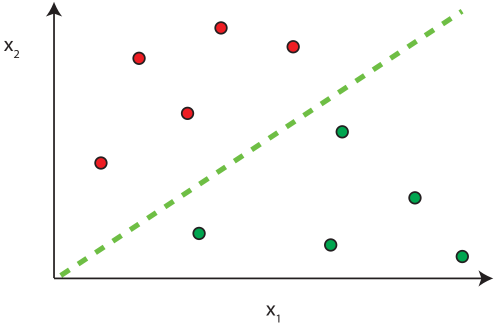
Overview

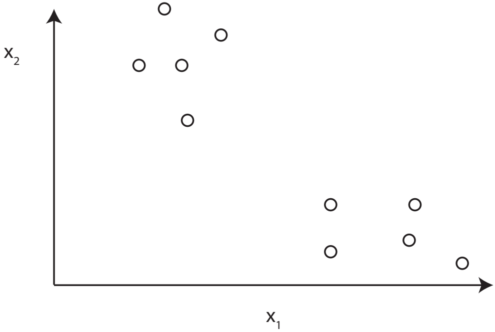
- Supervised vs Unsupervised Learning
- Clustering: k-means algorithm

Supervised Learning



- Training data: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(m)}, y^{(m)})\}$
- Training data is labelled i.e. we know $y^{(1)}$, $y^{(2)}$ etc

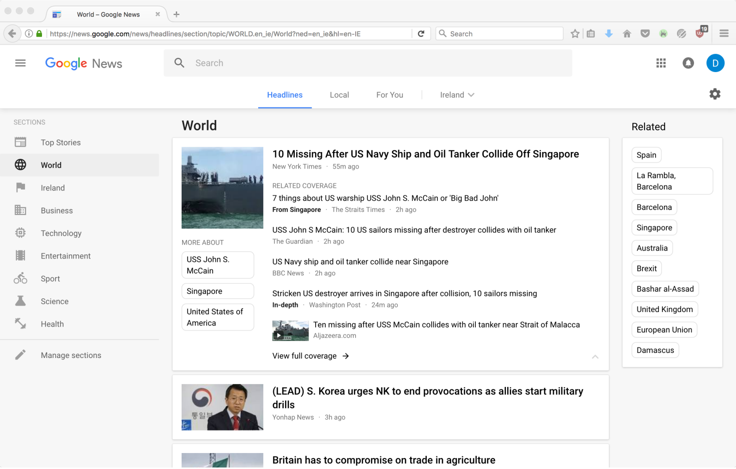
Unsupervised Learning



- Training data: $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$
- Training data is unlabelled i.e. we do not know $y^{(1)}$, $y^{(2)}$ etc
- We need algorithms that try to cluster the training data ...

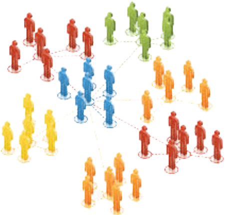
Applications

- Google News

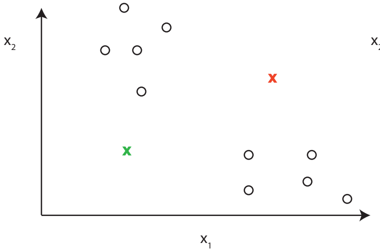


Applications

- Fraud detection - try to cluster into normal and anomalous activity based on observed features
- Market segmentation e.g. try to detect customers about to leave a service
- Social network analysis e.g. try to detect communities/groupings



k-means algorithm



k-means algorithm

Input:

- k, number of clusters
- Training data: $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$
- We'll drop the $x_0 = 1$ convention and use $x_1, \ldots, x_n$ as elements of x.

Randomly initialise k cluster centres $\mu^{(1)}, \ldots, \mu^{(k)}$. e.g. choose k points from training set and use these (need $k < m$).

- Repeat:
  cluster assignment:
  for $i = 1$ to m,
  $c^{(i)} :=$ index of cluster centres closest to $x^{(i)}$
  update centres:
  for $j = 1$ to k
  $\mu^{(j)} :=$ average (mean) of points assigned to cluster j
- Stop when assignments no longer change

k-means algorithm: optimisation objective

$c^{(i)}$ = index of cluster to which example $x^{(i)}$ is assigned
μ_j = centre of cluster j
$\mu_{c^{(i)}}$ = cluster centre to which example $x^{(i)}$ is assigned
$\|x - c\|^2 = \sum_{j=1}^{n}(x_j - c_j)^2$ (Euclidean distance)

Goal: minimise
$J(c^{(1)}, \ldots, c^{(m)}, \mu^{(1)}, \ldots, \mu^{(k)}) = \frac{1}{m} \sum_{i=1}^{m} \|x^{(i)} - \mu^{(c^{(i)})}\|^2$

k-means algorithm: optimisation objective

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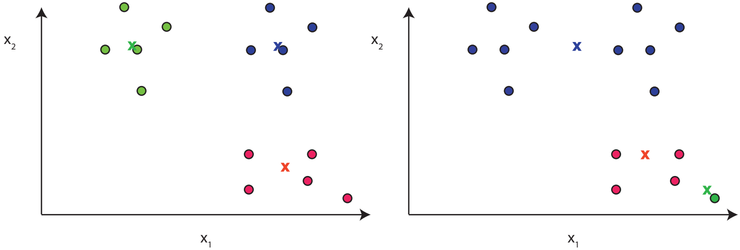
$J(c^{(1)}, \dots, c^{(m)}, \mu^{(1)}, \dots, \mu^{(k)}) = \frac{1}{m} \sum_{i=1}^{m} \|x^{(i)} - \mu^{(c^{(i)})}\|^2$

- Repeat:
  cluster assignment:
  for $i = 1$ to m,
  $c^{(i)}$:= index of cluster centres closest to $x^{(i)}$
  i.e. select $c^{(1)}, \dots, c^{(m)}$ to minimise
  $J(c^{(1)}, \dots, c^{(m)}, \mu^{(1)}, \dots, \mu^{(k)})$
  update centres:
  for $j = 1$ to k
  μ_j := average (mean) of points assigned to cluster j
  $= \frac{1}{|C_K|} \sum_{k \in C_j} x^k$ where $C_j = \{i : c^{(i)} = j\}$
  i.e. select $\mu^{(1)}, \dots, \mu^{(k)}$ to minimise
  $J(c^{(1)}, \dots, c^{(m)}, \mu^{(1)}, \dots, \mu^{(k)})$ (a least squares task)
- Stop when assignments no longer change

k-means algorithm: local optima

- k-means algorithm can converge to a local optimum, rather than a global optimum. e.g.



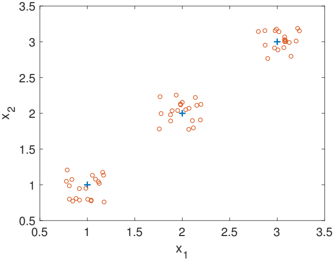
k-means algorithm: local optima

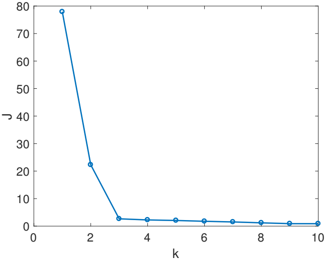
Use random initialisation and multiple runs of algorithm:

for $i = 1$ to 100
  randomly initialise the k centres $\mu^{(1)}, \ldots, \mu^{(k)}$
  run k-means algorithm
  compute cost function $J(c^{(1)}, \ldots, c^{(m)}, \mu^{(1)}, \ldots, \mu^{(k)})$

Pick clustering that gives lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu^{(1)}, \ldots, \mu^{(jk)})$

k-means algorithm: choosing the number of clusters

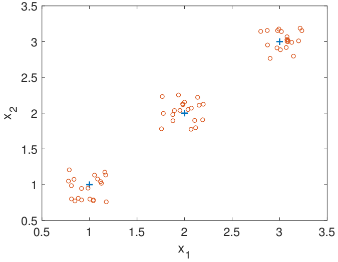


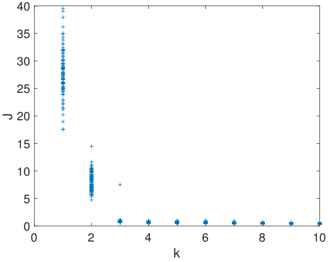


Elbow method:

- Vary k and pick value at "elbow"
- Problem: there might not be an elbow, or at least not a clear one

k-means algorithm: choosing the number of clusters





Cross-validation:

- Randomly select a subset of training data
- run k means algorithm
- Calculate cost $J(c^{(1)}, \ldots, c^{(m)}, \mu^{(1)}, \ldots, \mu^{(k)})$ for the test data not used for training
- Repeat for multiple random subsets and several values of k.