Advanced Statistical Inference
Clustering

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Unsupervised learning

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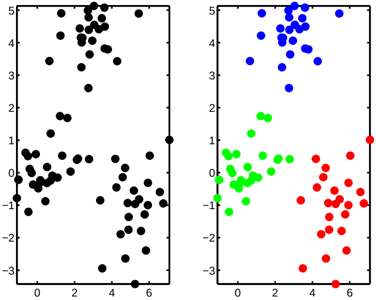
- We'll also cover *projection* (later in the course)

Aims

- This is the only lecture on clustering.
- By the end, you should:
    - Understand what clustering is.
    - Understand the K-means algorithm.
    - Understand the idea of mixture models.
    - Be able to derive the update expression for mixture model parameters.

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

- 2 algorithms:
  - K-means
  - Mixture models
- The two are somewhat related.
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- Each cluster is defined by a position in the input space:

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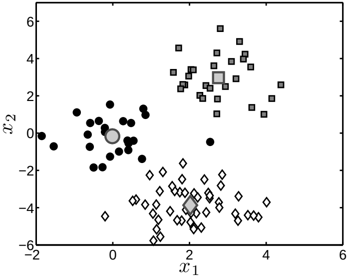

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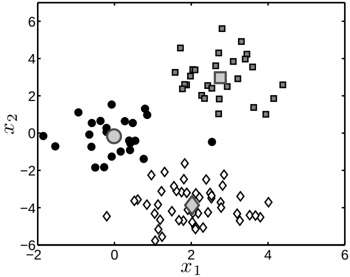

- Distance is normally Euclidean distance:

$$d_{nk} = (\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T}(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

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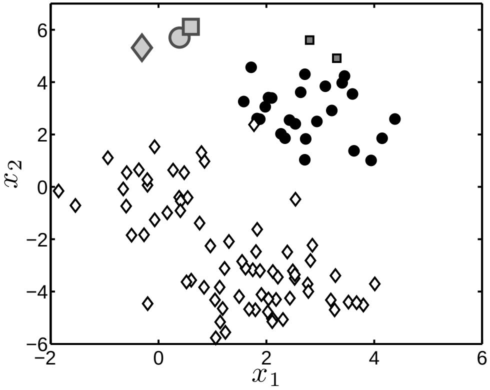
- Algorithm will converge....it will reach a point where the assignments don't change.

K-means – example



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

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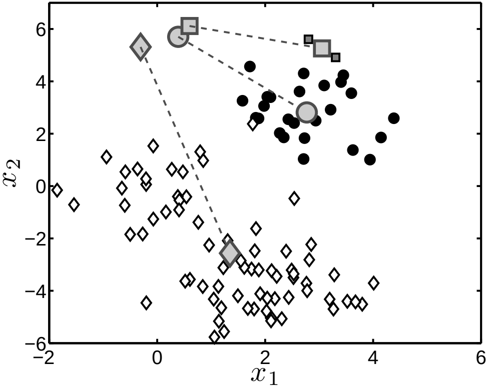

- Cluster means updated to mean of assigned points.

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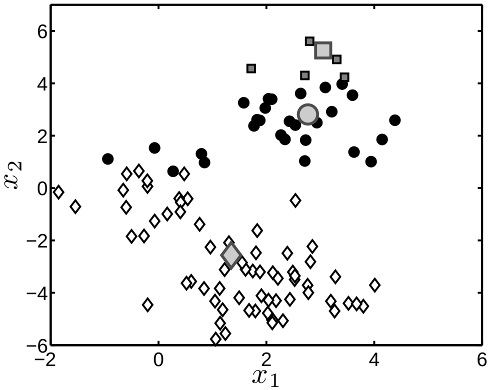
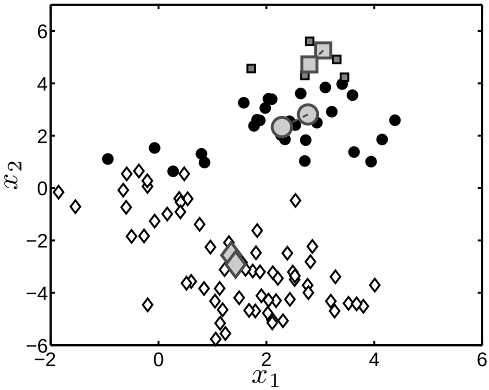


- Points re-assigned to closest mean.

K-means – example



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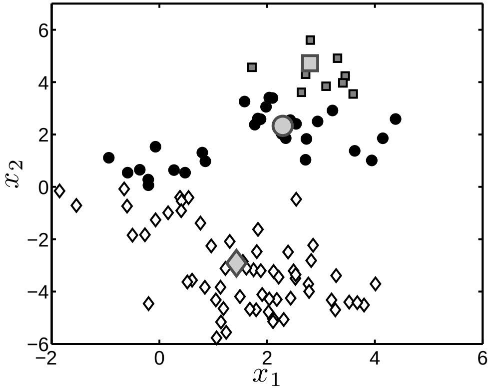

- Assign point to closest mean.

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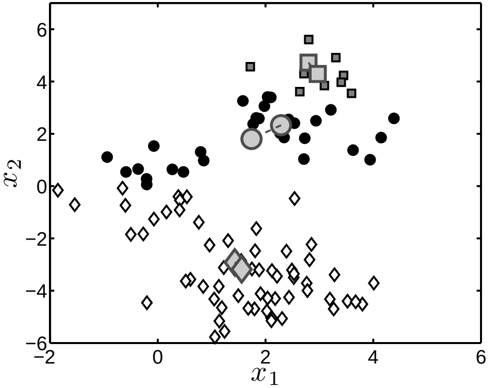
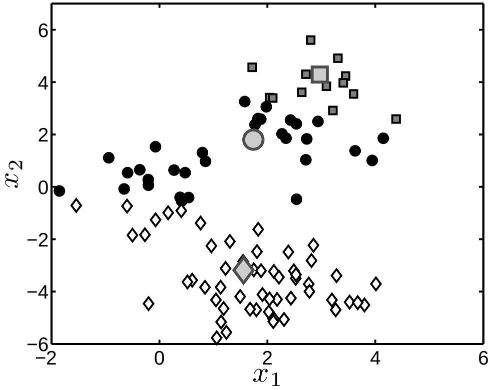


- Update mean.

K-means – example



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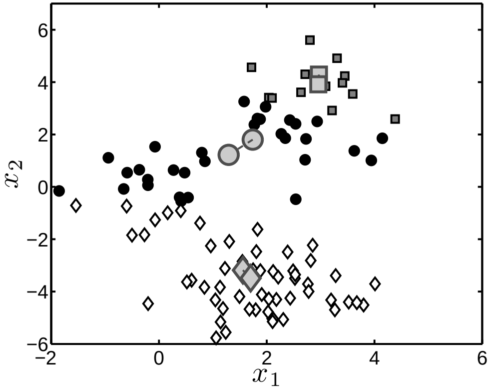

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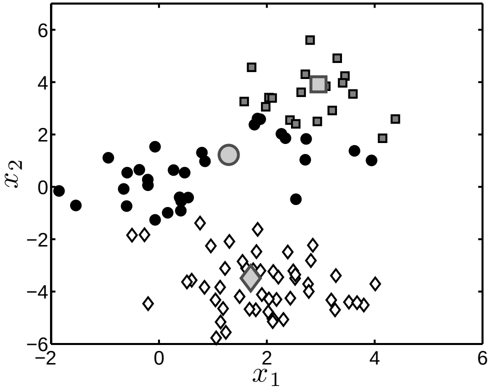

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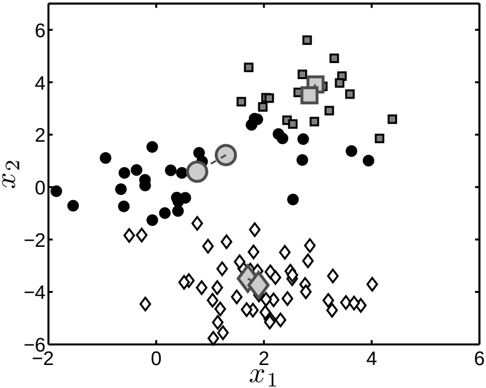

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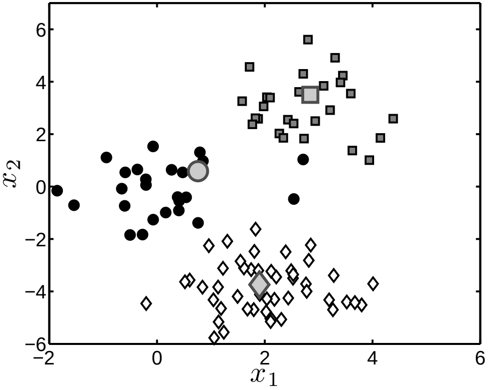

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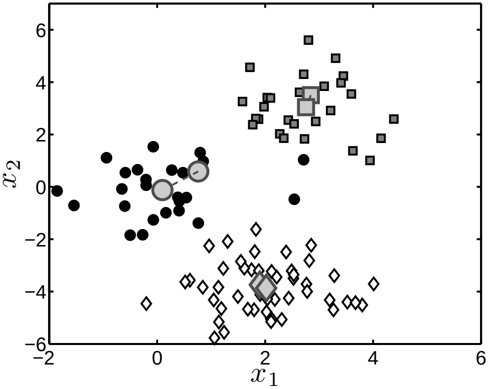

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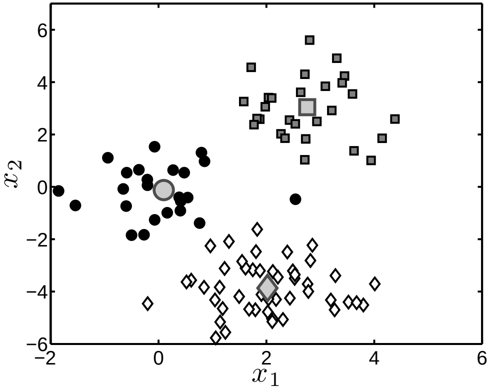

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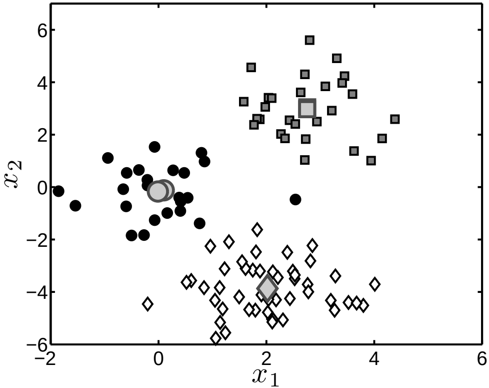

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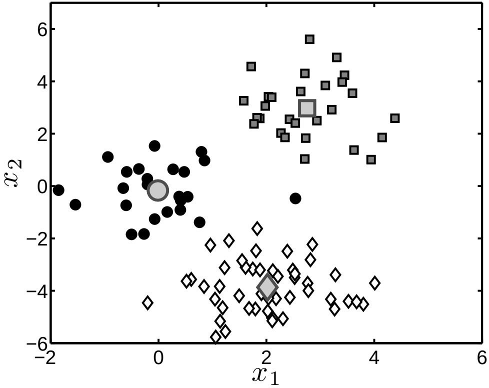
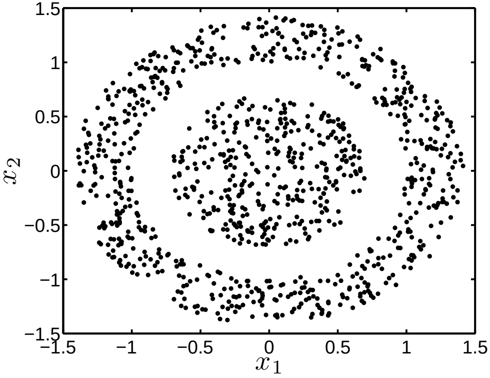


- Solution at convergence.

When does K-means break?



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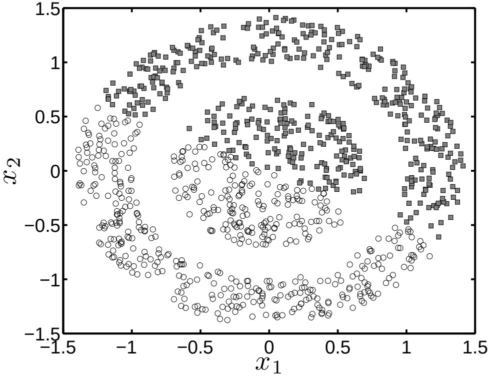

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- Distances can be written as (defining $N_k = \sum_n z_{nk}$):

$$(\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T}(\mathbf{x}_n - \boldsymbol{\mu}_k) = \left(\mathbf{x}_n - N_k^{-1}\sum_{m=1}^N z_{mk}\mathbf{x}_m\right)^\mathsf{T}\left(\mathbf{x}_n - N_k^{-1}\sum_{m=1}^N z_{mk}\mathbf{x}_m\right)$$

Kernelizing K-means

- Multiply out:

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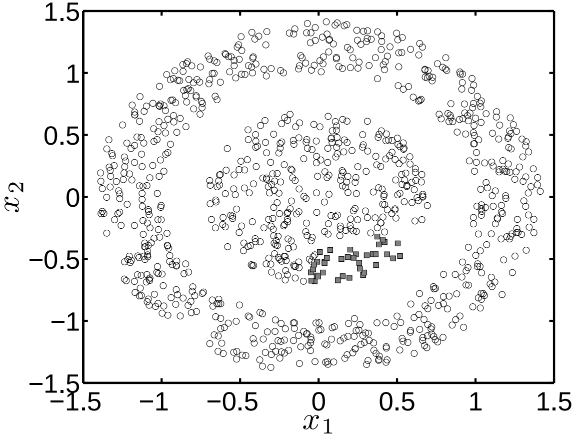
- Note – no $\boldsymbol{\mu}_k$. This would be $N_k^{-1} \sum_n z_{nk} \phi(\mathbf{x}_n)$ but we don't know $\phi(\mathbf{x}_n)$ for kernels. We only know $\phi(\mathbf{x}_n)^\mathsf{T} \phi(\mathbf{x}_m)$...

Kernel K-means – example



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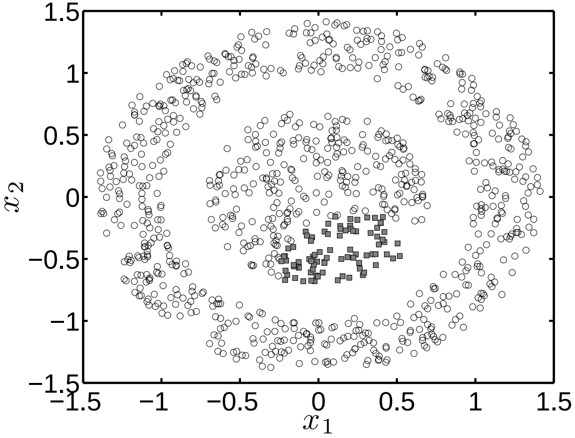

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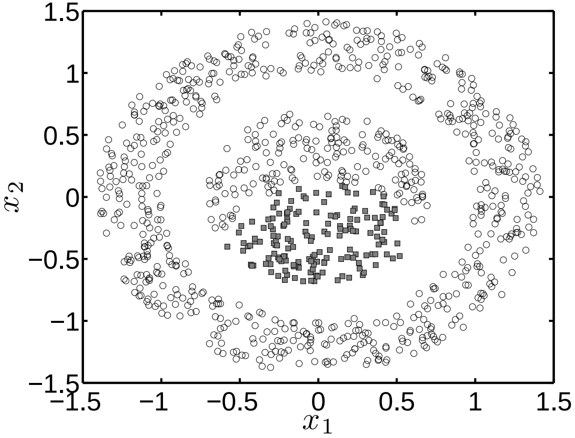

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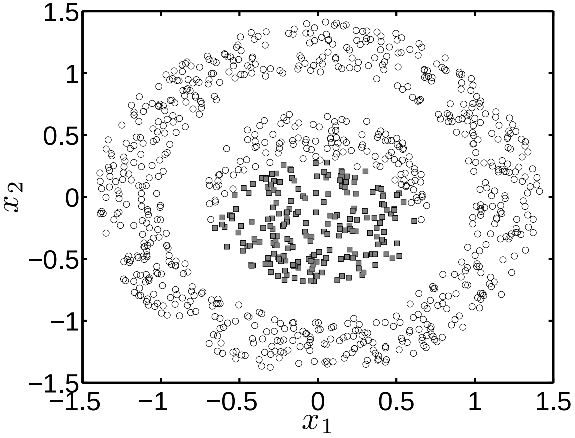

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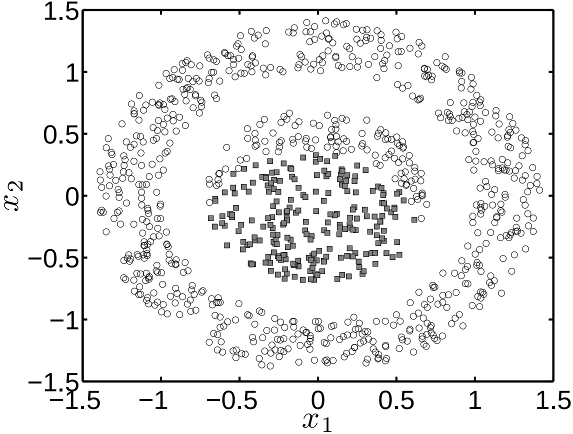

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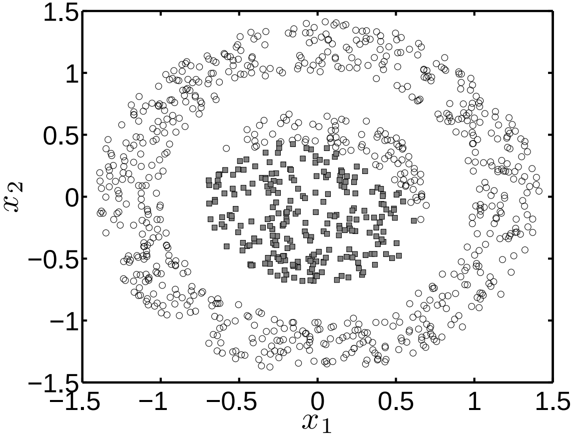

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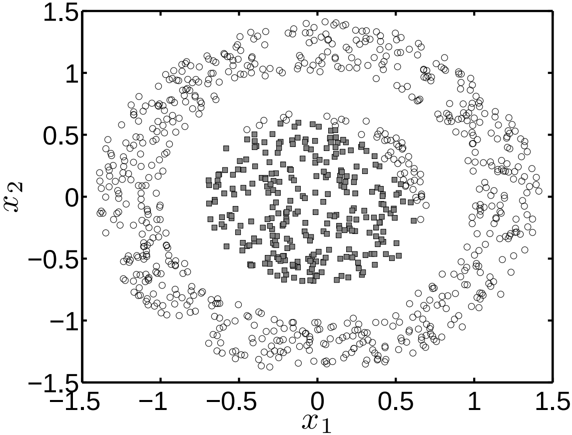

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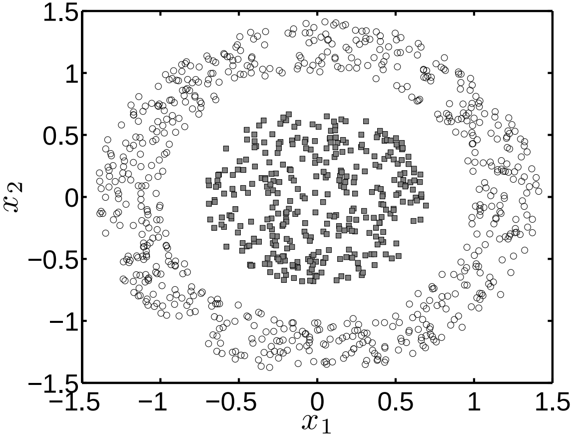

- Solution at convergence.

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.

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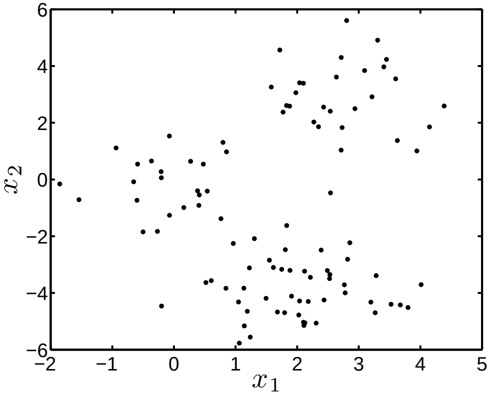
- How do we choose K?
  - Tricky: Quantity above always decreases as K increases.
  - Can use CV if we have a measure of 'goodness'.
  - For clustering these will be application specific.

Mixture models – thinking generatively



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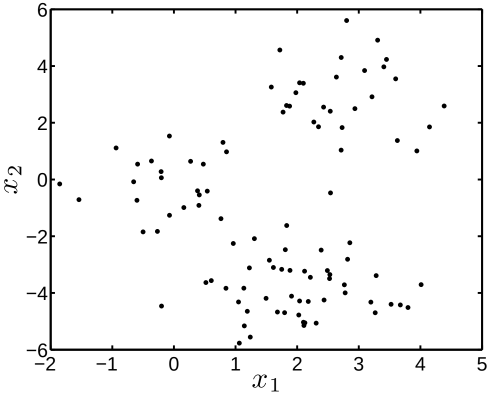

- Could we hypothesis a model that could have created this data?
- Each $\mathbf{x}_n$ seems to have come from one of three distributions.

A generative model

- Assumption:Each $\mathbf{x}_n$ comes from one of different K distributions.
- To generate $\mathbf{X}$:
- For each n:
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- Maximize the likelihood!

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- Then, un-marginalize k:

$$\begin{aligned}p(\mathbf{X}|\Delta) &= \prod_{i=1}^{N}\sum_{k=1}^{K}p(\mathbf{x}_n,z_{nk}=1|\Delta)\\ &= \prod_{i=1}^{N}\sum_{k=1}^{K}p(\mathbf{x}_n|z_{nk}=1,\Delta_k)p(z_{nk}=1|\Delta)\end{aligned}$$

Mixture model likelihood

- So, we have a likelihood:

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- Log of a sum is bad – we need some help....

Jensen's inequality

$$\log \mathbf{E}_{p(x)} \{f(x)\} \geq \mathbf{E}_{p(x)} \{\log f(x)\}$$

- How does this help us?
- Our log likelihood:

$$L = \sum_{n=1}^{N} \log \sum_{k=1}^{K} p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) p(z_{nk} = 1 | \Delta)$$

- Add a (arbitrary looking) distribution $q(z_{nk} = 1)$ (s.t. $\sum_k q(z_{nk} = 1) = 1$):

$$L = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \frac{q(z_{nk} = 1)}{q(z_{nk} = 1)} p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) p(z_{nk} = 1 | \Delta)$$

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- We now have an expectation:

$$L = \sum_{n=1}^{N} \log \mathbf{E}_{q(z_{nk}=1)} \left\{ \frac{1}{q(z_{nk} = 1)} p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) p(z_{nk} = 1 | \Delta) \right\}$$

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- So, using Jensen's:

$$\begin{aligned} L &\geq \sum_{n=1}^{N} \mathbf{E}_{q(z_{nk}=1)} \left\{ \log \frac{1}{q(z_{nk}=1)} p(\mathbf{x}_n | z_{nk}=1, \Delta_k) p(z_{nk}=1|\Delta) \right\} \\ &= \sum_{n=1}^{N} \sum_{k=1}^{K} q(z_{nk}=1) \log \left\{ \frac{1}{q(z_{nk}=1)} p(\mathbf{x}_n | z_{nk}=1, \Delta_k) p(z_{nk}=1|\Delta) \right\} \end{aligned}$$

Lower bound on log-likelihood

$$
\begin{aligned}
L &\geq \sum_{n=1}^{N}\sum_{k=1}^{K} q(z_{nk}=1)\log\left\{\frac{1}{q(z_{nk}=1)}p(\mathbf{x}_n|z_{nk}=1,\Delta_k)p(z_{nk}=1|\Delta)\right\} \\
&= \sum_{n=1}^{N}\sum_{k=1}^{K} q(z_{nk}=1)\log p(z_{nk}=1|\Delta) + \dots \\
&\quad \sum_{n=1}^{N}\sum_{k=1}^{K} q(z_{nk}=1)\log p(\mathbf{x}_n|z_{nk}=1,\Delta_k) - \dots \\
&\quad \sum_{n=1}^{N}\sum_{k=1}^{K} q(z_{nk}=1)\log q(z_{nk}=1)
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- Define $q_{nk} = q(z_{nk}=1)$, $\pi_k = p(z_{nk}=1|\Delta)$ (both just scalars).

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\end{aligned}
$$

- Define $q_{nk}=q(z_{nk}=1)$, $\pi_k=p(z_{nk}=1|\Delta)$ (both just scalars).
- Differentiate lower bound w.r.t q_{nk}, π_k and Δ_k and set to zero to obtain **iterative** update equations.

Optimizing lower bound

- Updates for Δ_k, π_k will depend on q_{nk}.
- Update q_{nk} and then use these values to update Δ_k and π_k etc.

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- This is a form of the Expectation-Maximization algorithm (EM) but we've derived it differently.
- Best illustrated with an example....

Gaussian mixture model

- Assume component distributions are Gaussians with diagonal covariance:

$$p(\mathbf{x}_n | z_{nk} = 1, \boldsymbol{\mu}_k, \sigma_k^2) = \mathcal{N}(\boldsymbol{\mu}, \sigma^2 \mathbf{I})$$

- Update for π_k. Relevant bit of bound:

$$\sum_{n,k} q_{nk} \log(\pi_k)$$

- Now, we have a constraint: $\sum_k \pi_k = 1$. So, add a Lagrangian:

$$\sum_{n,k} q_{nk} \log \pi_k - \lambda \left(\sum_k \pi_k - 1 \right)$$

- Differentiate and set to zero:

$$\frac{\partial}{\partial \pi_k} = \frac{1}{\pi_k} \sum_n q_{nk} - \lambda = 0$$

- Re-arrange:

$$\sum_n q_{nk} = \lambda \pi_k$$

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- Substitute and re-arrange:

$$\pi_k = \frac{\sum_n q_{nk}}{\sum_{n,j} q_{nj}} = \frac{1}{N} \sum_k q_{nk}$$

Update for q_{nk}

- Now for q_{nk}. Whole bound is relevant.
- Add Lagrange term $-\lambda(\sum_k q_{nk} - 1)$
- Differentiate:

$$\frac{\partial}{\partial q_{nk}} = \log \pi_k + \log p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) - (\log q_{nk} + 1) - \lambda$$

- Re-arranging ($\lambda' = f(\lambda)$):

$$\pi_k p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) = \lambda' q_{nk}$$

- Sum over k to find λ' and re-arrange:

$$q_{nk} = \frac{\pi_k p(\mathbf{x}_n | z_{nk} = 1, \Delta_k)}{\sum_{j=1}^{K} \pi_j p(\mathbf{x}_n | z_{nj} = 1, \Delta_j)}$$

Updates for $\boldsymbol{\mu}_k$ and σ_k^2

- These are easier – no constraints.
- Differentiate the following and set to zero (D is dimension of $\mathbf{x}_n$):

$$\sum_{n,k} q_{nk} \log \left\{ \frac{1}{(2\pi\sigma_k^2)^{D/2}} \exp\left(-\frac{1}{2\sigma_k^2} (\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T} (\mathbf{x}_n - \boldsymbol{\mu}_k) \right) \right\}$$

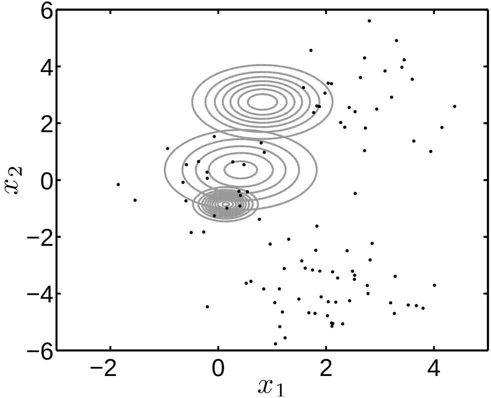
- Result:

$$\begin{aligned} \boldsymbol{\mu}_k &= \frac{\sum_n q_{nk} \mathbf{x}_n}{\sum_n q_{nk}} \\ \sigma_k^2 &= \frac{\sum_n q_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T} (\mathbf{x}_n - \boldsymbol{\mu}_k)}{D \sum_n q_{nk}} \end{aligned}$$

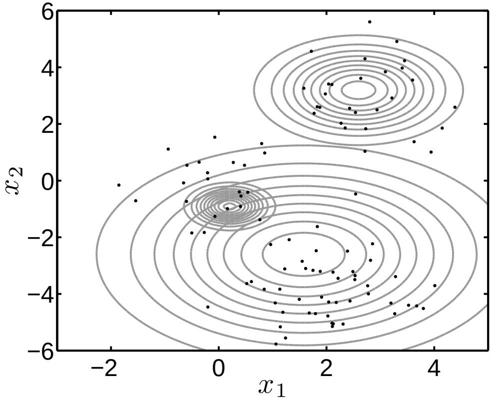
Mixture model optimization – algorithm

- Following optimization algorithm:
  1. Guess $\boldsymbol{\mu}_k, \sigma_k^2, \pi_k$
  2. Compute q_{nk}
  3. Update $\boldsymbol{\mu}_k, \sigma_k^2$
  4. Update π_k
  5. Return to 2 unless parameters are unchanged.
- Guaranteed to converge to a local maximum of the lower bound.
- Note the similarity with kmeans.

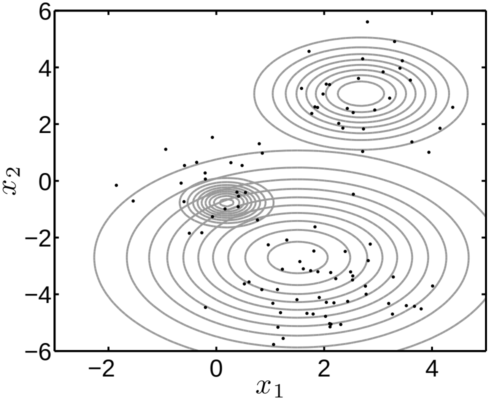
Algorithm in operation



- Initial parameter values.



- Update q_{nk} and then other parameters.



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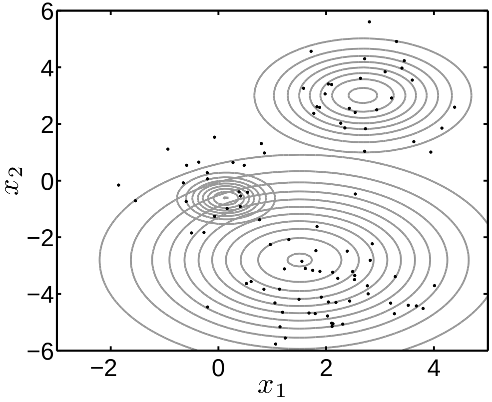

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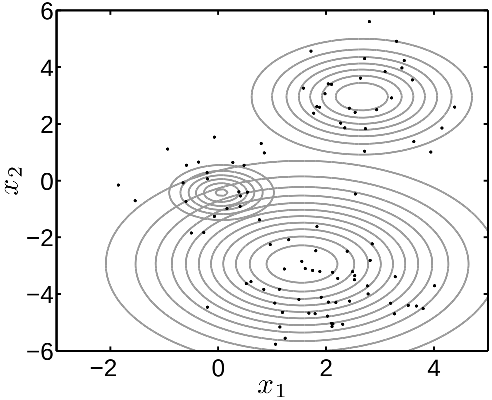

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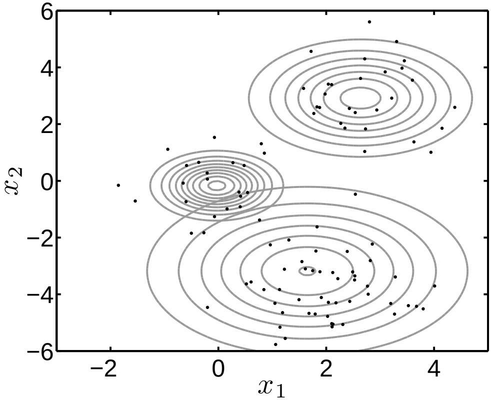

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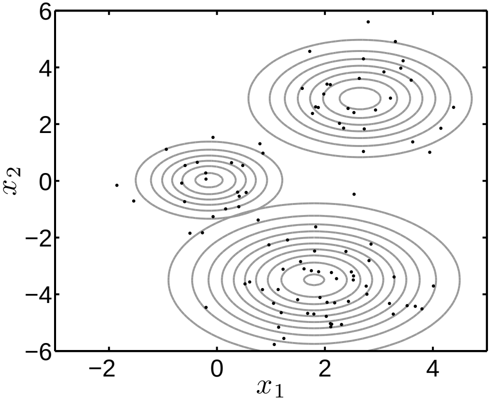

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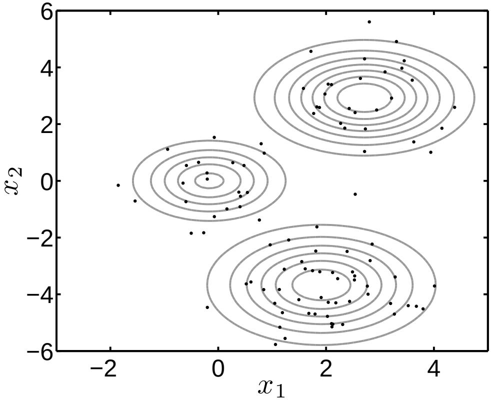

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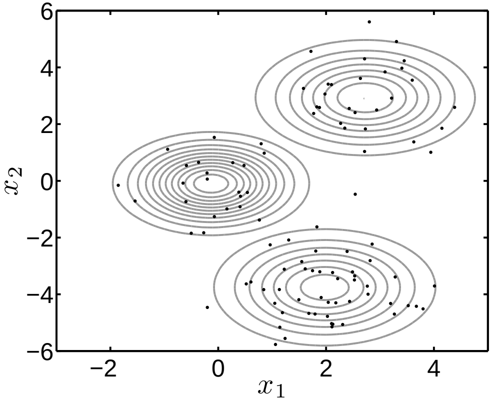

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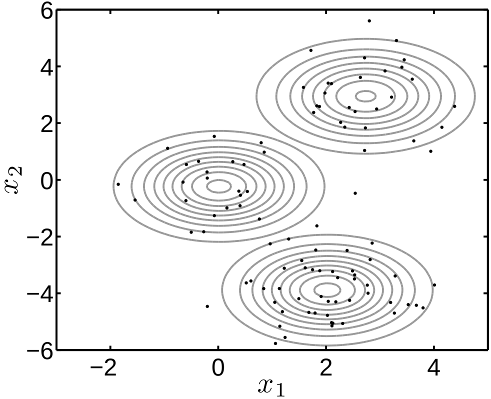

- Solution at convergence.

Mixture model clustering

- So, we've got the parameters, but what about the assignments?
- Which points came from which distributions?

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$$q_{nk} = P(z_{nk} = 1 | \mathbf{x}_n, \mathbf{X})$$

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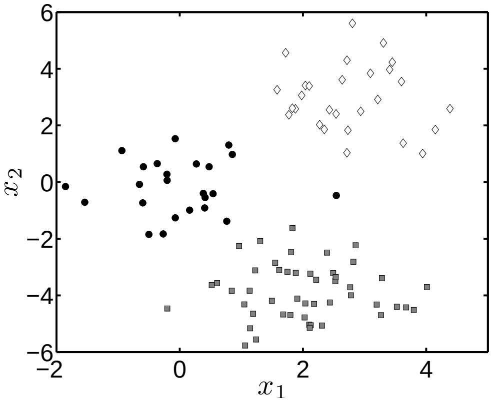
$$q_{nk} = P(z_{nk} = 1|\mathbf{x}_n, \mathbf{X})$$

- Can stick with probabilities or assign each $\mathbf{x}_n$ to it's most likely component.

Mixture model clustering



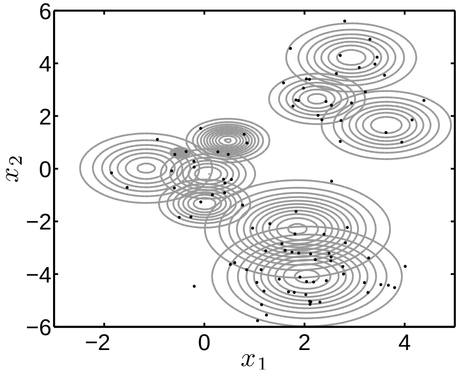
- Points assigned to the cluster with the highest q_{nk} value.

Mixture model – issues

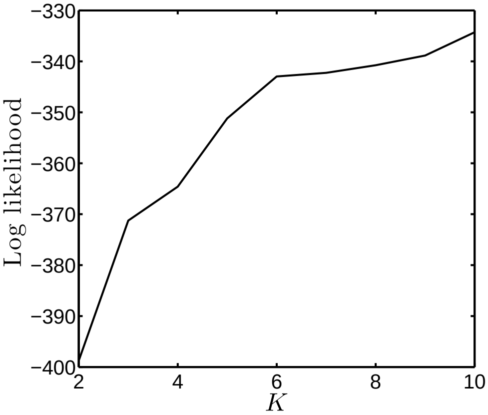
- How do we choose K?
- What happens when we increase it?

Mixture model – issues

- How do we choose K?
- What happens when we increase it?
- $K = 10$



Likelihood increase



- Likelihood always increases as σ_k^2 decreases.

What can we do?

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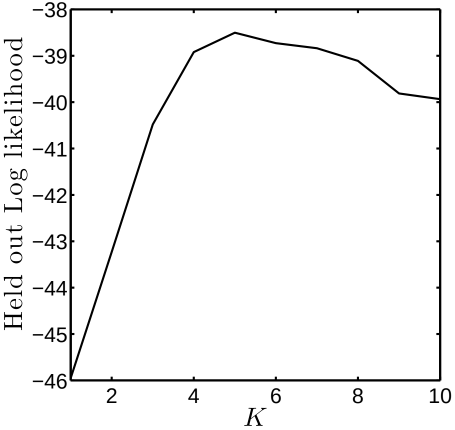
What can we do?

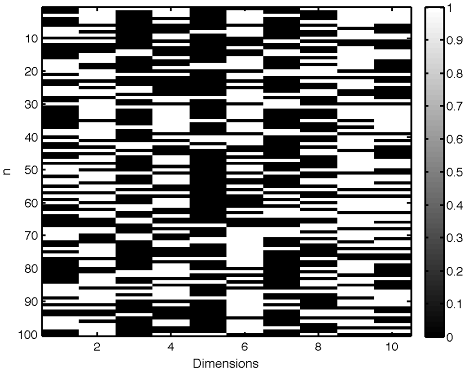
- What can we do?
- Cross-validation...



- 10-fold CV. Maximum is close to true value (3)

Mixture models – other distributions

- We've seen Gaussian distributions.
- Can actually use anything....
- As long as we can define $p(\mathbf{x}_n | z_{nk} = 1, \Delta_k)$
- e.g. Binary data:



Binary example

- $\mathbf{x}_n = [0, 1, 0, 1, 1, \ldots, 0, 1]^\mathsf{T}$ (D dimensions)
- $p(\mathbf{x}_n | z_{nk} = 1, \Delta_k) = \prod_{d=1}^{D} p_{kd}^{x_{nd}} (1 - p_{kd})^{1 - x_{nd}}$

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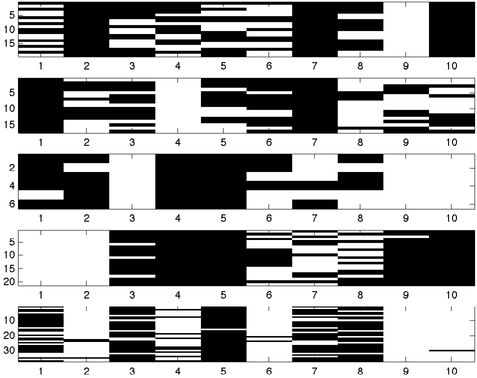
- q_{nk} and π_k are the same as before...
- Initialize with random p_{kd} ($0 \leq p_{kd} \leq 1$)

Results



- $K = 5$ clusters.
- Clear structure present.

Summary

- Introduced two clustering methods.
- K-means
  - Very simple.
  - Iterative scheme.
  - Can be kernelized.
  - Need to choose K.
- Mixture models
  - Create a model of each class (similar to Bayes classifier)
  - Iterative sceme (EM)
  - Can use any distribution for the components.
  - Can set K by cross-validation (held-out likelihood)
  - State-of-the-art: Don't need to set K – treat as a variable in a Bayesian sampling scheme.