A Bit of History

- [J. B. MacQueen, 1967]
- [http://img1.wikia.nocookie.net/_cb20110723073418/pixar/images/b/b2/Lightning_mcqueen_cars_2.png]

- [H. Steinhaus 57], [S. Lloyd 57], [E. W. Forgy 65]
- Vector Quantisation/Clustering/Bunching/Grouping
- Old, but often still the first choice!
- Learning: Supervised, Unsupervised, Reinforcement, Semi-supervised
- Two flavours of K-Means: K as a parameter, & the distance threshold as a parameter
- Crisp boundaries: grading, states on a linguistic basis(hmm...), f'print image ROI.Fuzzy: signal-noise separation, concept of well-built (h, w)

Xpdf: k_means_em.pdf

Types of Algorithms

[https://images-na.ssl-images-amazon.com/images/M/MV5BOTU5NDkzNTM5MV5BMl5BanBnXkFtZTgwMDU4ODE5MDE@._V1_QL50_.jpg]

- The Good: Polynomial Time Complexity, $\mathcal{O}(n^k)$
  Sorting, DFT, FFT
- The Bad: Exponential Time Complexity, $\mathcal{O}(k^n)$

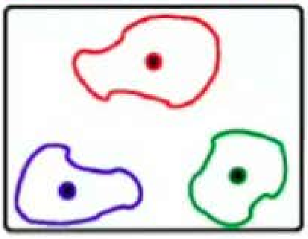
  NP–Hard

  NP–Complete

  Boolean functions of n variables: minterms, combinations of minterms; TSP
- The Ugly: Opt converge with prob 1, but infinite time

The Goal

- N points $\{\mathbf{x}_1 \ldots \mathbf{x}_N\}$ to be grouped into K clusters
- $\boldsymbol{\mu}_j$: prototype of the jth cluster (e.g., centre)
- such that the sum of squared distances of each data point to its closest vector $\boldsymbol{\mu}_j$ is a minimum
- Vector Quantisation: $\boldsymbol{\mu}_j$: codebook vectors
- Objective Function (Distortion Measure):



$$J \triangleq \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} \, ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$$

- Binary Indicator variable $r_{ij} \triangleq 1$: ith data point assigned to jth cluster, & $\triangleq 0$, otherwise
- Find $\{r_{ij}\}$ & $\{\boldsymbol{\mu}_j\}$ such that J is minimised

One way to solve this: two phases, EM-framework

Choose K initial cluster centres $\{\boldsymbol{\mu}_j\}$

1. Fixed $\{\boldsymbol{\mu}_j\}$, find assignment $\{r_{ij}\}$: Expectation
2. Keep $\{r_{ij}\}$ fixed, find $\{\boldsymbol{\mu}_j\}$: Maximisation

REPEAT till convergence/fixed max# of iterations

Convergence: each step provably convergent!

- Expectation Step: $\{\boldsymbol{\mu}_j\}$ fixed, minimise J wrt $\{r_{ij}\}$

$J \stackrel{\triangle}{=} \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} \, ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$ This is linear in $\{r_{ij}\}$.
For $\mathbf{x}_i$, assign it to the closest cluster centre.

- Minimisation Step: $\{r_{ij}\}$ fixed, minimise J wrt $\{\boldsymbol{\mu}_j\}$

$J \triangleq \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} ||\mathbf{x}_i - \boldsymbol{\mu}_j||^2$ This is quadratic in $\{\boldsymbol{\mu}_j\}$.

$$\frac{\partial J}{\partial \{\boldsymbol{\mu}_j\}} = 0 \implies \sum_{i=1}^{N} 0 + 0 + \ldots + 2 r_{ij}(\mathbf{x}_i - \{\boldsymbol{\mu}_j\}) + \ldots = 0$$

$$\implies \sum_{i=1}^{N} r_{ij}(\mathbf{x}_i - \{\boldsymbol{\mu}_j\}) = 0 \implies$$

$$\sum_{i=1}^{N} r_{ij}\mathbf{x}_i = \left(\sum_{i=1}^{N} r_{ij}\right)\boldsymbol{\mu}_j \implies \boxed{\boldsymbol{\mu}_j = \frac{\sum_{i=1}^{N} r_{ij}\mathbf{x}_i}{\sum_{i=1}^{N} r_{ij}}}$$

Sum of points in cluster j / # of points in cluster j

= Mean of all points in cluster j!

ALGORITHM K-Means
INITIALISATION: Fix $\boldsymbol{\mu}_j$
1. [E-Step] $\{\boldsymbol{\mu}_j\}$ (centres) fixed, find $\{r_{ij}\}$ (assignment) Assign points to closest cluster prototype ($J \downarrow$)
1. [M-Step] $\{r_{ij}\}$ (assignment) fixed, find $\{\boldsymbol{\mu}_j\}$ (centres) Recompute cluster centres ($J \downarrow$)
REPEAT till no change in assign't/max iterations

K-Means: Some Points

- Could converge to a local min
- Initialisation: random subset of size K of the data points as the cluster prototypes
- E-Step: distance computations b/w every data point & every prototype vector $\mathcal{O}(KN)$
- E-step: $\mathcal{O}(KN)$; M-Step: $\mathcal{O}(N)$ Can run for each $\binom{N}{K}$ start seeds, or a max. Run for few K
- Alternate formulation with distance threshold: on-line algo, works as data comes in
- Limitations: e.g., data in concentric circles

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- Generalisation: prob/fuzzy assignment of $\{r_{ij}\}$

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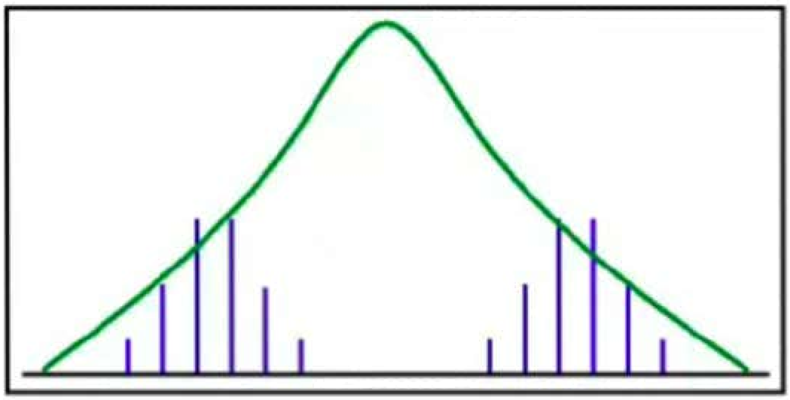
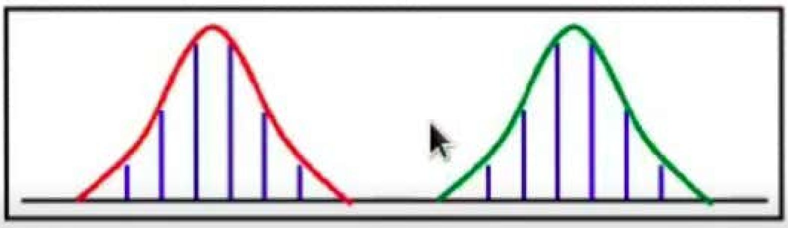
M-of-Gs: Curve-Fitting

- Almost any parameterised curve can be fitted to a bunch of points with an associated error cost
- Gaussian: computationally nice: 2 moments
  - any hump/bump:one Gaussian
  - const region: many closely-spaced Gaussians
- 

  1-G: bad fit as most prob region doesn't have many samples
- 

  2-G: better fit