K-means Clustering

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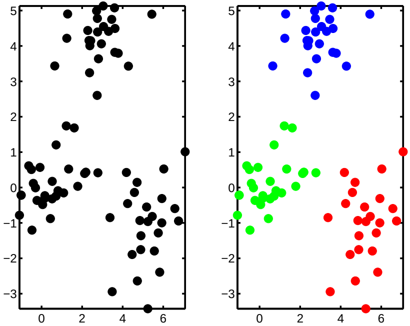
- *Supervised Learning is just the icing on the cake which is unsupervised learning.*
  Yann Le Cun, NIPS 2016

Clustering



- In this example each object has two attributes:

$$\mathbf{x}_n = [x_{n1}, x_{n2}]^{\mathsf{T}}$$

- Left: data.
- Right: data after clustering (points coloured according to cluster membership).

What we'll cover

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  - Mixture models
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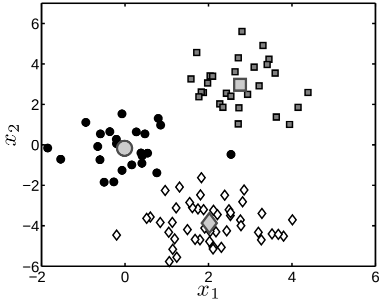

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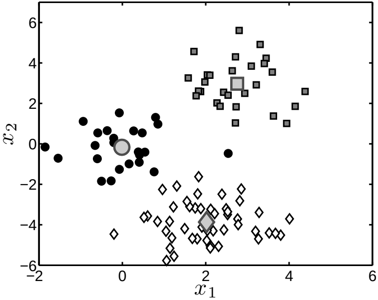

- Distance is normally Euclidean distance, but other choices are also feasible.

How do we find $\boldsymbol{\mu}_k$?

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- Use an iterative algorithm:

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$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$$

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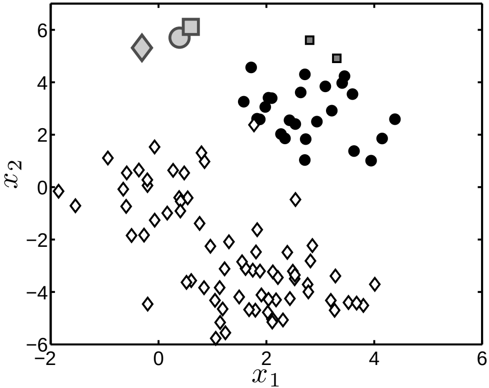
- Algorithm will converge....it will reach a point where the assignments don't change.

K-means – example



- Cluster means randomly assigned (top left).
- Points assigned to their closest mean.

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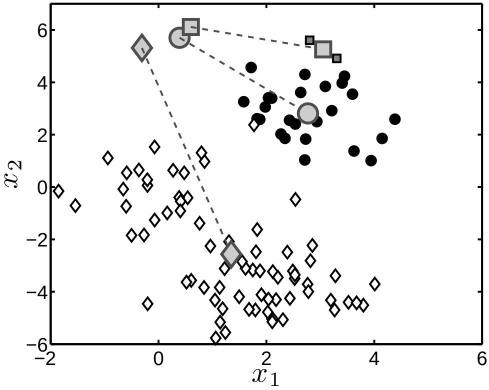

- Cluster means updated to mean of assigned points.

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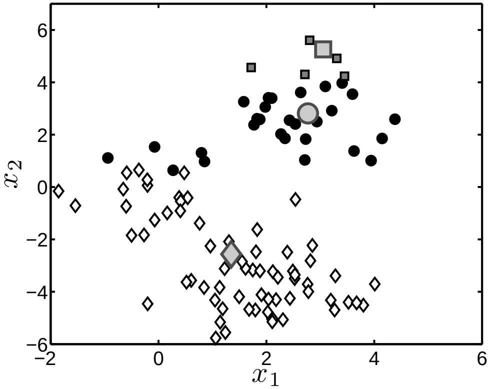

- Points re-assigned to closest mean.

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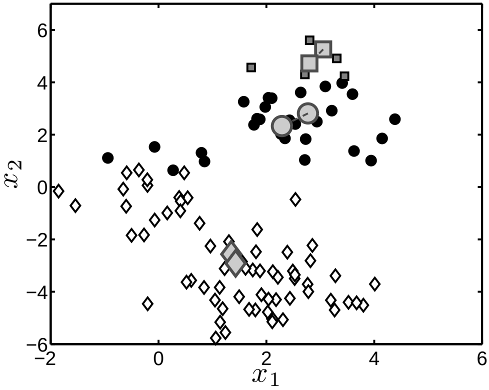

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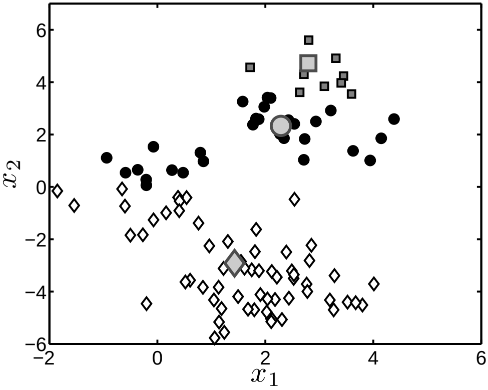

- Assign point to closest mean.

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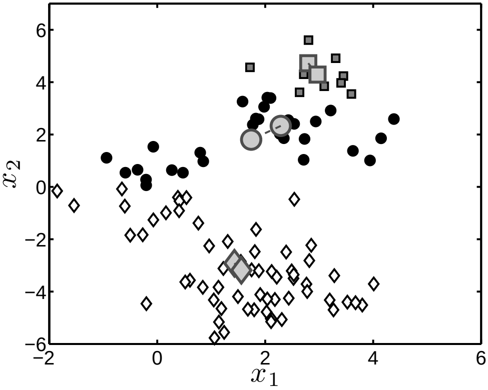

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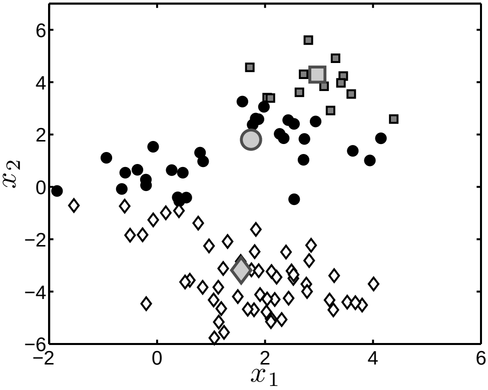

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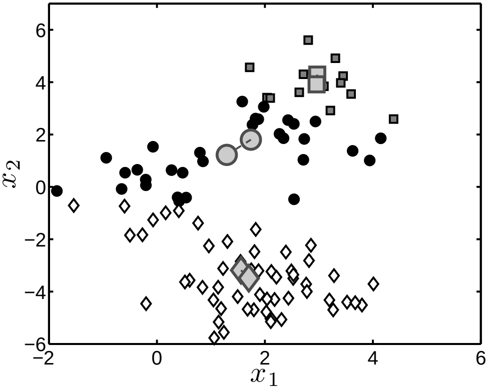

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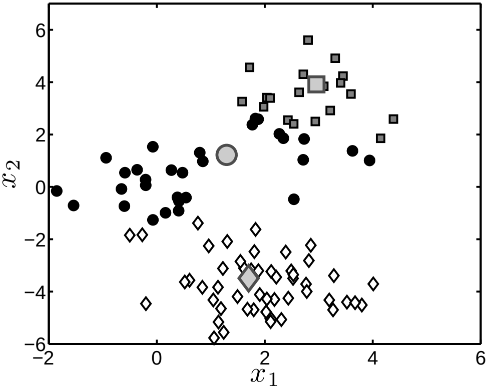

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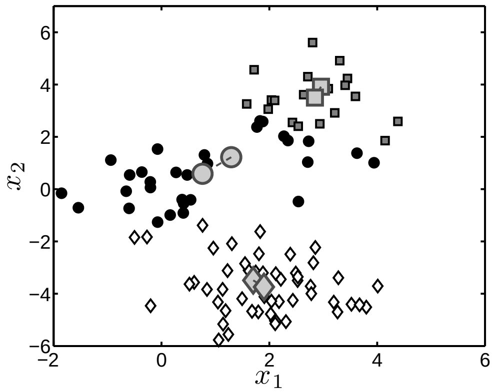

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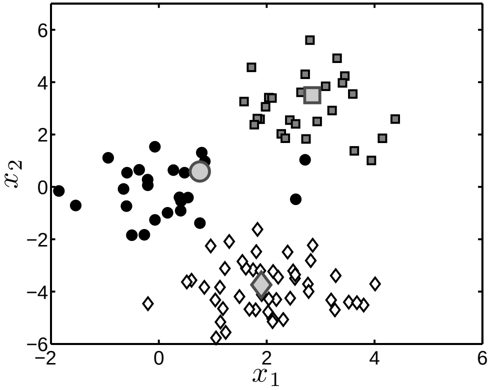

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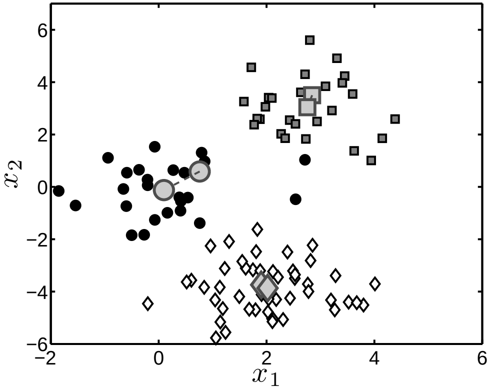

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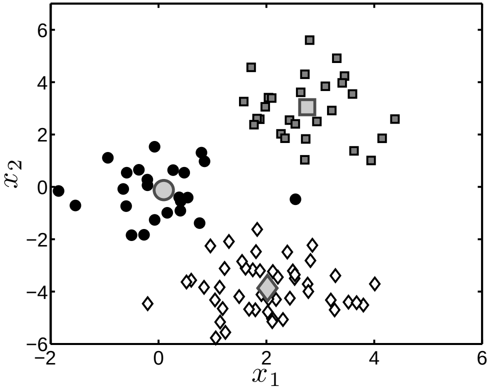

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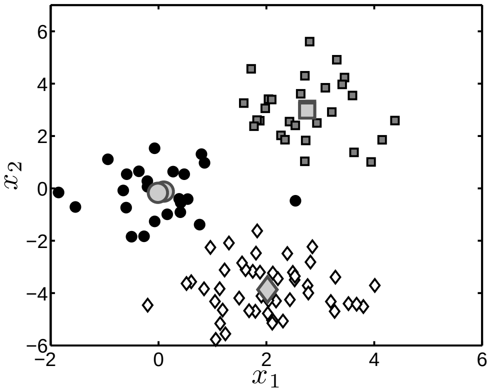

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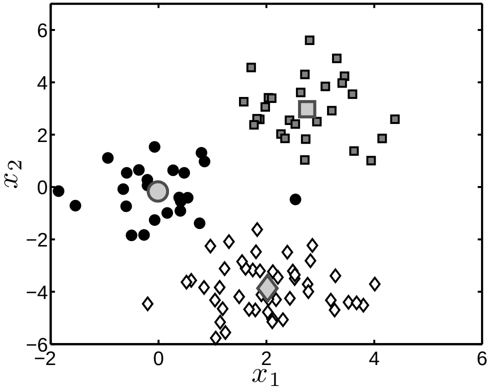

- Solution at convergence.

K-means – Cost Function

- Simple (and effective) clustering strategy.
- Converges to (local) minima of:

$$\sum_n \sum_k z_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathsf{T}} (\mathbf{x}_n - \boldsymbol{\mu}_k)$$

- under which conditions?

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$$\text{such that: } z_{nk} \in \{0, 1\},$$

$$\sum_k z_{nk} = 1, \forall n.$$

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- Both these significantly affect resulting clustering.

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- Pick a random input point for first center, next center at a point as far away from this as possible, next as far away from first two ...

k–Means++ (D. Arthur and S. Vassilvitskii (2007)

- Start with $C_1 := \{\mathbf{x}\}$ where $\mathbf{x}$ is chosen at random from input points.
- For $2 \leq k \leq K$,
  1. pick a new unselected point $\mathbf{x}$ according to a probability distribution ν_k: (this distribution is computed over the unselected data points)

$$\nu_k(\mathbf{x}) = \frac{d^2(\mathbf{x}, C_{k-1})}{\sum_{\mathbf{x}'} d^2(\mathbf{x}', C_{k-1})}$$

     $d^2(\mathbf{x}, C_{k-1})$ is the squared distance between $\mathbf{x}$ and the nearest center that has already been chosen in C_{k-1}.
  2. set $C_k := C_{k-1} \cup \{\mathbf{x}\}$.

Gives a provably good $O(\log K)$ approximation to optimal clustering.

Choosing K

- Intra-cluster variance:

$$W_k := \frac{1}{|C_k|} \sum_{\mathbf{x} \in C_k} (\mathbf{x} - \boldsymbol{\mu}_k)^2.$$

- $W := \sum_k W_k$.
- Pick k to minimize W_k
- Elbow heuristic, Gap Statistic ...

Sum of Norms (SON) Formulation

SON Relaxation (Lindsten et al 2011)

$$\min_{\boldsymbol{\mu}} \sum_{n} \|\mathbf{x}_n - \boldsymbol{\mu}(\mathbf{x}_n)\|^2 + \lambda \sum_{p,q:p<q} \|\boldsymbol{\mu}_p - \boldsymbol{\mu}_q\|_2.$$

where $\boldsymbol{\mu}(\mathbf{x}_n)$ indicates the centroid of the cluster that $\mathbf{x}_n$ is assigned to.

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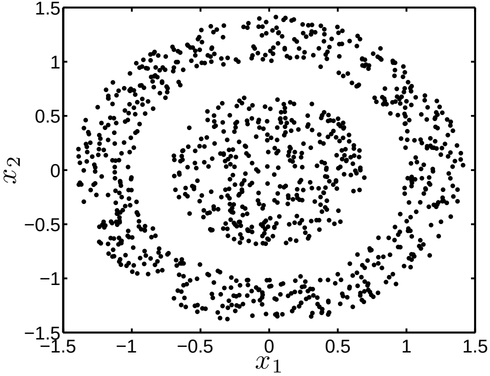
- ... $\boldsymbol{\mu}_p = \boldsymbol{\mu}_q$ for all p, q (thus, $K = 1$).
- By varying λ, we steer between these two extremes.
- Do not need to know K in advance and do not need to do careful initialization.

When does K-means break?



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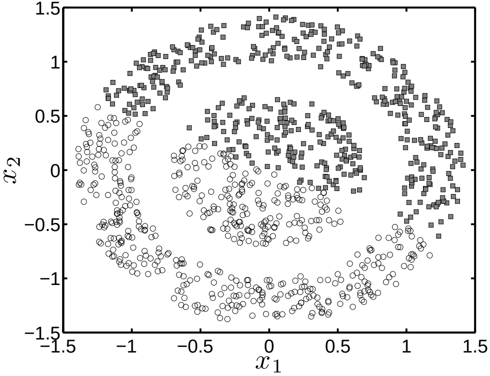

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- Distances can be written as (defining $N_k = \sum_n z_{nk}$):
$$(\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T}(\mathbf{x}_n - \boldsymbol{\mu}_k) = \left(\mathbf{x}_n - N_k^{-1}\sum_{m=1}^{N} z_{mk}\mathbf{x}_m\right)^\mathsf{T}\left(\mathbf{x}_n - N_k^{-1}\sum_{m=1}^{N} z_{mk}\mathbf{x}_m\right)$$

Kernelising K-means

- Multiply out:

$$\mathbf{x}_n^\mathsf{T}\mathbf{x}_n - 2N_k^{-1}\sum_{m=1}^{N} z_{mk}\mathbf{x}_m^\mathsf{T}\mathbf{x}_n + N_k^{-2}\sum_{m,l} z_{mk}z_{lk}\mathbf{x}_m^\mathsf{T}\mathbf{x}_l$$

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- Kernel substitution:

$$k(\mathbf{x}_n, \mathbf{x}_n) - 2N_k^{-1}\sum_{m=1}^{N} z_{mk}k(\mathbf{x}_n, \mathbf{x}_m) + N_k^{-2}\sum_{m,l=1}^{N} z_{mk}z_{lk}k(\mathbf{x}_m, \mathbf{x}_l)$$

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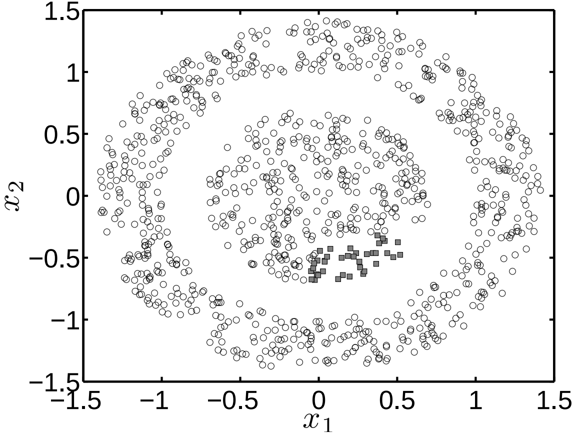
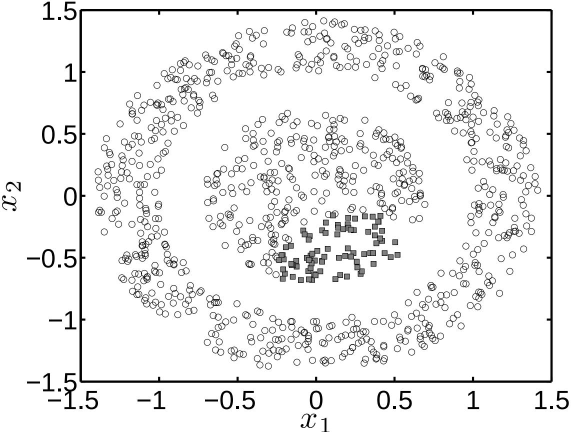
- Note – no $\boldsymbol{\mu}_k$. This would be $N_k^{-1} \sum_n z_{nk} \phi(\mathbf{x}_n)$ but we don't know $\phi(\mathbf{x}_n)$ for kernels. We only know $\phi(\mathbf{x}_n)^\mathsf{T} \phi(\mathbf{x}_m)$ ...

Kernel K-means – example



Kernel K-means – example



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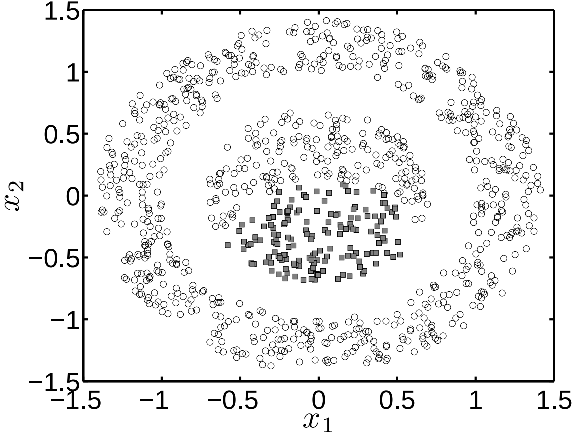

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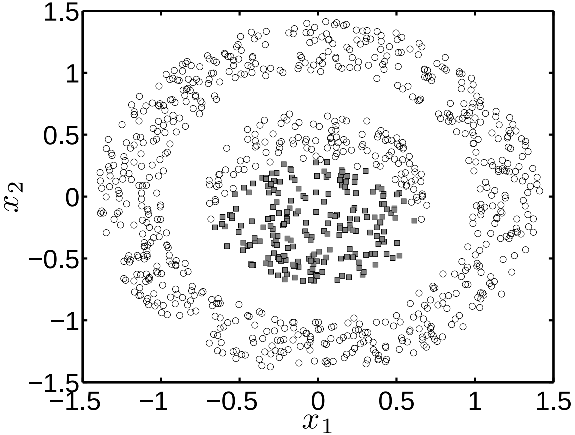

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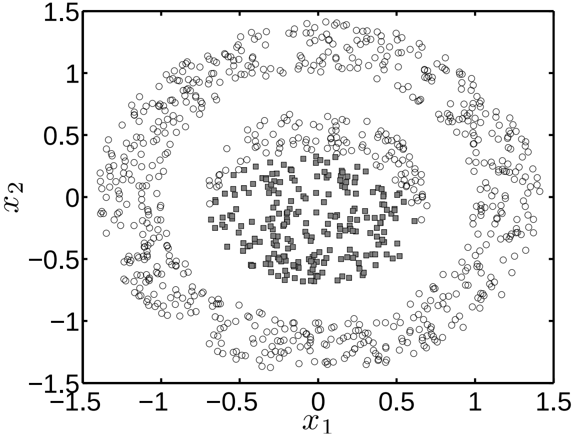

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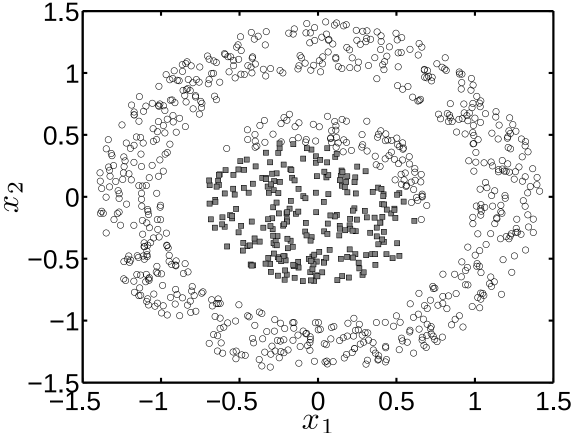

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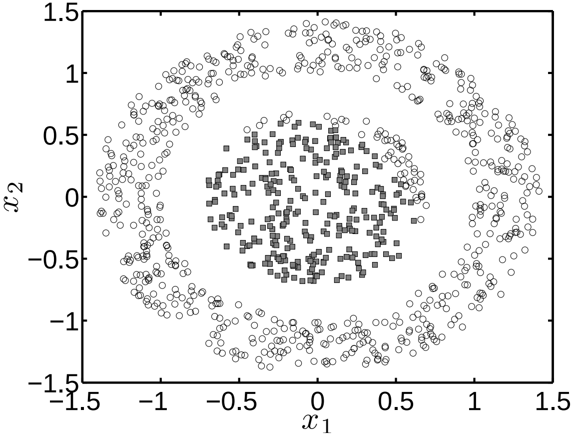

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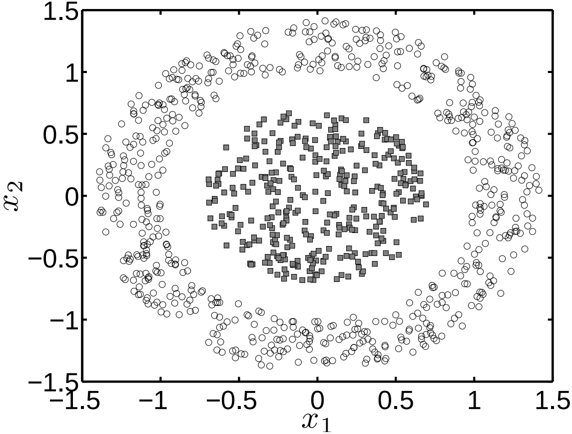

- Solution at convergence.

Kernel K-means

- Makes simple K-means algorithm more flexible.
- But, have to now set additional parameters.
- Very sensitive to initial conditions – lots of local optima.

K-means – summary

- Simple (and effective) clustering strategy.

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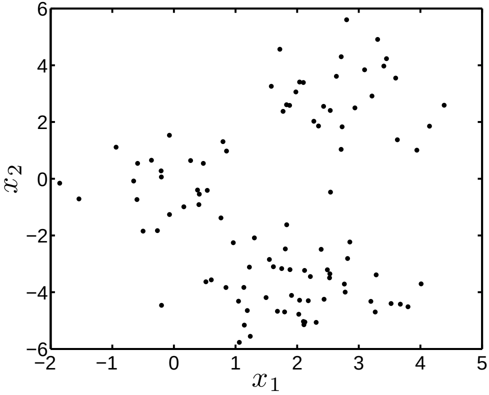
- Sensitive to initialisation.
- How do we choose K?
  - Tricky, several heuristics have been proposed.
  - The Sum of Norms method.
  - Can we use CV (Cross-Validation)?

Mixture models – thinking generatively



- Could we hypothesis a model that could have created this data?

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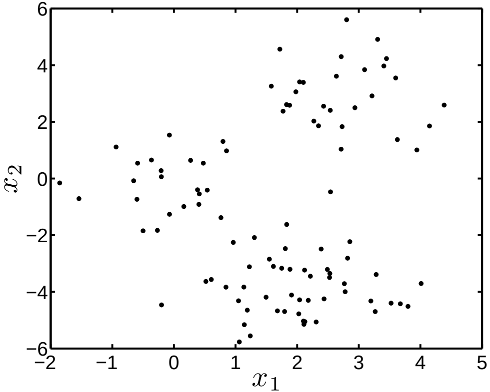

- Could we hypothesis a model that could have created this data?
- Each $\mathbf{x}_n$ seems to have come from one of three distributions.