13: Clustering

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Unsupervised learning - introduction

- Talk about **clustering**
  - **Learning from unlabeled data**
- Unsupervised learning
  - Useful to contras 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"
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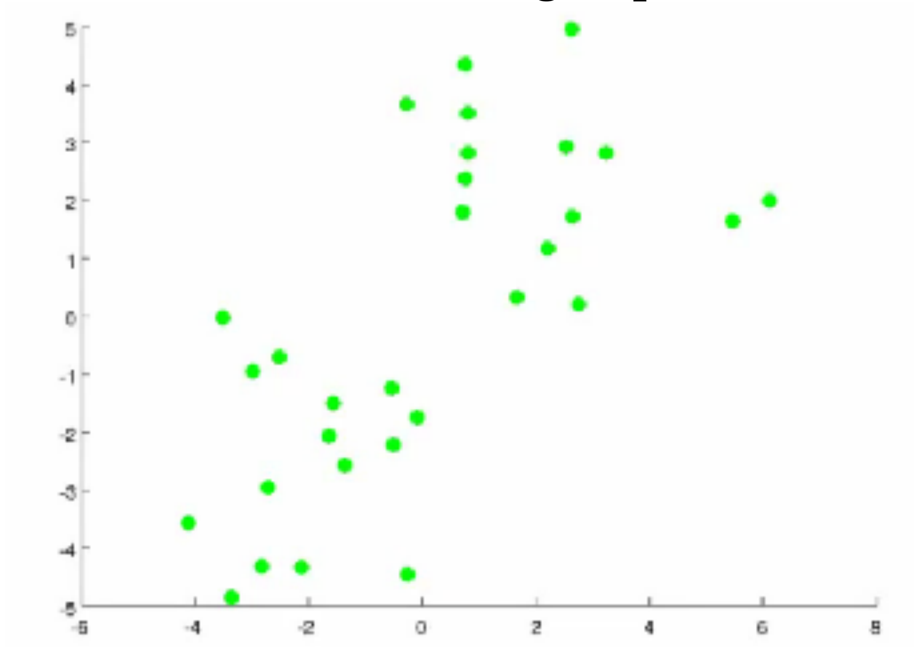
  - **Astronomical data analysis** - Understanding galaxy formation

K-means algorithm

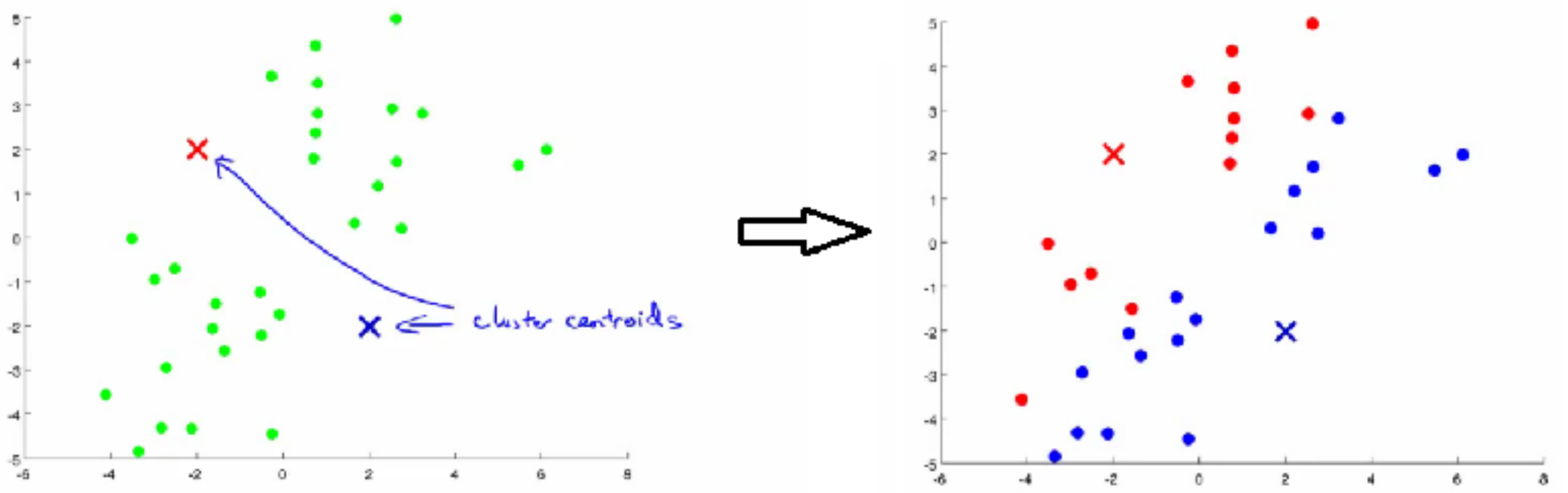
- Want an algorithm to automatically group the data into coherent clusters
- K-means is **by far** the most widely used clustering algorithm

Overview

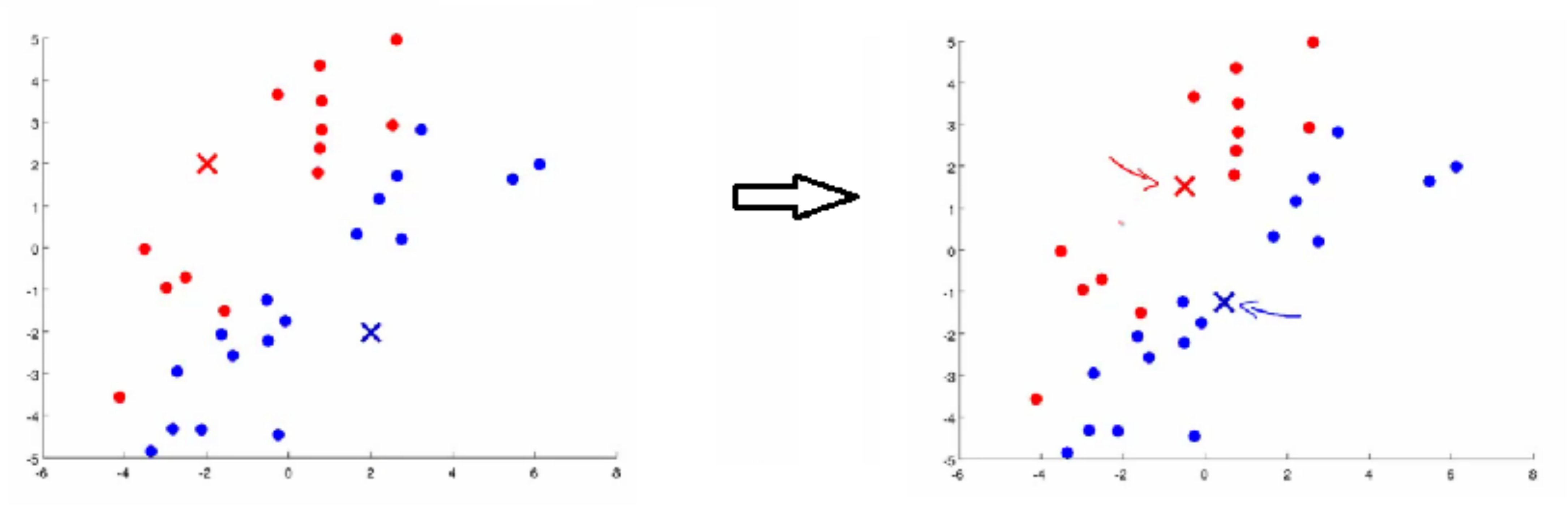
- Take unlabeled data and group into two clusters



- 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



  - 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
    - **Input:**
        - K (number of clusters in the data)
        - Training set {x^1, x^2, x^3 ..., x^n)
    - **Algorithm:**
        - Randomly initialize K cluster centroids as {μ_1, μ_2, μ_3 ... μ_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 $k$  }
```

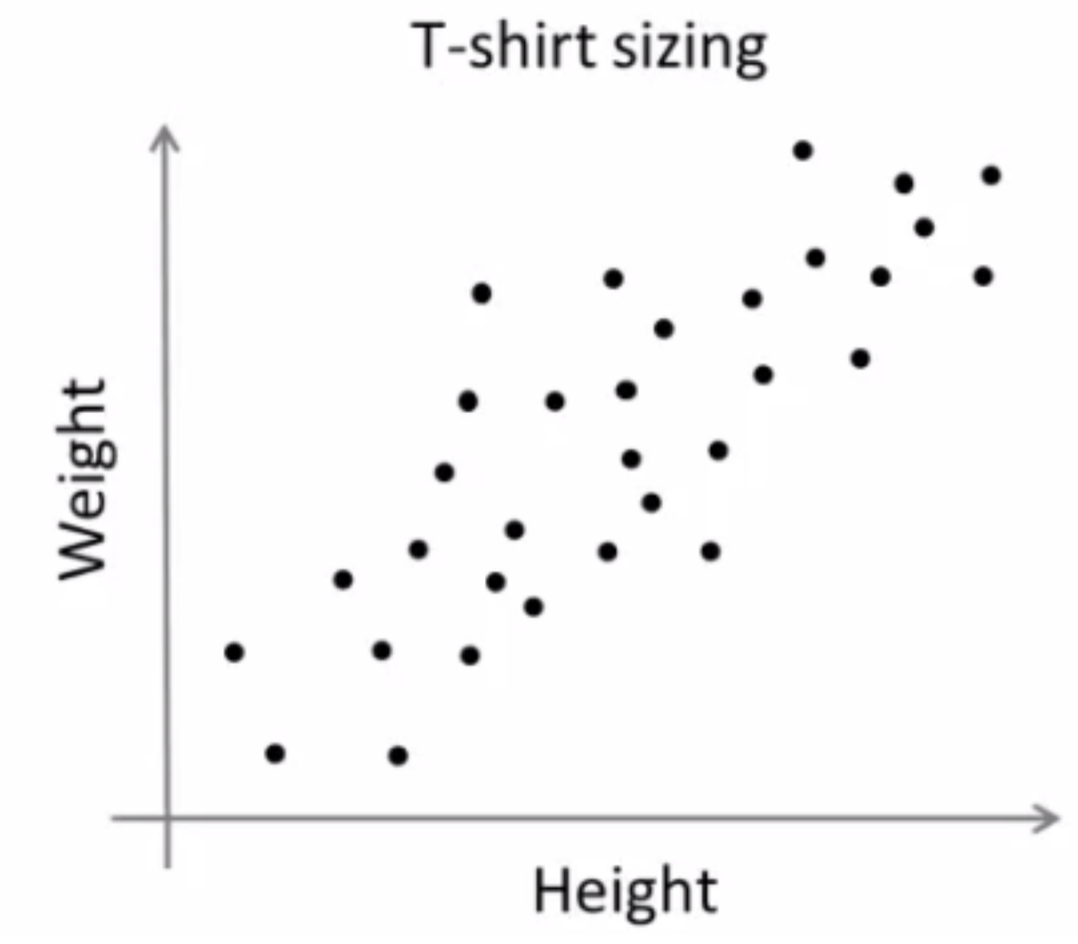
            - Loop 1
                - This inner loop repeatedly sets the $c^{(i)}$ variable to be the index of the closes variable of cluster centroid closes to x^i
                - i.e. take ith example, measure squared distance to each cluster centroid, assign $c^{(i)}$to the cluster closest

$$\min_{k} \|x^{(i)} - \mu_k\|^2 \quad k \rightarrow c^{(i)}$$

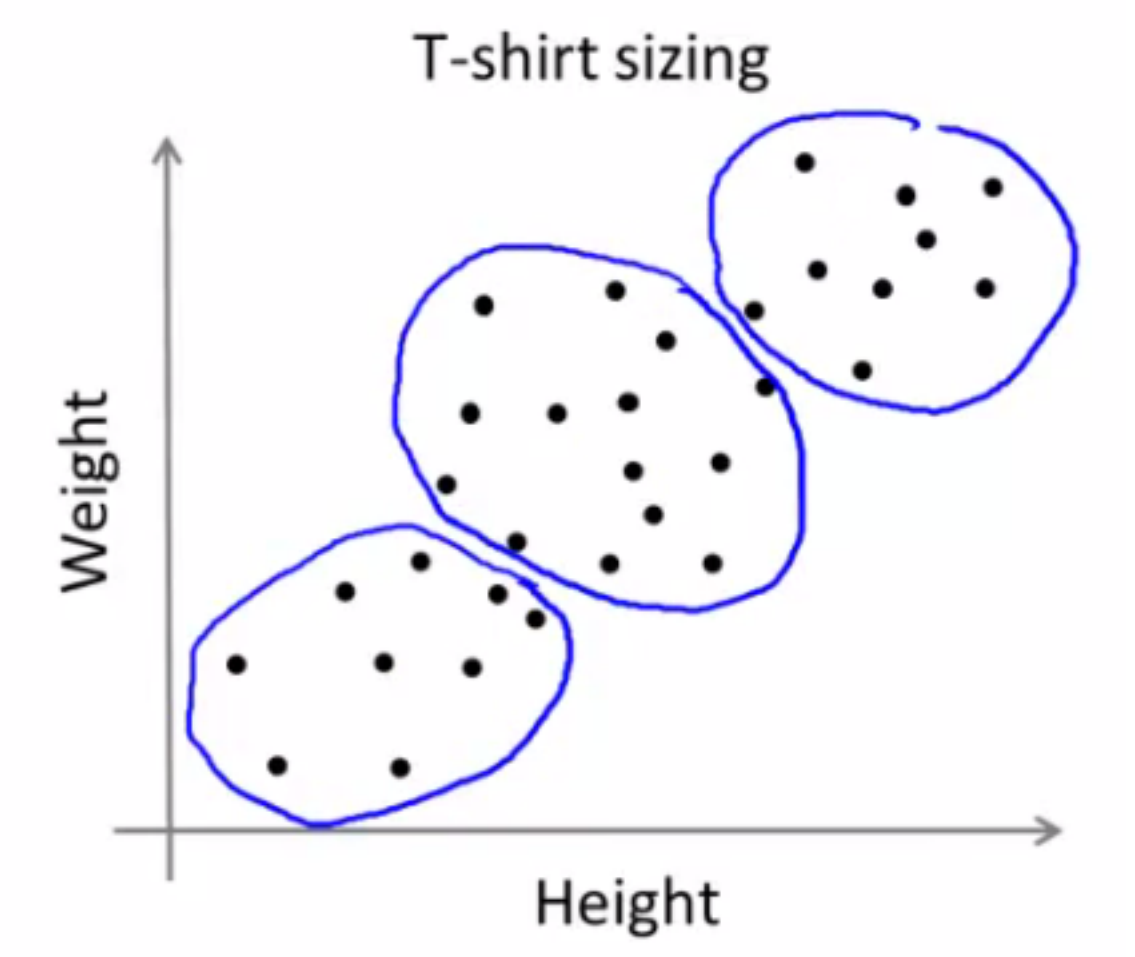
            - Loop 2
                - Loops over each centroid calculate the average mean based on all the points associated with each centroid from $c^{(i)}$
        - What if there's a centroid with no data
            - Remove that centroid, so end up with K-1 classes
            - Or, randomly reinitialize 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



- 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

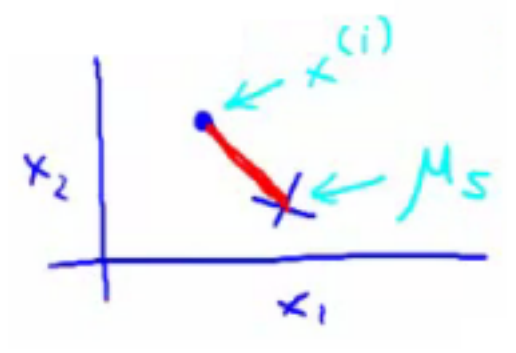
K means optimization objective

- 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, ..., 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 the 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
    - $\mu_c{}^i$, 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;



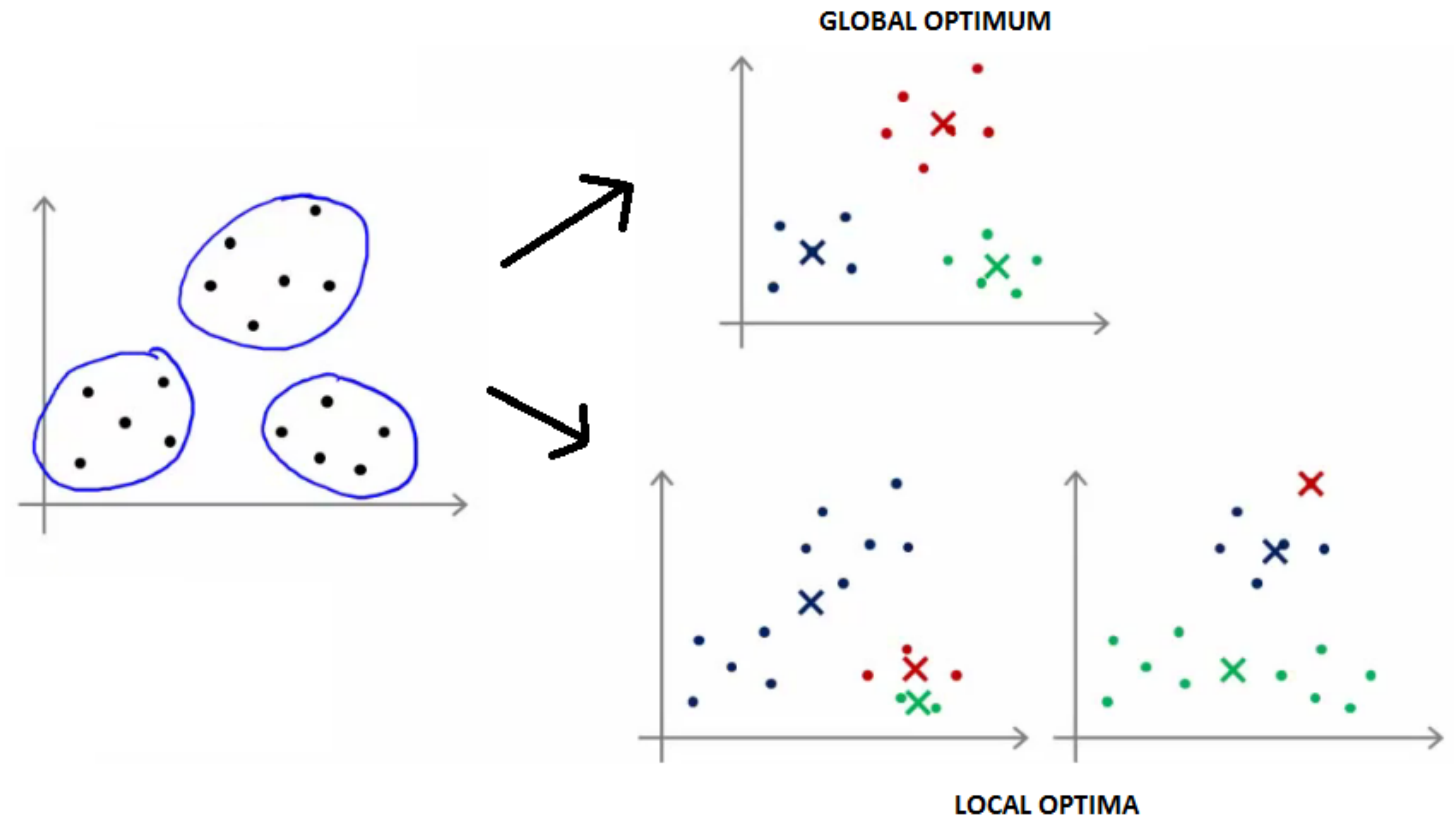
    - The red line here shows the distances between the example x^i and the cluster to which that example has been assigned
        - Means that when the example is very close to the cluster, this value is small
        - When the cluster is very far away from the example, the value is large
  - This is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

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

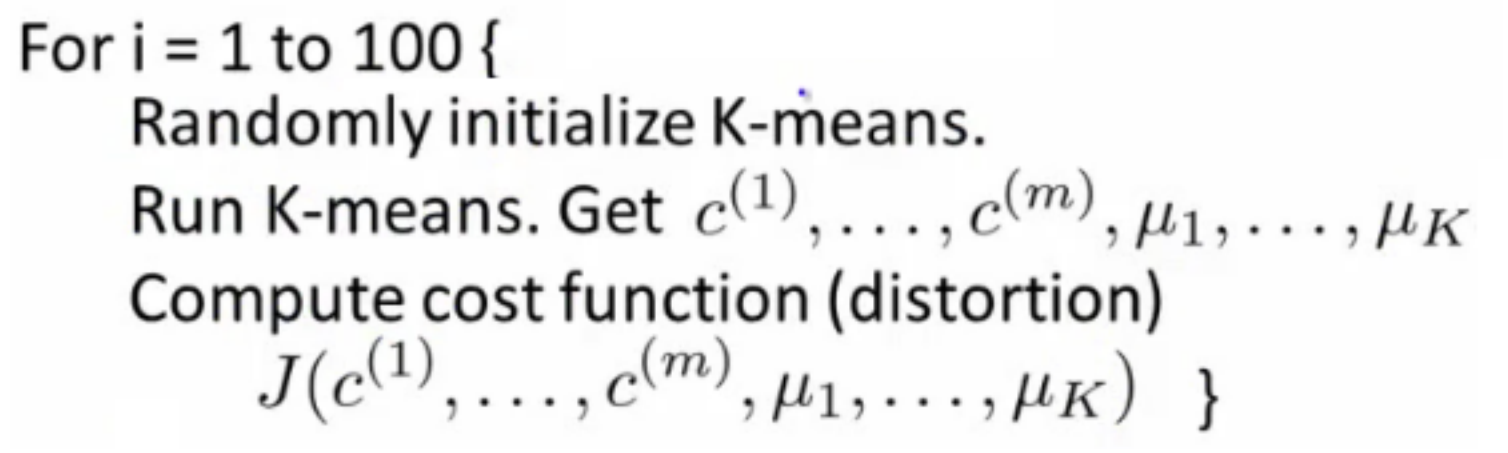
- If we consider the k-means algorithm
  - The **cluster assigned step** is minimizing J(...) with respect to $c^1, c^2 \dots c^i$
    - i.e. find the centroid closest to each example
    - Doesn't change the centroids themselves
  - The **move centroid step**
    - We can show this step is choosing the values of μ which minimizes J(...) 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)o
  - 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 $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$
    Compute cost function (distortion)
        $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$ }
```

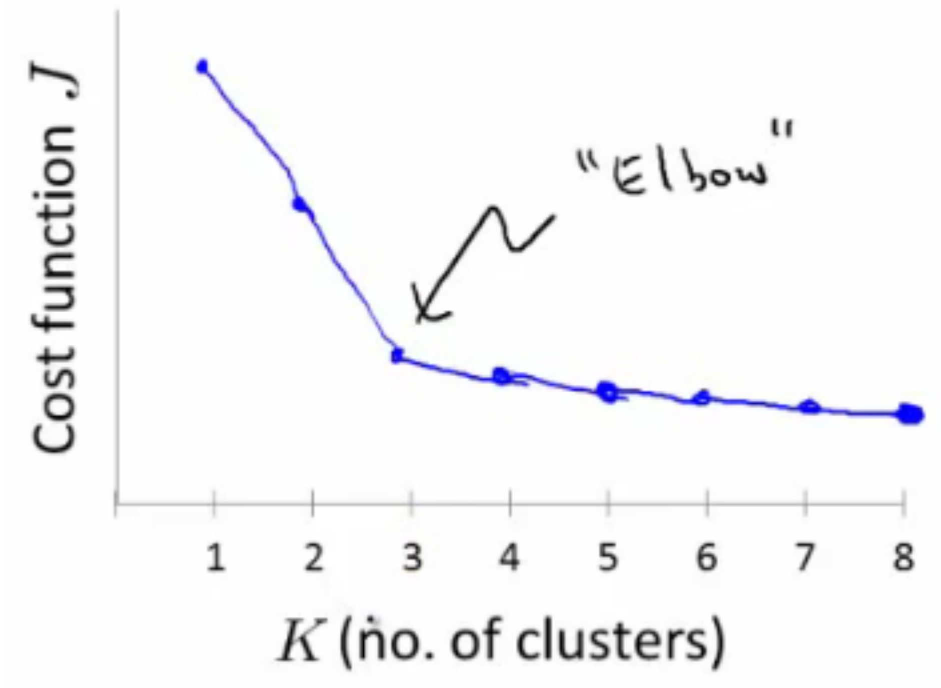
    - A typical number of times to initialize K-means is 50-1000
    - Randomly initialize K-means
        - For each 100 random initialization run K-means
        - Then compute the distortion on the set of cluster assignments and centroids at convergent
        - End with 100 ways of cluster the data
        - 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

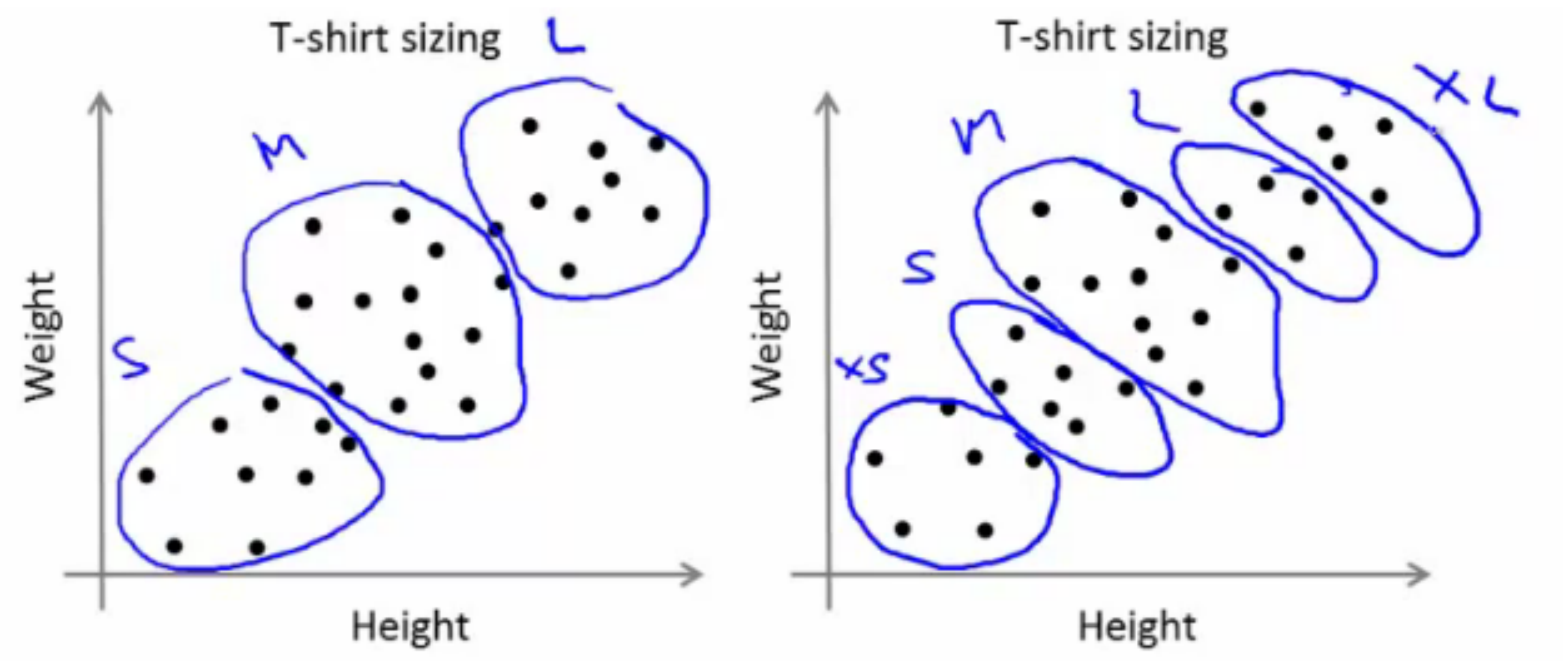
- Vary K and compute cost function at a range of K values
- As K increases J(...) minimum value should decrease (i.e. you decrease the granularity so centroids can better optimize)
    - Plot this (K vs J())
- Look for the "elbow" on the graph



- 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