Unsupervised Learning

Clustering

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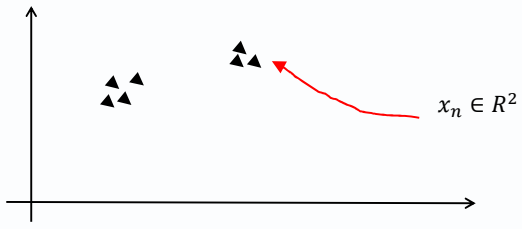
Unsupervised Learning

By contrast to supervised learning the training set consists of only data points (no 'target data').

Goal: Find some structure in the data

$$X = \{x_n | n = 1 \dots m\}$$



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Clustering

Given the hue and size (features) of fruits, group them into clusters

Possible uses: Find hidden structure in the data

- news clustering, genes clustering, image clustering, audio clustering.

Slide no: 0-3

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K - means clustering

Given: $X = \{x_n | i = 1 \dots m\}$ $x_n \in R^N$ and the number of clusters K

Find: $\{c_n | n = 1 \dots m\}, c_n \in [1 \dots K]$ and $\{\mu_k | k = 1 \dots \mathrm{K}\}, \mu_k \in R^N$

The K-Means clustering algorithm works as follows. First initialize K centres $\boldsymbol{\mu}_k$ (for example by picking K input samples randomly) then iteratively repeat the following steps.

$\mathrm{Step} - 1$: classify x_n to the cluster k with the nearest centre μ_k

$c_n = k$ (or $x_n \in C_k$) if $\|x_n - \mu_{c_n}\| < \|x_n - \mu_j\|$ for all $j \neq k$

$\mathrm{Step} - 2$: re$-$compute μ_k to be the mean of the class C_k

$$\mu_k = \frac{\sum_{x_n \in C_k} x_n}{\sum_{x_n \in C_k} 1} = \frac{1}{|C_k|} \sum_{x_n \in C_k} x_n$$

Until the solution stabilizes (i.e. until clusters of x_n stop changing in Step 1).

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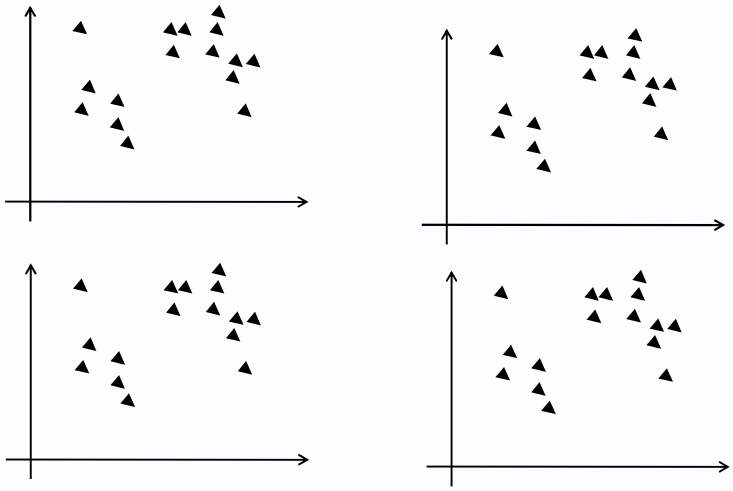
K - means clustering (example)



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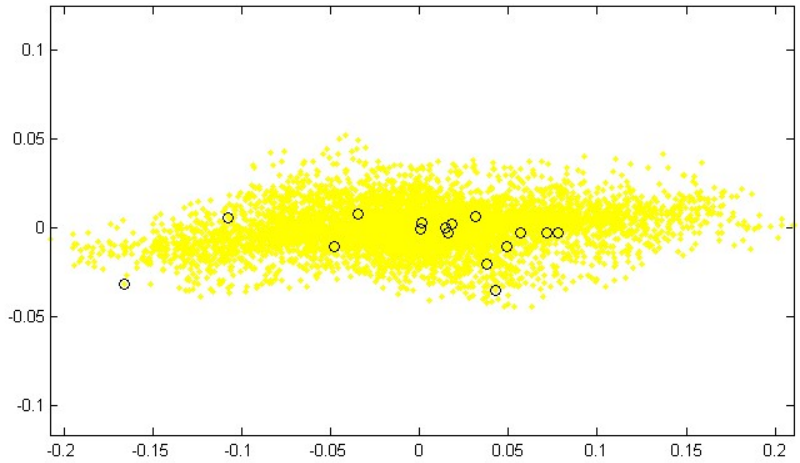
K - means: Initialisation



We have used random initialisation – more sophisticated schemes exist

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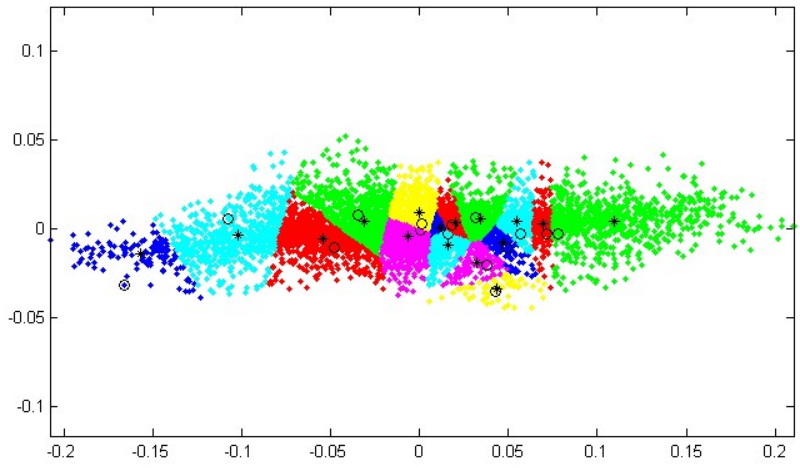
K - means: 1st iteration



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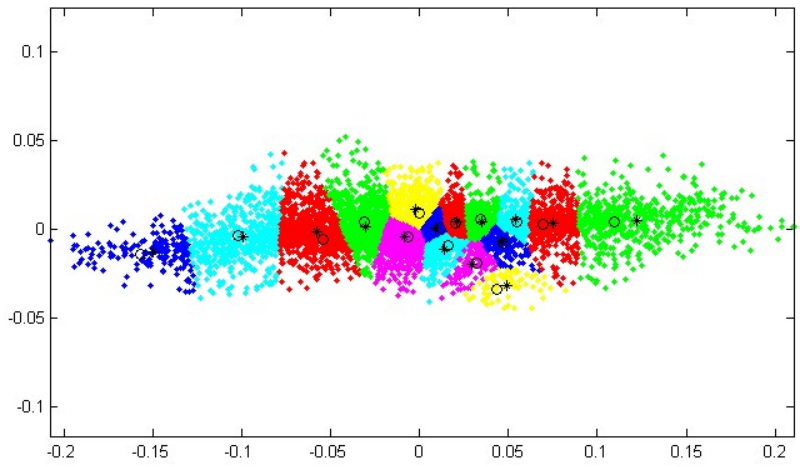
K - means: 2nd iteration



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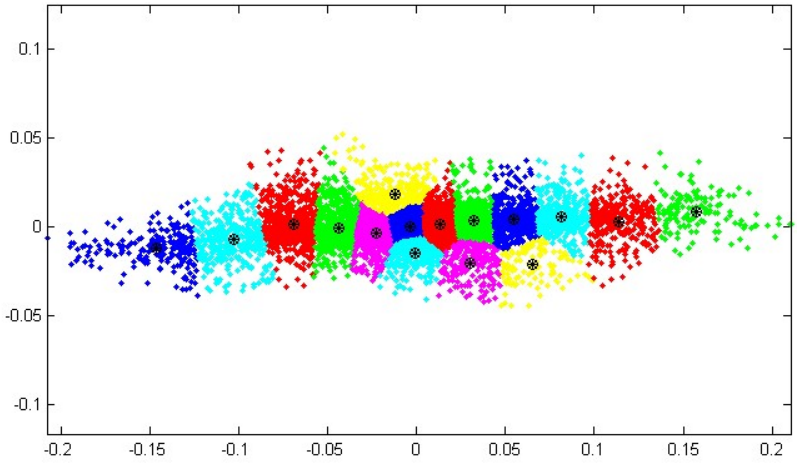
K - means: converged (20th iteration)



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Convergence of K - means

We can now show that the two steps of K-means optimise a cost function

$$J(c_1, \ldots, c_n, \mu_1, \ldots, \mu_K) = \sum_n \|x_n - \mu_{c_n}\|^2$$

Where $c_n \in [1 \ldots K]$ indicates the cluster to which x_n belongs.

Non convex function, may have local minima, difficult to optimize.

K-means follows an optimisation scheme called co-ordinate descent (or ascent if the objective needs to be maximised)

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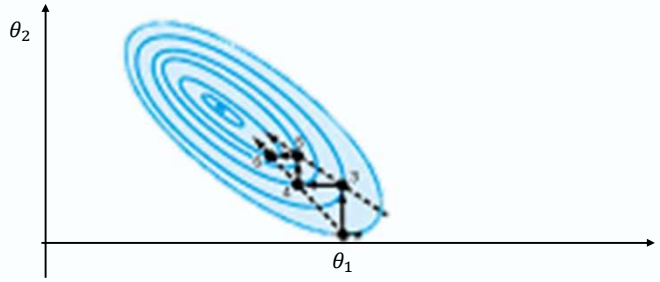
Coordinate descent

Minimize $J(\theta_1, \theta_2)$ by iterating between two steps:

Step 1: Keep θ_2 fixed and optimise w.r.t. θ_1, i.e., $\theta_1^{k+1} = argmin\, J(\theta_1, \theta_2^k)$

Step 2: Keep θ_1 fixed and optimise w.r.t θ_2, i.e., $\theta_2^{k+1} = argmin\, J(\theta_1^{k+1}, \theta_2)$

Until convergence



Given some conditions, the procedure converges to a local minimum

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"Optimality" of K - means (1)

Cost function $J(c_1, \ldots, c_m, \mu_1, \ldots, \mu_K) = \sum_n \|x_n - \mu_{c_n}\|^2$

Step 1: Optimise w.r.t $c_1, \ldots, c_m$

$$c_n^* = \text{argmin}_{c_n} \sum_{n=1} \|x_n - \mu_{c_n}\|^2 = \text{argmin}_{c_n} \|x_n - \mu_{c_n}\|^2$$

Thus to minimise the cost with respect to classifications we choose $\mathbf{c_n}$ to be the cluster k for which $||x_n - \mu_k||^2$ is smallest (i.e. we choose the closest centre).

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"Optimality" of K - means (1)

Cost function $J(c_1, \dots, c_m, \mu_1, \dots, m_k) = \sum_{n=1}^{m} \left|\left|x_n - \mu_{c_n}\right|\right|^2$

Step 2: Optimise w.r.t μ_k by setting the derivative wrt it to zero.

$$\nabla_{\mu_k} J(\dots) = \sum_{x_n \in C_k} -2\mu_k(x_n - \mu_k)$$

$$\nabla_{\mu_k} J(\dots) = 0 \Rightarrow \mu_k = \frac{\sum_{x_n \in C_k} x_n}{\sum_{x_n \in C_k} 1} = \frac{1}{|C_k|} \sum_{x_n \in C_k} x_n$$

Where $|C_k|$ are the number of points assigned to cluster k

That is, the μ_k that minimizes the cost function is the average of the points that belong to cluster k.

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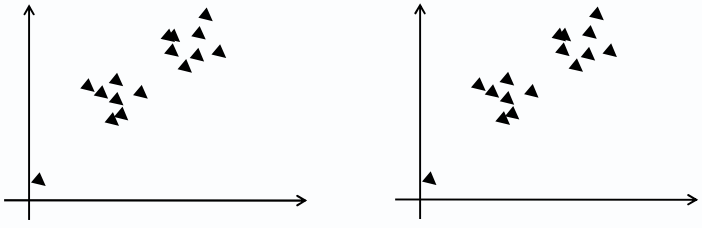
Local minima

K-means converges only to a local minimum.



Usually K-means is run several times with different initialisations.

The quality of each solution is determined by evaluating the cost function

The solution leading to the lowest cost is chosen.

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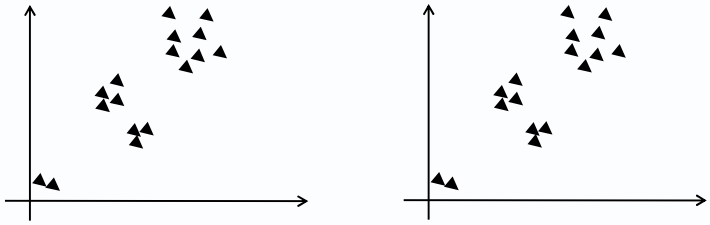
How many clusters?

Ambiguous! Not well posed problem.



Cost function is monotonic wrt K. Larger K leads to smaller J

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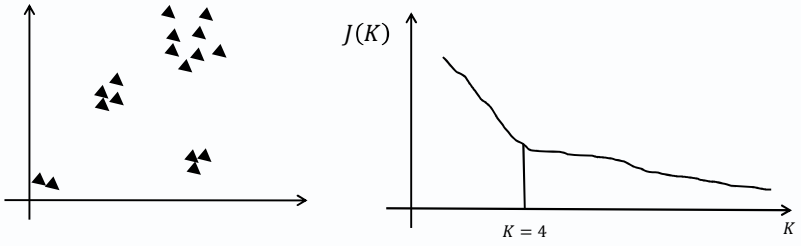
How many clusters?

1. Plot cost as function of K. Cost function is monotonic wrt K. Larger K leads to smaller J. In some cases, the shape may give a hint for the "correct" value of K.



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How many clusters?

2. Evaluate on the application. Obtain different clusters for different values of K. Calculate a measure $J'(K)$ that depends on the application

   Example a: News clustering:

   Evaluate: Present to actual users clustering results with different number of clusters. Asses whether they prefer fewer clusters (i.e. Broader topics) or more clusters (i.e. More specialized topics)

   Example b: A recommendation system cluster users into groups and gives recommendations according to which cluster it think that a user belongs.

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How many clusters?

3. Calculate a measure that penalises complex solutions / many clusters

$$J'(K) = \text{dK lnm+ } \sum_n x_n \ - \mu_{c_n}|_2^2$$

where d is the dimensionality

K the number of clusters

m the number of data points.

Related to Bayesian Information Criterion (BIC).

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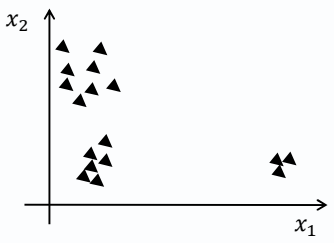
K-means issues: Data scaling

Is sensitive to data scaling.

$x_1 \leftarrow \alpha x_1$ can move the cluster of the points in the right arbitrarily to the left or right.



Normalisation (stretching) $x_1 \leftarrow \frac{x_1 - min_n\left\{x_1^{(n)}\right\}}{\max_n\left\{x_1^{(n)}\right\} - min_n\left\{x_1^{(n)}\right\}}$

Normalisation (by variance) $x_1 \leftarrow \sigma^{-1} x_1$

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Applications: Image Segmentation

Group together pixels that are homogenous in their properties (e.g., colour)

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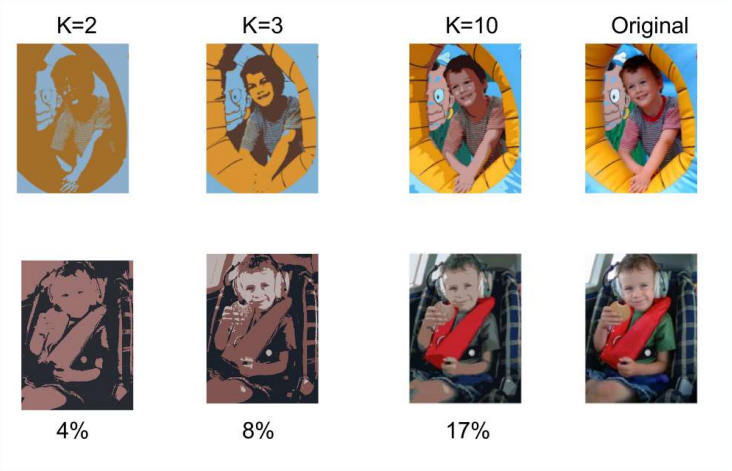
Applications: Image Segmentation



Represent each pixel with the mean of its cluster

$x \in R^3$ 3 colour channels

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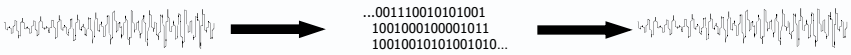
Applications: K - means for VQ

Problem: *What is the best (under MMSE) way to quantize vectors of* $x \in R^d$ *using N bits per sample?*

N bits means 2^N different representatives. (K = 2^N ☺

This is called Vector Quantization (VQ). It was the basis for speech codecs.



Vector Quantization for continuous speech signal:

1. Divide the signal into non overlapping segments of length d.
2. Cluster the segments (each one $\in R^d$) in to K clusters by K-means
3. Represent each segment by the index of the corresponding cluster using N bits coding. At the decoder side, decode using the corresponding cluster mean.

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Applications: VQ

FIGURE 14.9. *Sir Ronald A. Fisher* $(1890 - 1962)$ *was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a* 1024×1024 *grayscale image at* 8 *bits per pixel. The center image is the result of* 2×2 *block VQ, using* 200 *code vectors, with a compression rate of* 1.9 *bits/pixel. The right image uses only four code vectors, with a compression rate of* 0.50 *bits/pixel*

[Figure from Hastie *et al.* book]

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Summary

- Introduced the simple K-means clustering algorithm
- Limitations
- Convergence, optimality, scaling, number of clusters
- Applications

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