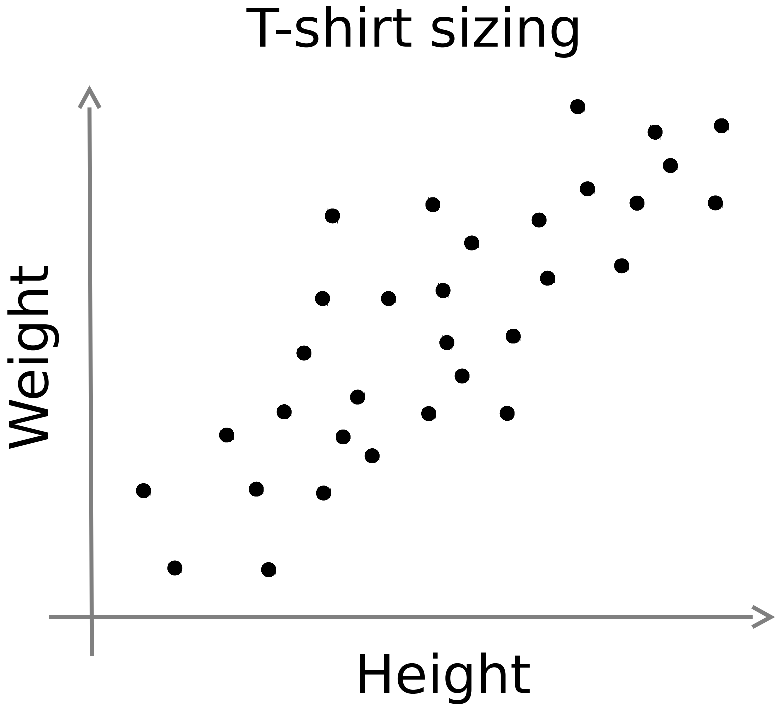
K-means for non-separated clusters



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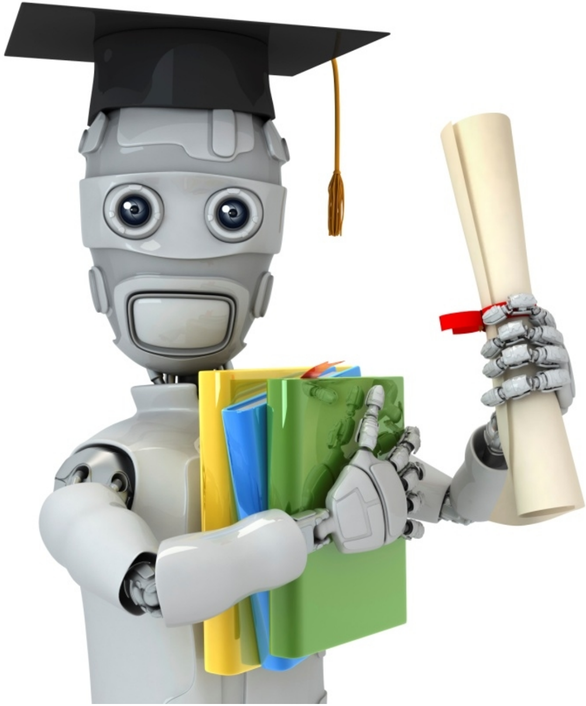


Machine Learning

Clustering Optimization objective

K-means optimization objective

$c^{(i)}$ = index of cluster (1,2,..., K) to which example $x^{(i)}$ is currently assigned

μ_k = cluster centroid k ($\mu_k \in \mathbb{R}^n$)

$\mu_{c^{(i)}}$ = cluster centroid of cluster to which example $x^{(i)}$ has been assigned

Optimization objective:

$$J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2$$

$$\min_{\substack{c^{(1)}, \dots, c^{(m)}, \\ \mu_1, \dots, \mu_K}} J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)$$

K-means algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

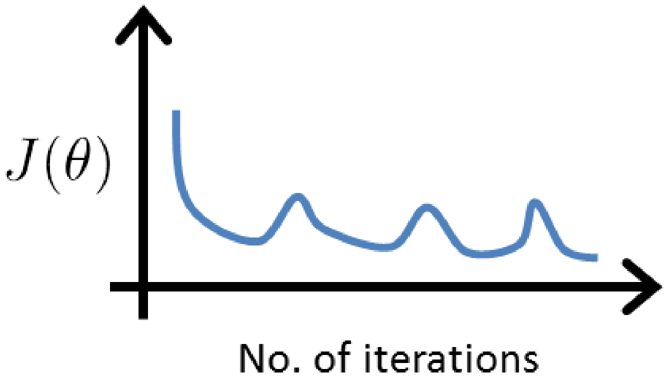
$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to cluster k

}

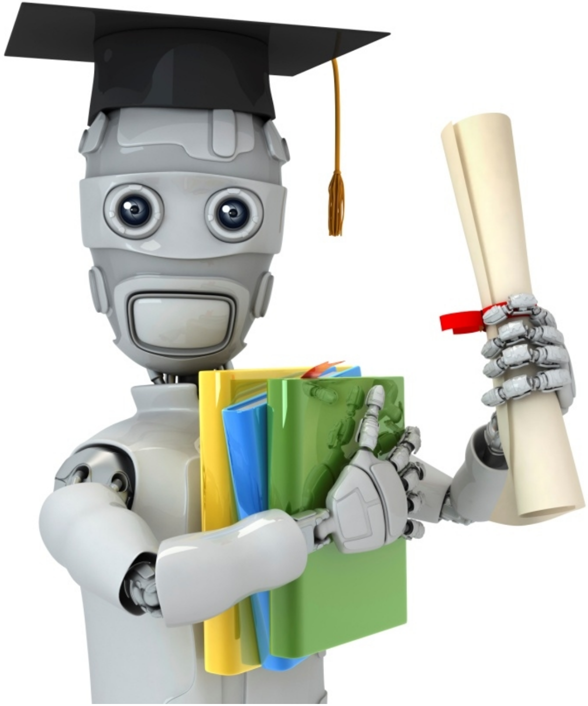
Suppose you have implemented k-means and to check that it is running correctly, you plot the cost function $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_k)$ as a function of the number of iterations. Your plot looks like this:



What does this mean?

- ○ The learning rate is too large.
- ○ The algorithm is working correctly.
- ○ The algorithm is working, but k is too large.
- ◉ It is not possible for the cost function to sometimes increase. There must be a bug in the code.

Correct Response



Machine Learning

Clustering

Random initialization

K-means algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to cluster k

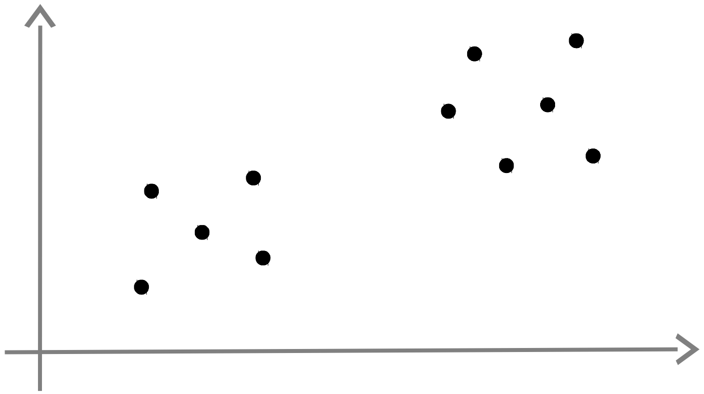
}

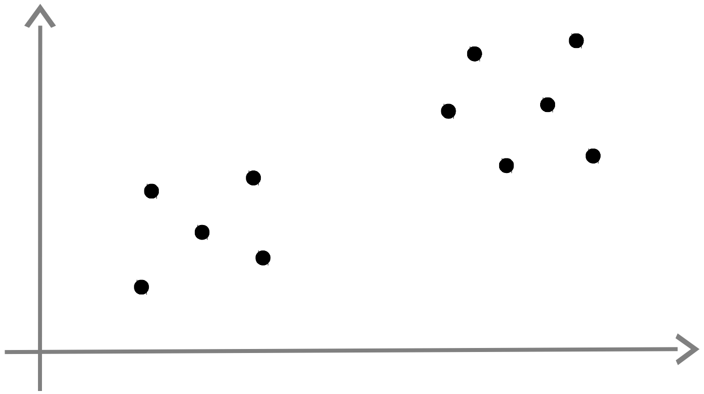
Random initialization

Should have $K < m$

Randomly pick K training examples.

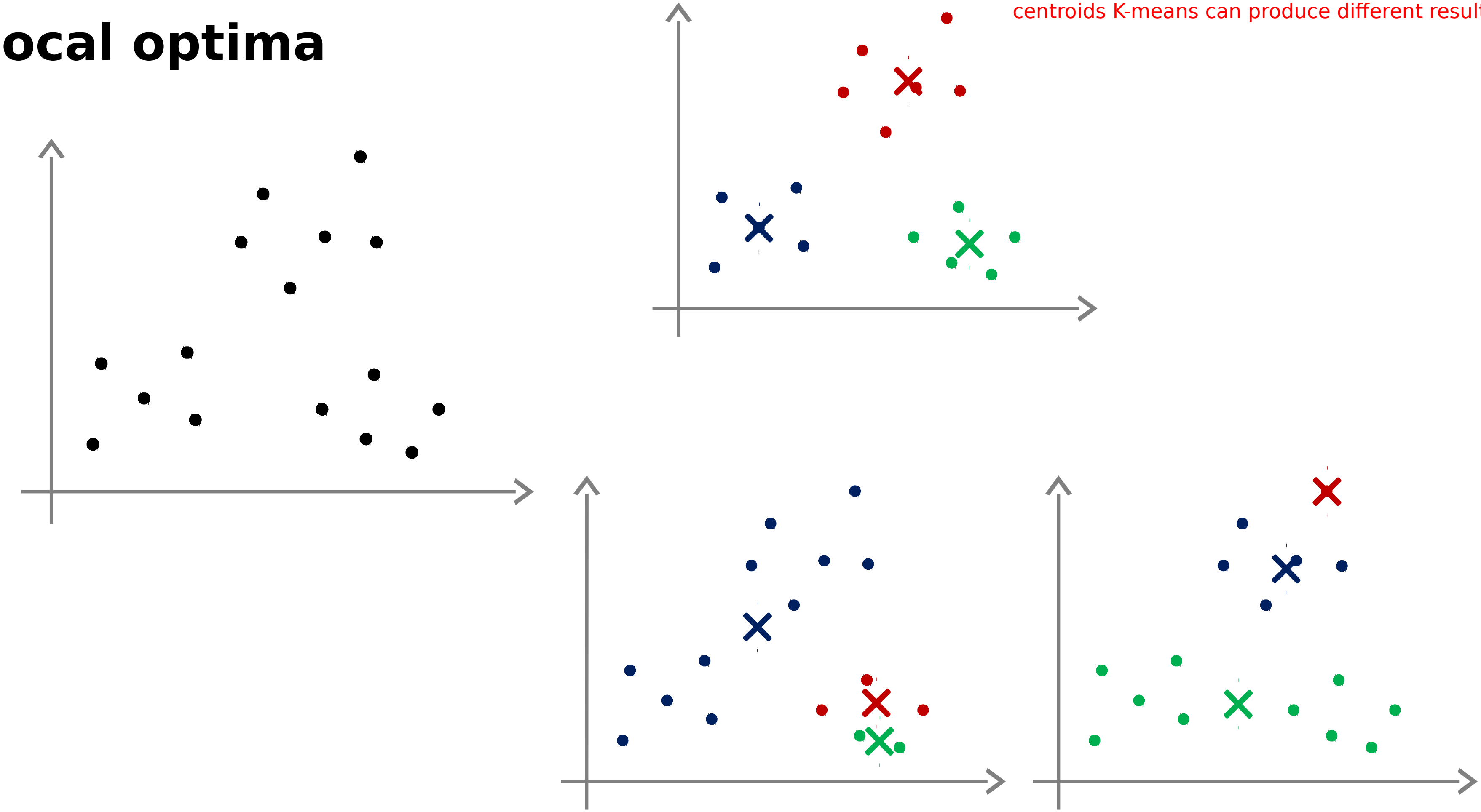
Set $\mu_1, \ldots, \mu_K$ equal to these K examples.





Local optima

Depending on the initialization of cluster centroids K-means can produce different results



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Random initialization

For i = 1 to 100 {

Randomly initialize K-means.
Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.
Compute cost function (distortion)

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

}

Pick clustering that gave lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

Which of the following is the recommended way to initialize k-means?

- Pick a random integer i from $\{1,\dots,k\}$. Set $\mu_1 = \mu_2 = \dots = \mu_k = x^{(i)}$.

- Pick k distinct random integers $i_1,\dots,i_k$ from $\{1,\dots,k\}$.

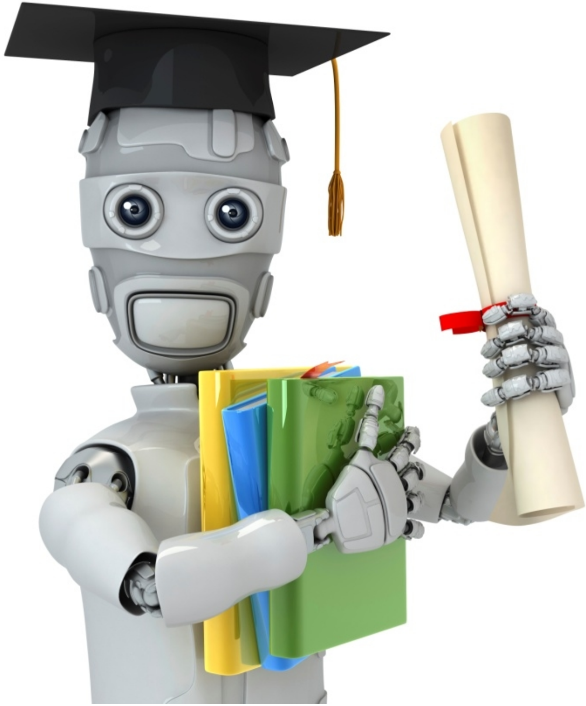
  Set $\mu_1 = x^{(i_1)}, \mu_2 = x^{(i_2)}, \dots, \mu_k = x^{(i_k)}$.

- Pick k distinct random integers $i_1,\dots,i_k$ from $\{1,\dots,m\}$.

  Set $\mu_1 = x^{(i_1)}, \mu_2 = x^{(i_2)}, \dots, \mu_k = x^{(i_k)}$.

  Correct Response

- Set every element of $\mu_i \in \mathbb{R}^n$ to a random value between $-\epsilon$ and ϵ, for some small ϵ.

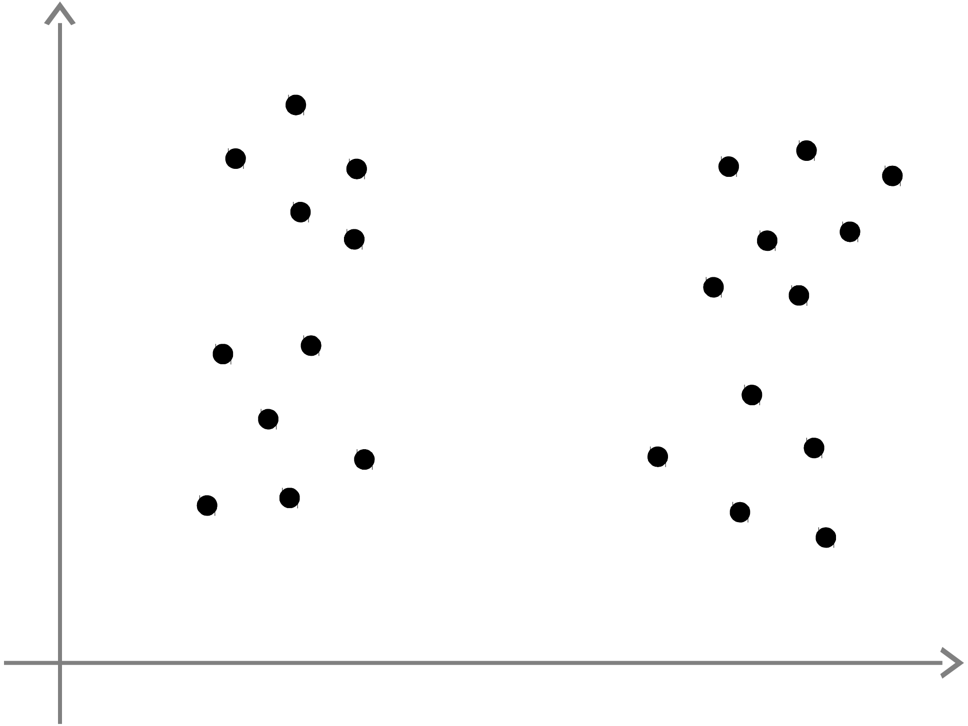


Machine Learning

Clustering

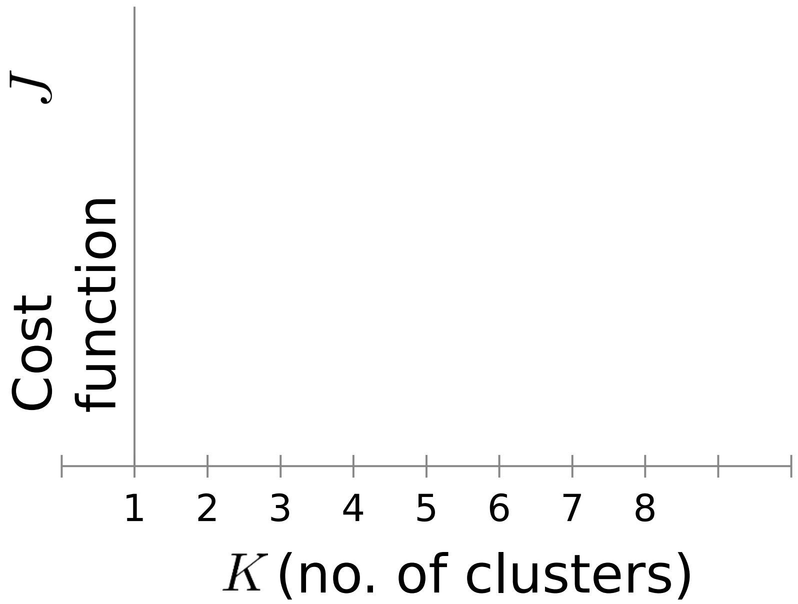
Choosing the number of clusters

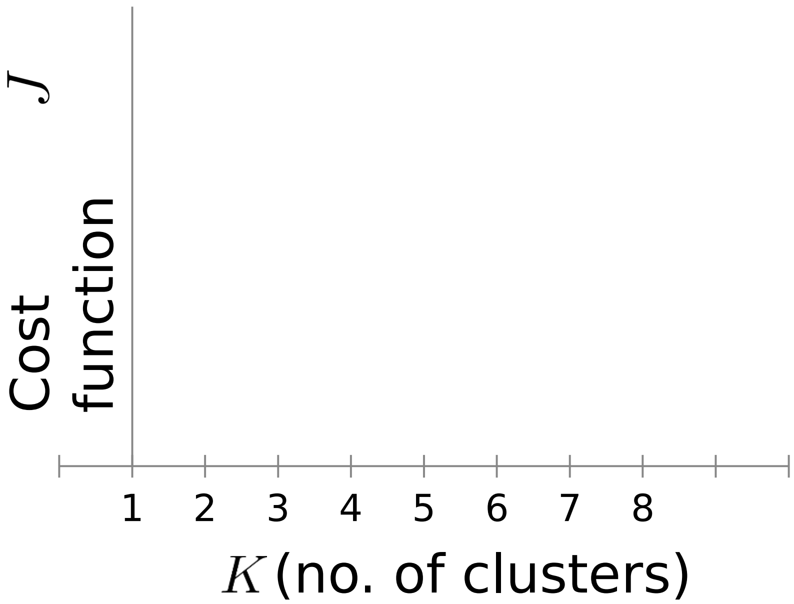
What is the right value of K?



Choosing the value of K

Elbow method:





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Suppose you run k-means using k = 3 and k = 5. You find that the cost function J is much higher for k = 5 than for k = 3. What can you conclude?

- ○ This is mathematically impossible. There must be a bug in the code.
- ○ The correct number of clusters is k = 3.
- ◉ In the run with k = 5, k-means got stuck in a bad local minimum. You should try re-running k-means with multiple random initializations.

  Correct Response

- ○ In the run with k = 3, k-means got lucky. You should try re-running k-means with k = 3 and different random initializations until it performs no better than with k = 5.

Choosing the value of K

Sometimes, you're running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose.

E.g.