Simple and Quick: k-means

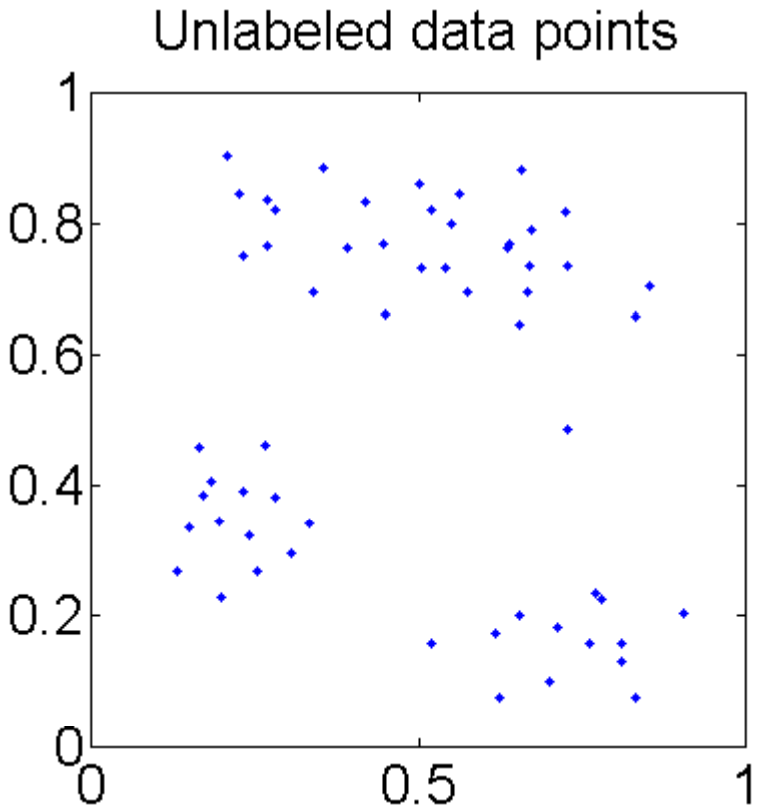
Description

Failings

Challenges

By David Jackson, 9/13/07

The problem:



- We have data points, we want to find assign data points to k clusters. What should we do?

K-means

- Suppose you have data X_n we want to assign binary indicator variable $r_{nk} \in \{0,1\}$ where $k = 1, \dots K$ If x_j is in cluster l then $r_{jk} = \begin{cases} 1 \; if \; l=k \\ 0 \; otherwise \end{cases}$

- How do we assign r_{nk} ?
- Objective function: Distortion

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \| x_n - \mu_k \|^2$$

or

$$J = \sum_{k=1}^{K} \sum_{\{n:r_{n,l=k}\}}^{N} \| x_{nk} - \mu_k \|^2$$

Argument based on Bishop P.R.M.L 2006, section 9.1

Running K-means

- We want to minimize J.
- Step 1. Expectation, assign r_{nk} to the cluster that increases the distortion by the smallest amount:

$$r_{nk} = \begin{cases} 1 \; if \; k = \arg\min_k \|x_n - \mu_k\|^2 \\ 0 \; otherwise \end{cases}$$

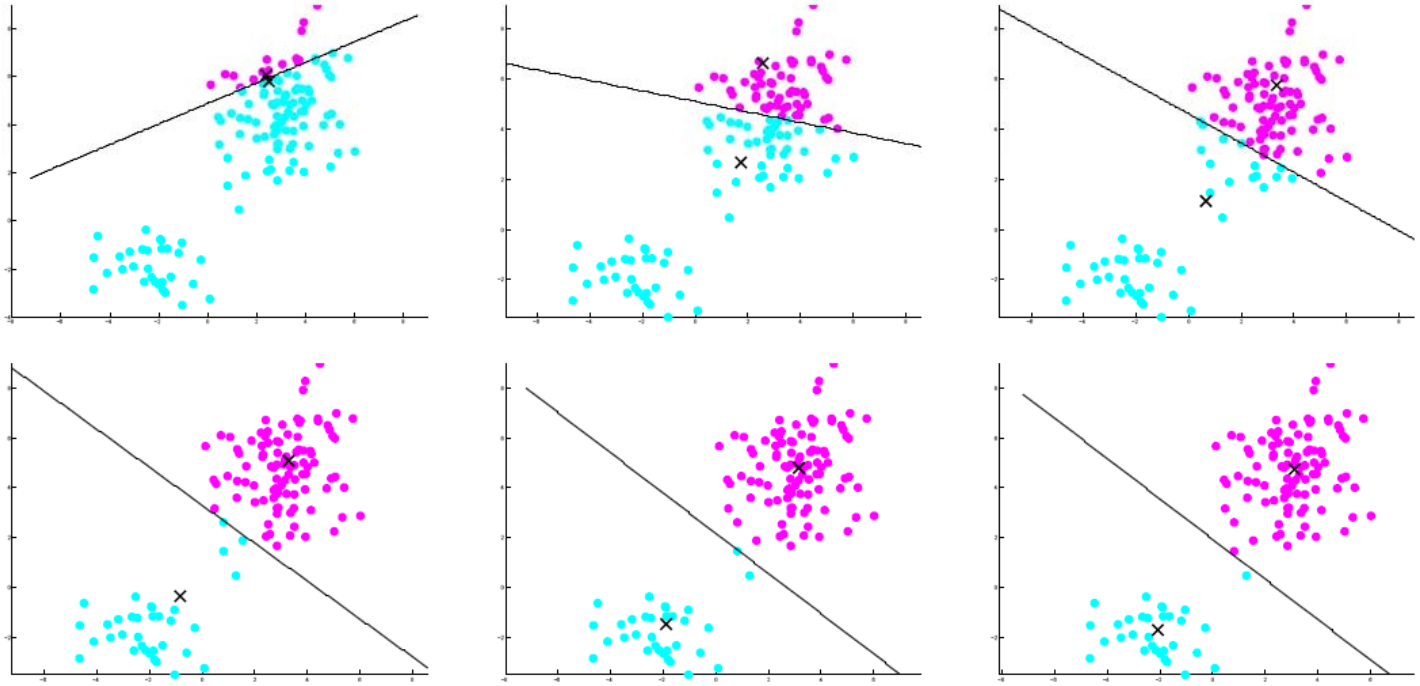
- Maximization step, take the derivative of J

$$2\sum_{n=1}^{N} r_{nk}(x_n - \mu_k) = 0$$

Solve for u_k:

$$\mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$$

K-means: an Example



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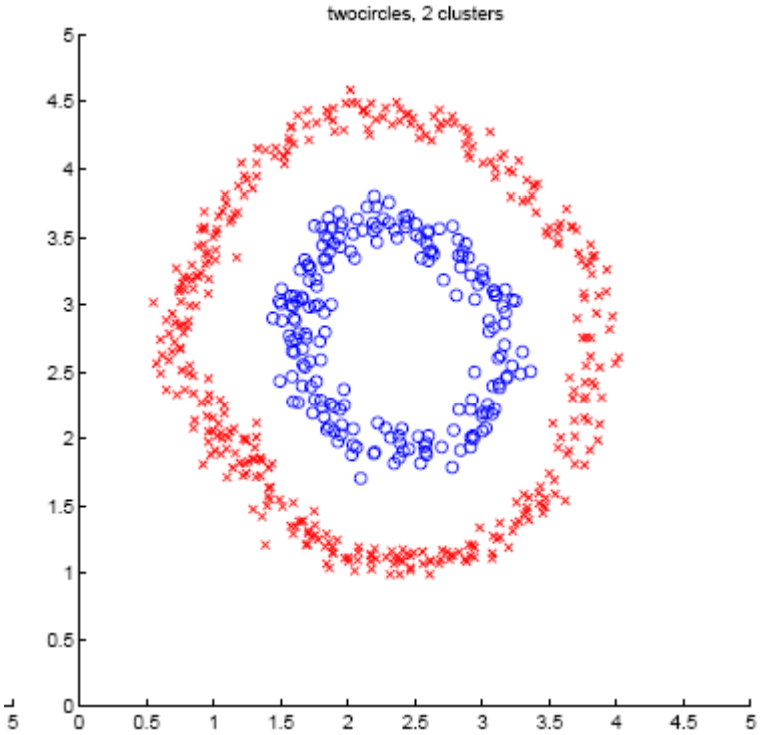
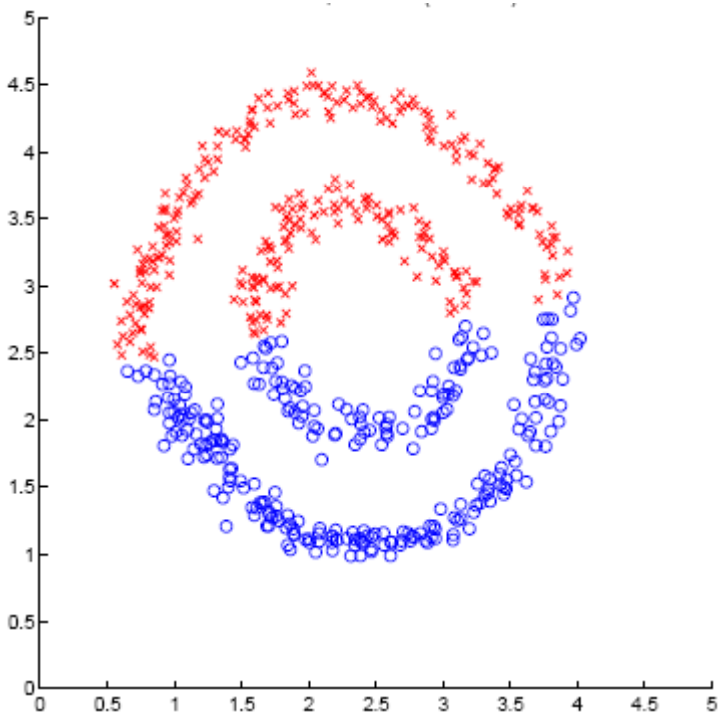
Why not ? (part 1)

We humans have an idea of continuity between data points in the same cluster:

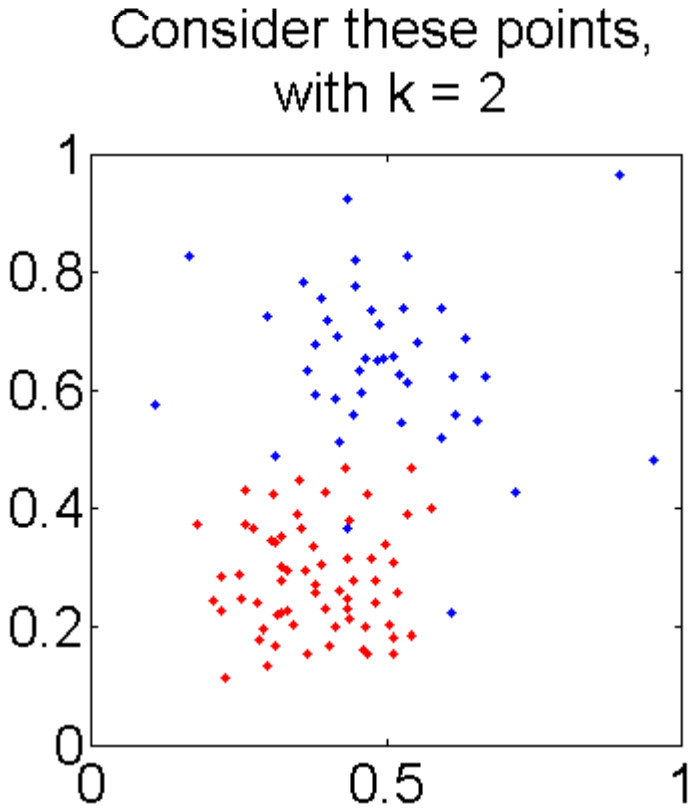




Looking at J, assigning points to concentric circles represents the worst case scenario!

[Images: Ng 2001]

Why not? (part 2)



What is K? (a Challenge)

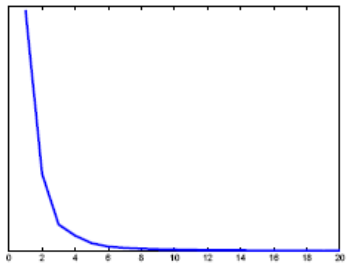
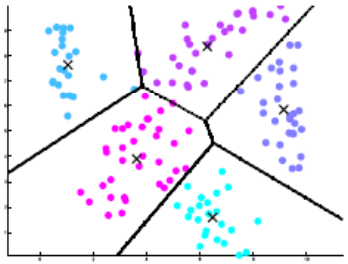
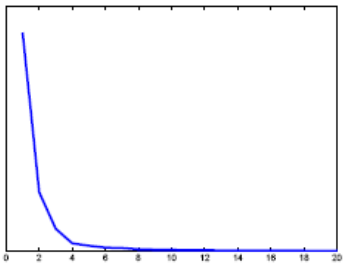
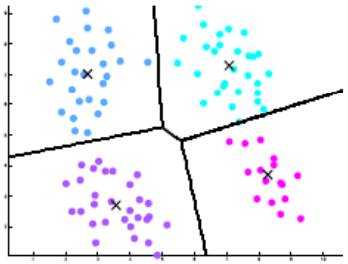
- With most clustering techniques (EM, spectral, amalgamative) the choice of K, the number of clusters, is often somewhat arbitrary but crucial.
- Some modern non-parametric methods/procedures have been created to address this issue.

What is K? (a Heuristic)

- How can we set k?
- The relevant statistic: *within-class dissimilarity*

$$W_k = \sum_{c=1}^{k} \sum_{y_i=y_j=c} \|\mathbf{x}_i - \mathbf{x}_j\|^2.$$

- A popular (heuristic) strategy: look for an "elbow" in W_k

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What is K? (an Answer?)

- We'll read a paper by Zoubin Ghahramani that proposes a way to "discover" K.

- Any good ideas on this question would be appreciated 1. by me, 2. by the field.