

13: Clustering

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Unsupervised learning - introduction

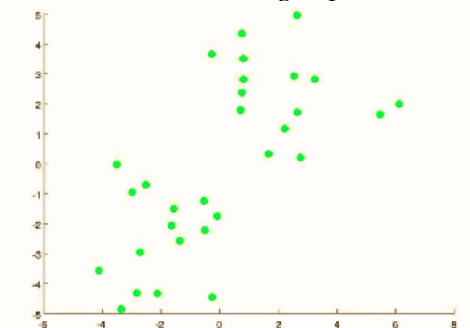
- Talk about **clustering**
 - **Learning from unlabeled data**
- Unsupervised learning
 - Useful to contrast with supervised learning
- Compare and contrast
 - Supervised learning
 - Given a set of labels, fit a hypothesis to it
 - Unsupervised learning
 - **Try and determining structure in the data**
 - **Clustering algorithm groups data together based on data features**
- What is clustering good for
 - **Market segmentation** - group customers into different market segments
 - **Social network analysis** - Facebook "smartlists"
 - **Organizing computer clusters** and data centers for network layout and location
 - **Astronomical data analysis** - Understanding galaxy formation

K-means algorithm

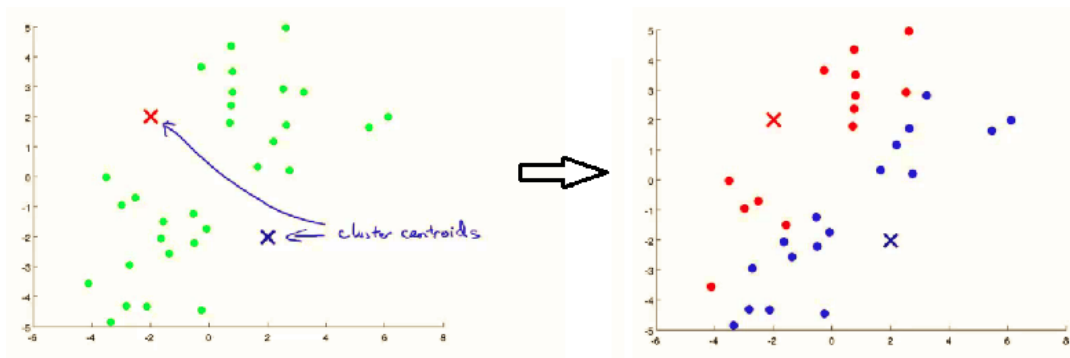
- Want an algorithm to automatically group the data into coherent clusters
- K-means is **by far** the most widely used clustering algorithm

Overview

- Take unlabeled data and group into two clusters

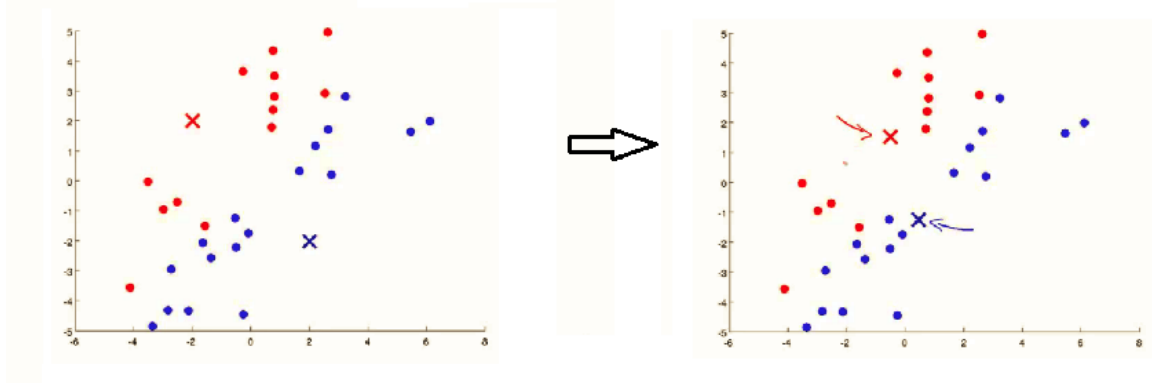


- Algorithm overview
 - 1) Randomly allocate two points as the **cluster centroids**
 - **Have as many cluster centroids as clusters you want to do (K cluster centroids, in fact)**
 - In our example we just have two clusters
 - 2) Cluster assignment step
 - **Go through each example and depending on if it's closer to the red or blue centroid assign each point to one of the two clusters**
 - To demonstrate this, we've gone through the data and "colour" each point red or blue



o 3) Move centroid step

- Take each centroid and move to the average of the correspondingly assigned data-points



- Repeat 2) and 3) until convergence

• More formal definition

o Input:

- K (number of clusters in the data)
- Training set $\{x^1, x^2, x^3, \dots, x^n\}$

o Algorithm:

- Randomly initialize K cluster centroids as $\{\mu_1, \mu_2, \mu_3, \dots, \mu_K\}$

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 }

■ Loop 1

- This inner loop repeatedly sets the $c^{(i)}$ variable to be the index of the closest variable of cluster centroid closest to x^i
- i.e. take i^{th} example, measure squared distance to each cluster centroid, assign $c^{(i)}$ to the cluster closest

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

\swarrow
 $c^{(i)}$

■ Loop 2

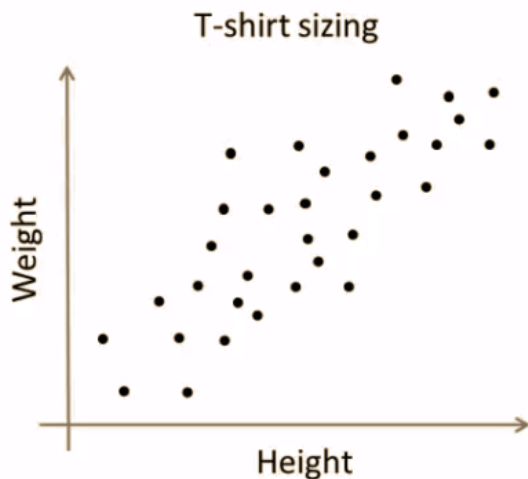
- Loops over each centroid calculate the average mean based on all the points associated with each centroid from $c^{(i)}$
- What if there's a centroid with no data

- Remove that centroid, so end up with K-1 classes
- Or, randomly reinitialize it
- Not sure when though...

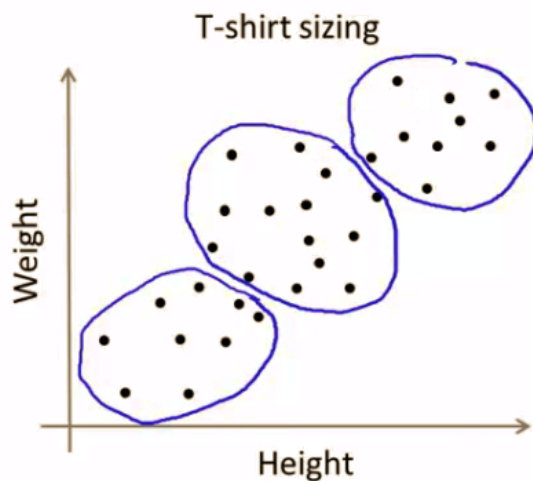
K-means for non-separated clusters

- So far looking at K-means where we have well defined clusters
- But often K-means is applied to datasets where there aren't well defined clusters
 - e.g. T-shirt sizing

eg. what should be in a given cluster is not well defined



- Not obvious discrete groups
- Say you want to have three sizes (S,M,L) how big do you make these?
 - One way would be to run K-means on this data
 - May do the following



- So creates three clusters, even though they aren't really there
- Look at first population of people
 - Try and design a small T-shirt which fits the 1st population
 - And so on for the other two
- This is an example of market segmentation
 - Build products which suit the needs of your subpopulations

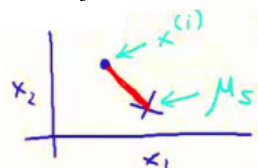
K means optimization objective

- Supervised learning algorithms have an optimization objective (cost function)
 - K-means does too
- K-means has an optimization objective like the supervised learning functions we've seen
 - Why is this good?

- Knowing this is useful because it helps for debugging
- Helps find better clusters
- While K-means is running we keep track of two sets of variables
 - c^i is the index of clusters $\{1, 2, \dots, K\}$ to which x^i is currently assigned
 - i.e. there are m c^i values, as each example has a c^i value, and that value is one of the clusters (i.e. can only be one of K different values)
 - μ_k is the cluster associated with centroid k
 - Locations of cluster centroid k
 - So there are K
 - So these the centroids which exist in the training data space
 - μ_{c^i} is the cluster centroid of the cluster to which example x^i has been assigned to
 - This is more for convenience than anything else
 - You could look up that example i is indexed to cluster j (using the c vector), where j is between 1 and K
 - Then look up the value associated with cluster j in the μ vector (i.e. what are the features associated with μ_j)
 - But instead, for easy description, we have this variable which gets exactly the same value
 - Lets say x^i as been assigned to cluster 5
 - Means that
 - $c^i = 5$
 - $\mu_{c^i} = \mu_5$
 - Using this notation we can write the optimization objective;

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

- i.e. squared distances between training example x^i and the cluster centroid to which x^i has been assigned to
 - This is just what we've been doing, as the visual description below shows;



- The red line here shows the distances between the example x^i and the cluster to which that example has been assigned
 - Means that when the example is very close to the cluster, this value is small
 - When the cluster is very far away from the example, the value is large
- This is sometimes called the **distortion (or distortion cost function)**
- So we are finding the values which minimizes this function;

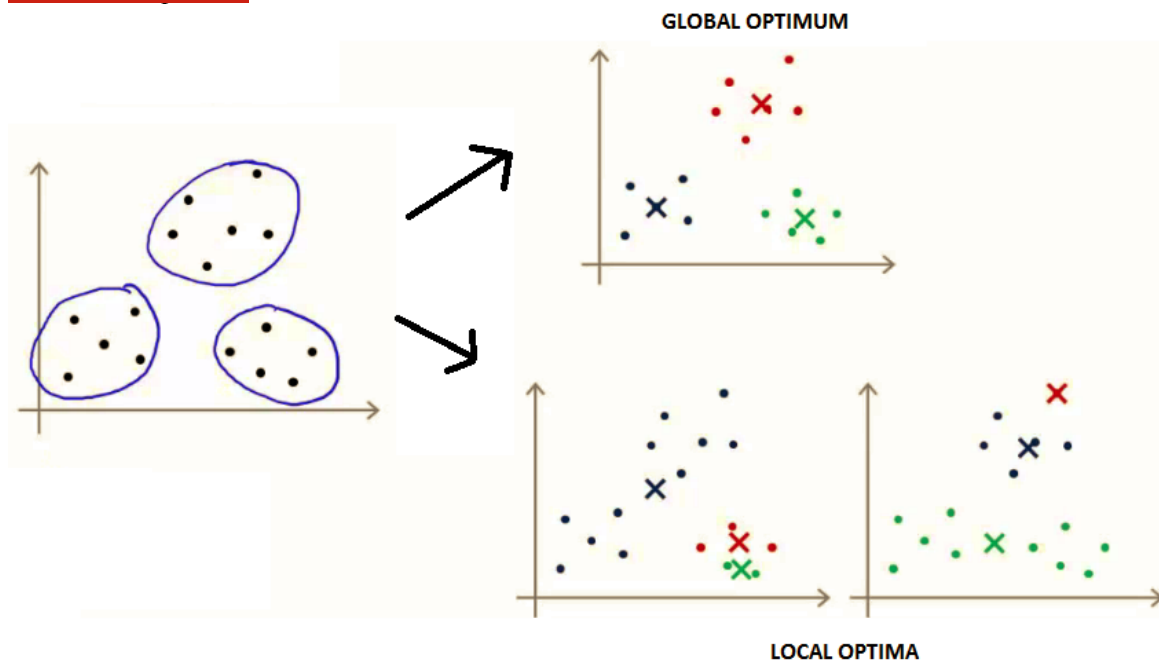
$$\min_{c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K} J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_K)$$

- If we consider the k-means algorithm
 - The **cluster assigned step** is minimizing $J(\dots)$ with respect to $c^1, c^2 \dots c^i$
 - i.e. find the centroid closest to each example
 - Doesn't change the centroids themselves
 - The **move centroid step**
 - We can show this step is choosing the values of μ which minimizes $J(\dots)$ with respect to μ
 - So, we're partitioning the algorithm into two parts
 - First part minimizes the c variables
 - Second part minimizes the J variables
- We can use this knowledge to help debug our K-means algorithm

Random initialization

- How we initialize K-means
 - And how avoid local optimum

- Consider clustering algorithm
 - Never spoke about how we initialize the centroids
 - A few ways - one method is most recommended
- Have number of centroids set to less than number of examples ($K < m$) (if $K > m$ we have a problem)
 - Randomly pick K training examples
 - Set μ_1 up to μ_K to these example's values
- K means can converge to different solutions depending on the initialization setup
 - Risk of local optimum



- The local optimum are valid convergence, but local optimum not global ones
- If this is a concern
 - We can do multiple random initializations
 - See if we get the same result - many same results are likely to indicate a global optimum
- Algorithmically we can do this as follows;


```

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

 - A typical number of times to initialize K-means is 50-1000
 - Randomly initialize K-means
 - For each 100 random initialization run K-means
 - Then compute the distortion on the set of cluster assignments and centroids at convergent
 - End with 100 ways of cluster the data
 - Pick the clustering which gave the lowest distortion
- If you're running K means with 2-10 clusters can help find better global optimum
 - If K is larger than 10, then multiple random initializations are less likely to be necessary
 - First solution is probably good enough (better granularity of clustering)

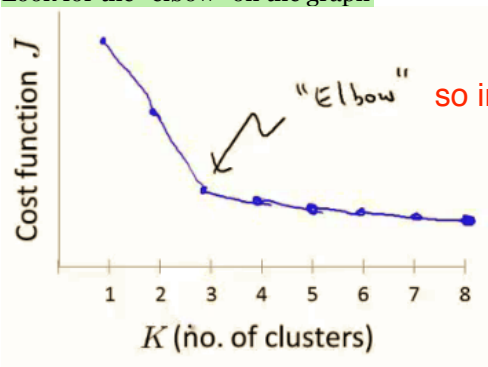
How do we choose the number of clusters?

- Choosing K ?
 - Not a great way to do this automatically
 - Normally use visualizations to do it manually
- What are the intuitions regarding the data?
- Why is this hard
 - Sometimes very ambiguous

- e.g. two clusters or four clusters
- Not necessarily a correct answer
- This is why doing it automatic this is hard

Elbow method

- Vary K and compute cost function at a range of K values
- As K increases $J(\dots)$ minimum value should decrease (i.e. you decrease the granularity so centroids can better optimize)
 - Plot this (K vs $J()$)
- Look for the "elbow" on the graph

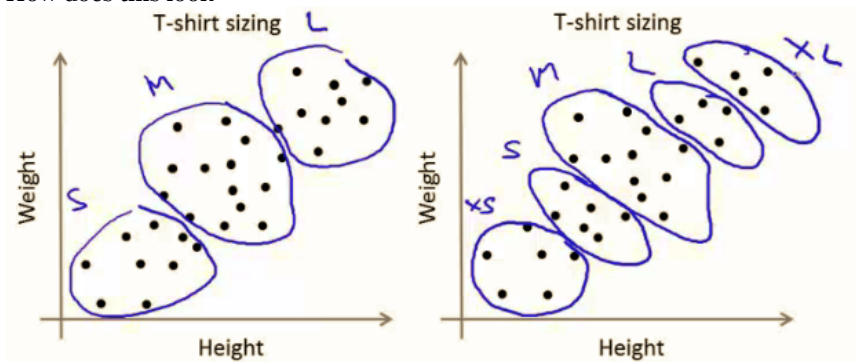


so in this case, 3 cluster centroids are good

- Chose the "elbow" number of clusters
- If you get a nice plot this is a reasonable way of choosing K
- **Risks**
 - Normally you don't get a a nice line -> no clear elbow on curve
 - Not really that helpful

Another method for choosing K

- Using K-means for market segmentation
- Running K-means for a later/downstream purpose
 - See how well different number of clusters serve you later needs
- e.g.
 - T-shirt size example
 - If you have three sizes (S,M,L)
 - Or five sizes (XS, S, M, L, XL)
 - Run K means where $K = 3$ and $K = 5$
 - How does this look



- This gives a way to chose the number of clusters
 - Could consider the cost of making extra sizes vs. how well distributed the products are
 - How important are those sizes though? (e.g. more sizes might make the customers happier)
 - So applied problem may help guide the number of clusters