



Machine Learning

# Clustering

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Unsupervised learning  
introduction

# Supervised learning



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

# Unsupervised learning



Clustering algorithm

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

# Applications of clustering



→ Market segmentation



→ Social network analysis



→ Organize computing clusters



→ Astronomical data analysis



Machine Learning

# Clustering

## K-means algorithm







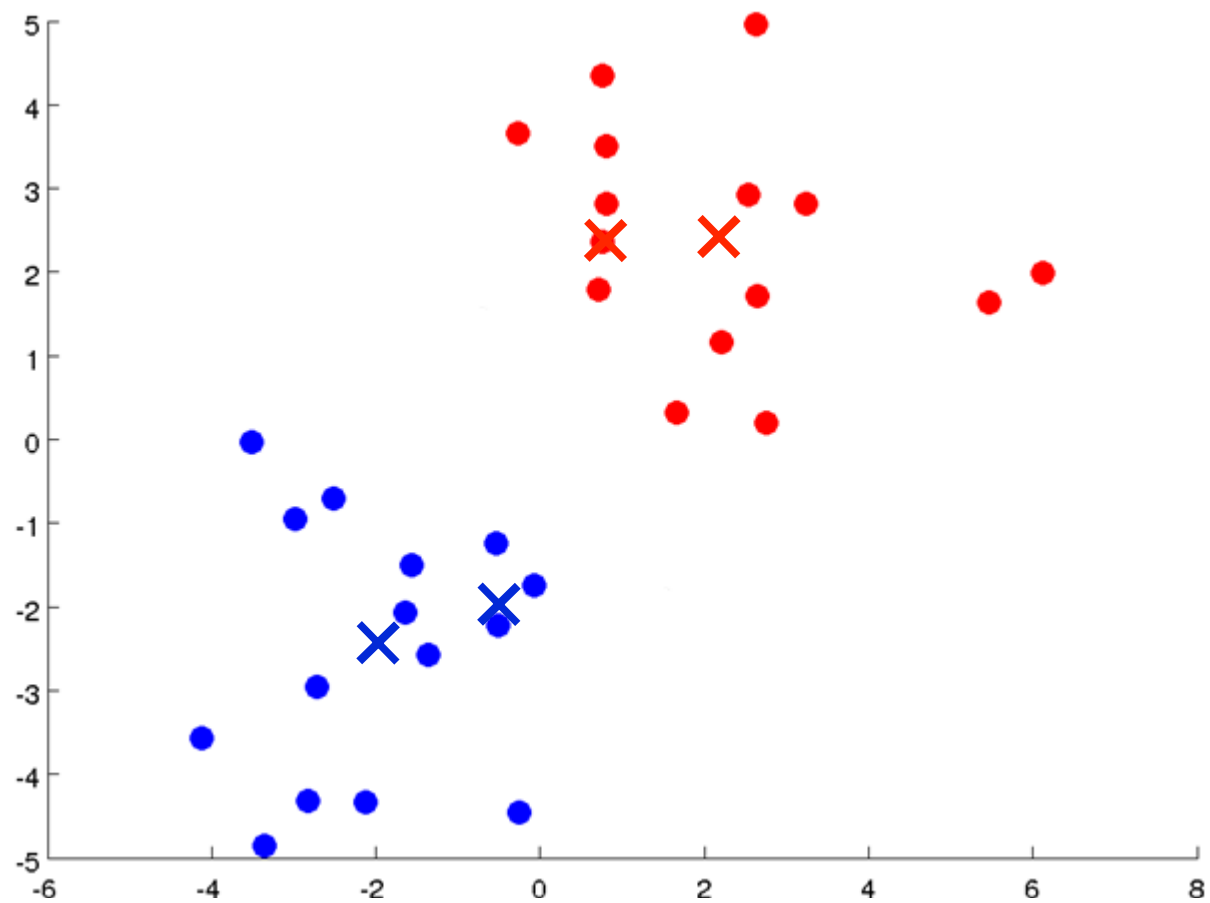


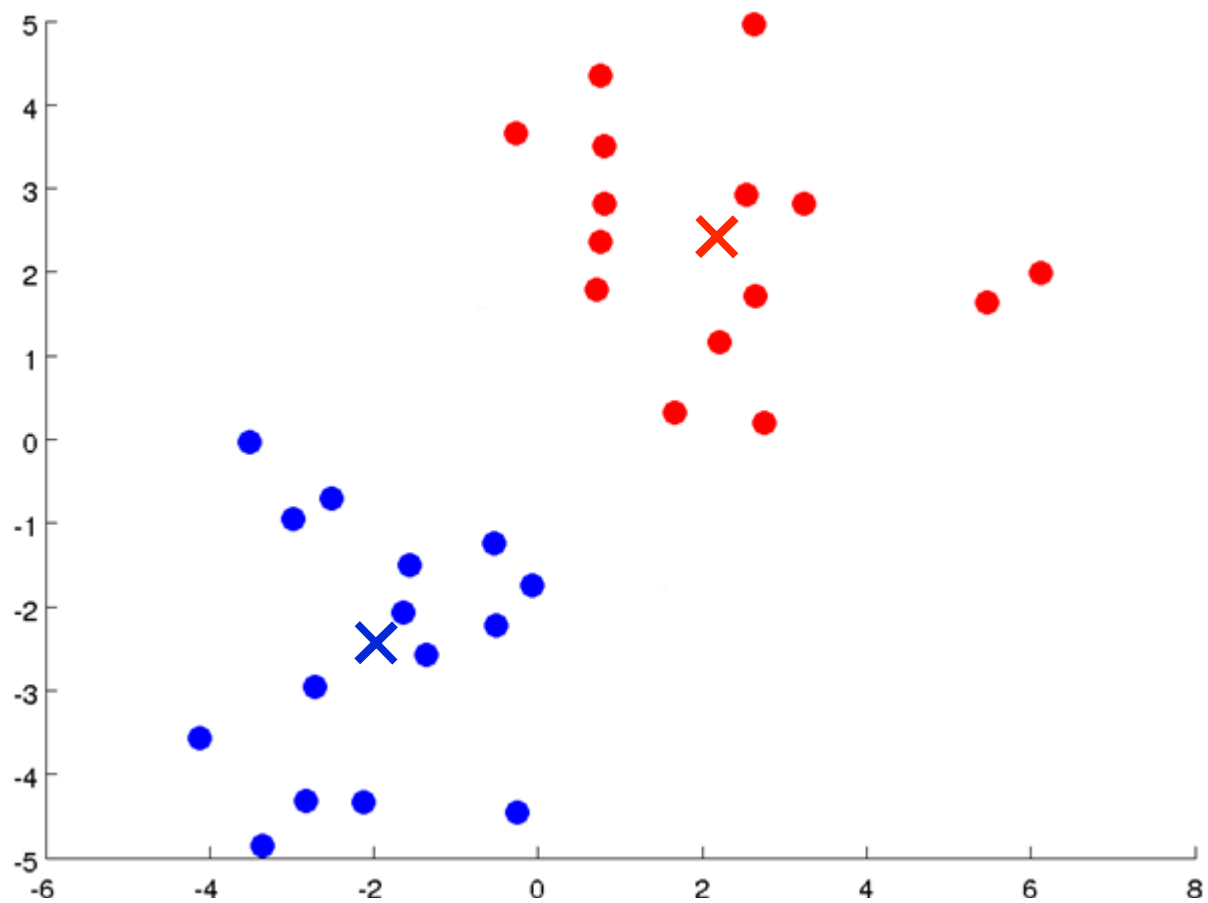












# K-means algorithm

Input:

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

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

# K-means algorithm

$$\mu_1 \quad \mu_2$$

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

Repeat {

Cluster assignment step

for  $i = 1$  to  $m$

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

$$\min_k \|x^{(i)} - \mu_k\|^2$$

$\uparrow$   
 $c^{(i)}$

for  $k = 1$  to  $K$

→  $\mu_k$  := average (mean) of points assigned to cluster  $k$

Move centroid

$$x^{(1)}, x^{(5)}, x^{(6)}, x^{(10)}$$

$$\rightarrow c^{(1)}=2, c^{(5)}=2, c^{(6)}=2, c^{(10)}=2$$

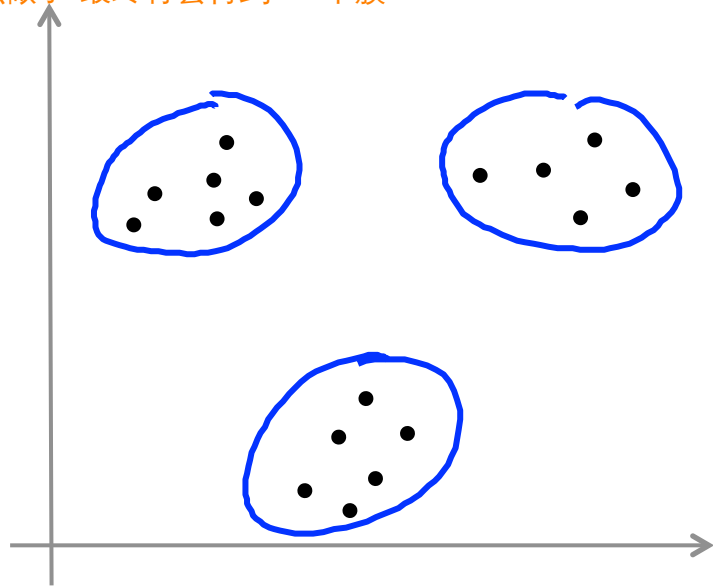
$$\mu_2 = \frac{1}{4} \begin{bmatrix} x^{(1)} + x^{(5)} + x^{(6)} + x^{(10)} \\ - \end{bmatrix} \in \mathbb{R}^n$$



# K-means for non-separated clusters

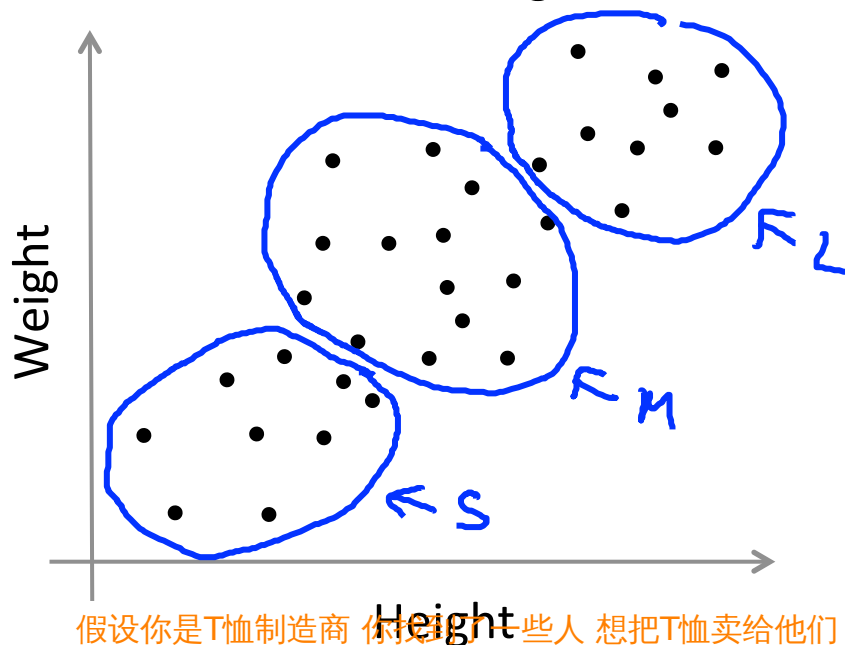
S, M, L

我要问的问题是 既然我们要让 $\mu_k$ 移动到分配给它的那些点的均值处 那么如果 存在一个 没有点分配给它的聚类中心 那怎么办?  
通常在这种情况下 我们就直接移除 那个聚类中心  
如果这么做了 最终将会得到K-1个簇



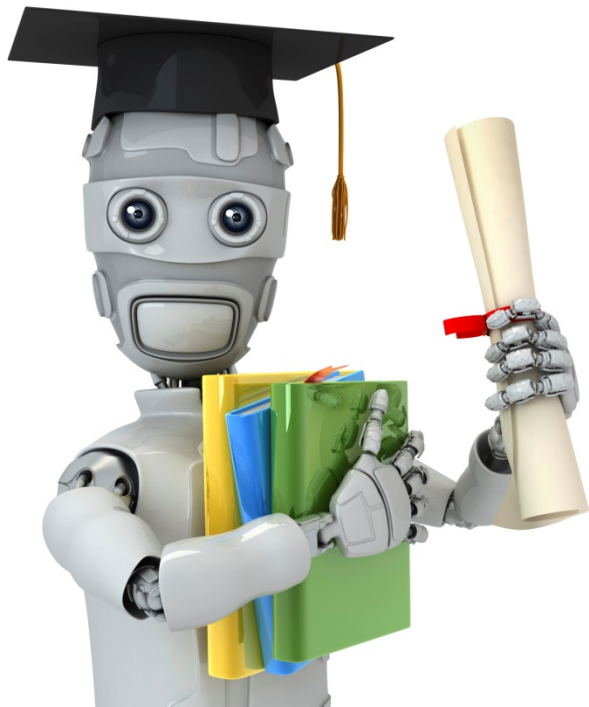
如果就是要K个簇 不多不少 但是有个 没有点分配给它的聚类中心  
你所要做的是 重新随机找一个聚类中心 但是直接移除那个中心  
是更为常见的方法 当你遇到了一个 没有分配点的 聚类中心  
不过在实际过程中 这个问题不会经常出现

T-shirt sizing



假设你是T恤制造商 你找到了一些人 想把T恤卖给他们 然后  
你搜集了一些 这些人的 身高和体重的数据 我猜 身高体重更  
重要一些 然后你可能 收集到了这样的样本 一些关于 人们  
身高和体重的样本 就像这个图所表示的 然后你想确定一

下T恤的大小 假设我们要设计 三种不同大小的t恤 小号 中号  
和大号 那么小号应该是多大的? 中号呢? 大号呢?



Machine Learning

# Clustering

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## Optimization objective

# K-means optimization objective

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

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

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

$K$   $k \in \{1, 2, \dots, K\}$   
 $x^{(i)} \rightarrow 5$   $\underline{c^{(i)} = 5}$   $\underline{\mu_{c^{(i)}} = \mu_5}$

Optimization objective:

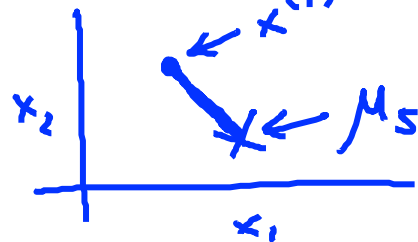
→  $\underline{J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)} = \frac{1}{m} \sum_{i=1}^m \left[ \|x^{(i)} - \mu_{c^{(i)}}\|^2 \right]$  ←

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

→  $\mu_1, \dots, \mu_K$

Distortion

K均值算法中 有时候也叫做distortion cost function



# K-means algorithm

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

Repeat {

*Cluster assignment step*  
Minimize  $J(\dots)$  w.r.t.  $c^{(1)}, c^{(2)}, \dots, c^{(m)} \leftarrow$   
(holding  $\mu_1, \dots, \mu_K$  fixed)

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

*move centroid*  
for  $k = 1$  to  $K$   
     $\mu_k :=$  average (mean) of points assigned to cluster  $k$

} *Minimize  $J(\dots)$  w.r.t.  $\mu_1, \dots, \mu_K$*



Machine Learning

# Clustering Random initialization

# K-means algorithm

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

Repeat {  
    for  $i = 1$  to  $m$   
         $c^{(i)} :=$  index (from 1 to  $K$ ) of cluster centroid  
            closest to  $x^{(i)}$   
    for  $k = 1$  to  $K$   
         $\mu_k :=$  average (mean) of points assigned to cluster  $k$   
}

# Random initialization

Should have  $K < m$

Randomly pick  $K$  training examples.

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

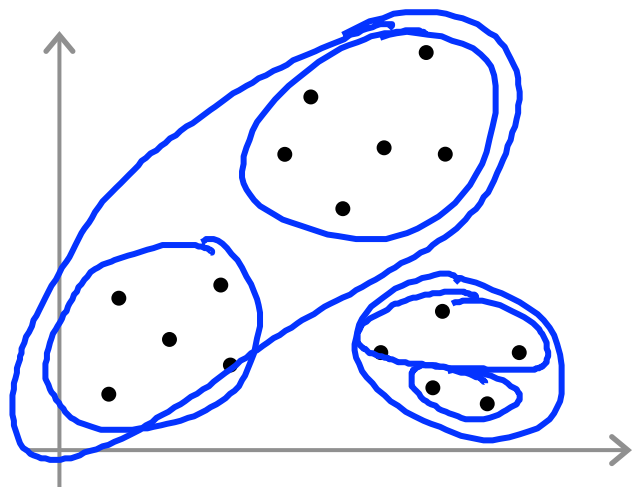
$$\begin{aligned}\mu_1 &= x^{(i)} \\ \mu_2 &= x^{(j)} \\ &\vdots\end{aligned}$$

$K=2$

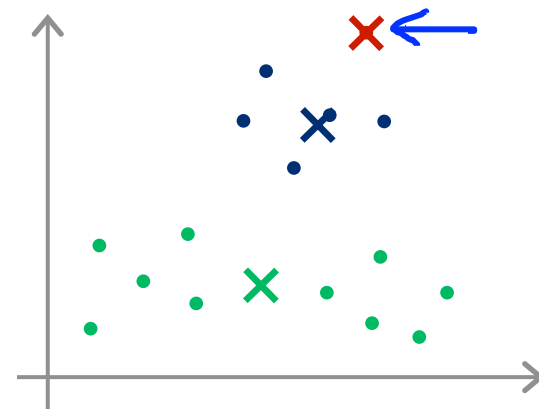
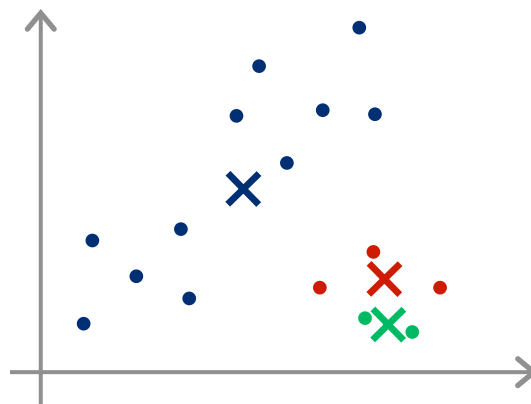
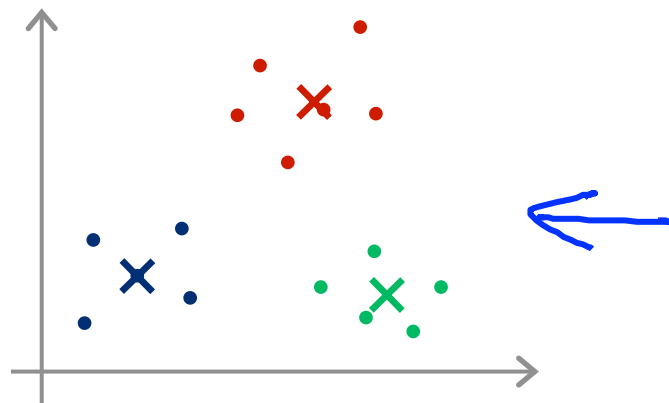


K均值方法 最终可能会得到 不同的结果 取决于 聚类簇的初始化方法 因此也就取决于随机的初始化  
尤其是如果K均值方法落在局部最优的时候

## Local optima



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





我们能做的是 初始化K均值很多次 并运行K均值方法很多次

## Random initialization

For  $i = 1$  to  $100$  {

Randomly initialize K-means.

Run K-means. Get  $c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K$ .

Compute cost function (distortion)

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

}

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



Machine Learning

# Clustering

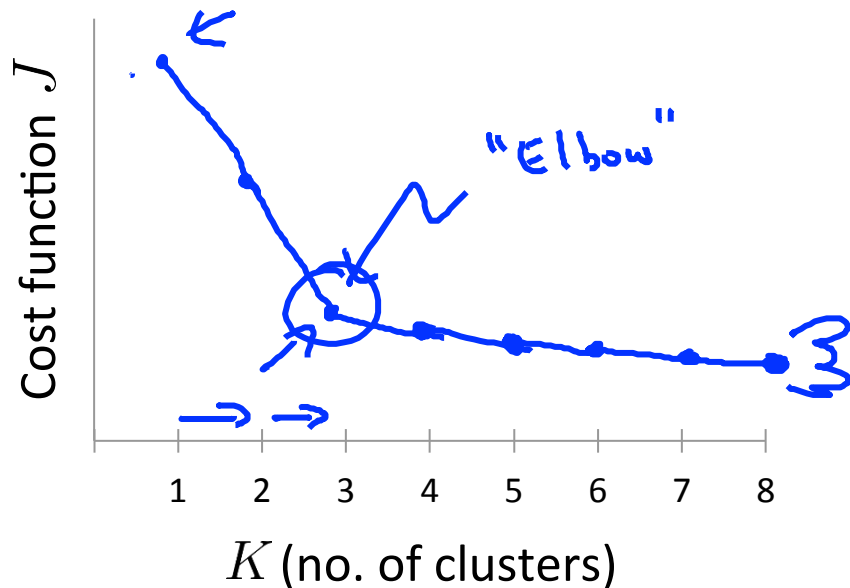
Choosing the  
number of clusters

What is the right value of K?

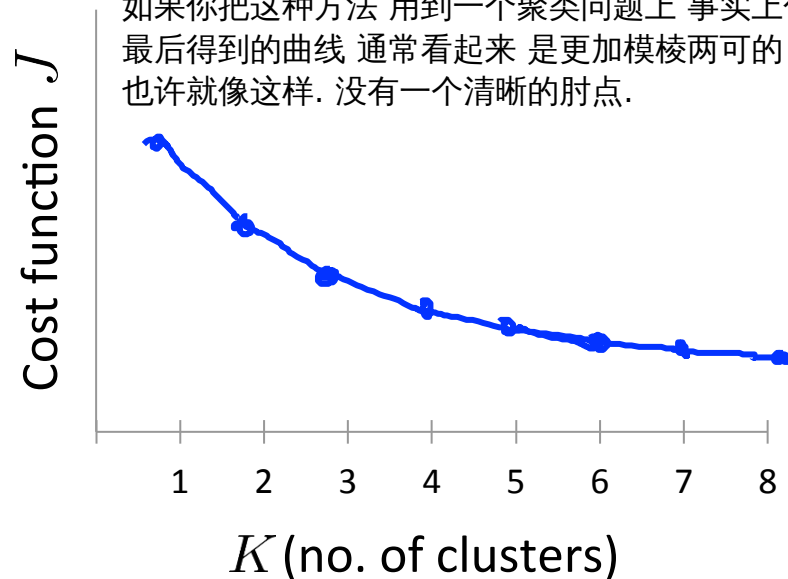


# Choosing the value of $K$

Elbow method:



而事实证明肘部法则 并不那么常用 其中一个原因是如果你把这种方法 用到一个聚类问题上 事实上你最后得到的曲线 通常看起来 是更加模棱两可的 也许就像这样. 没有一个清晰的肘点.



最后 有另外一种方法 来考虑如何选择K的值

**Choosing the value of K** 通常人们使用 K-均值聚类算法 是为了某些后面的用途 或者说某种下游的目的

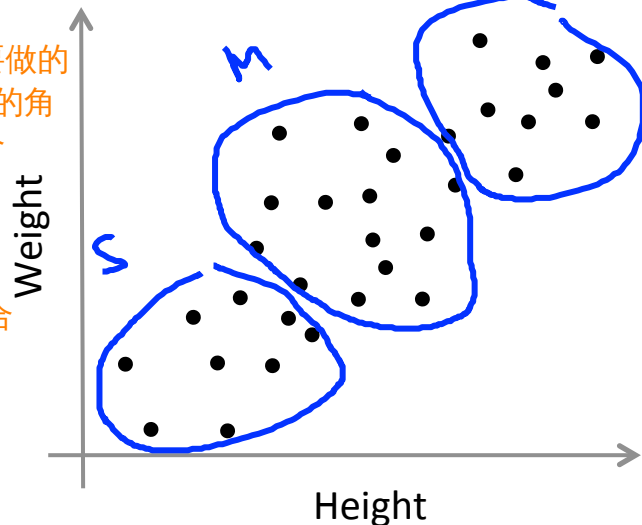
Sometimes, you're running K-means to get clusters to use for some later/downstream purpose. Evaluate K-means based on a metric for how well it performs for that later purpose. 看不同的聚类数量能为 后续下游的目的提供多好的结果

$K=3$  S, M, L

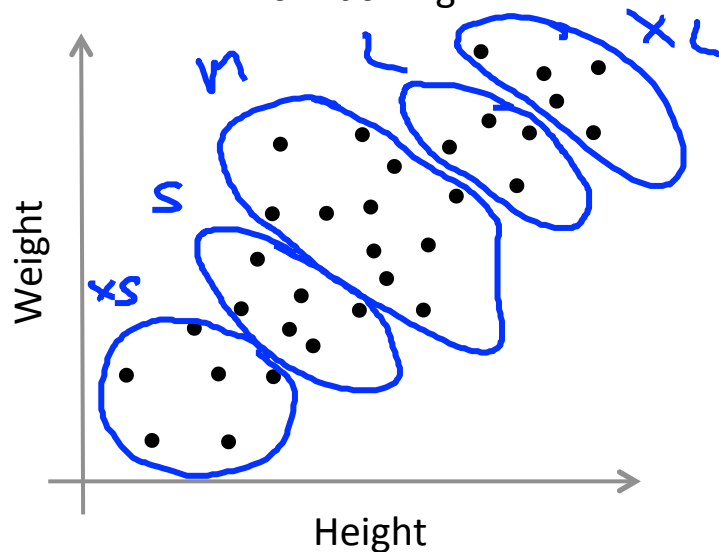
$K=5$  XS, S, M, L, XL

E.g.

T-shirt sizing



T-shirt sizing



具体来说 你要做的是 从T恤生意的角度 来思考这个事情 然后问 “如果我有5个分段 那么我的T恤有多适合我的顾客？”