Machine Learning & Artificial Intelligence for Data Scientists: Clustering (Part 2)

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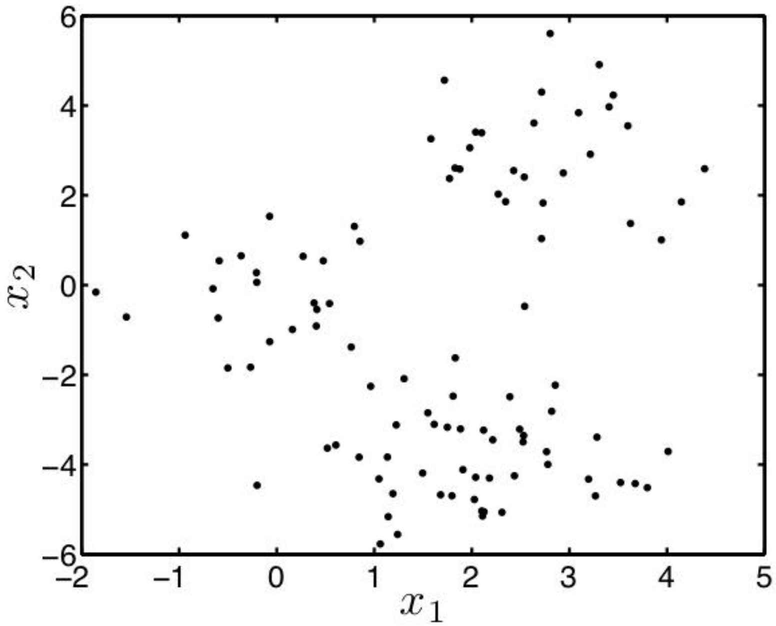
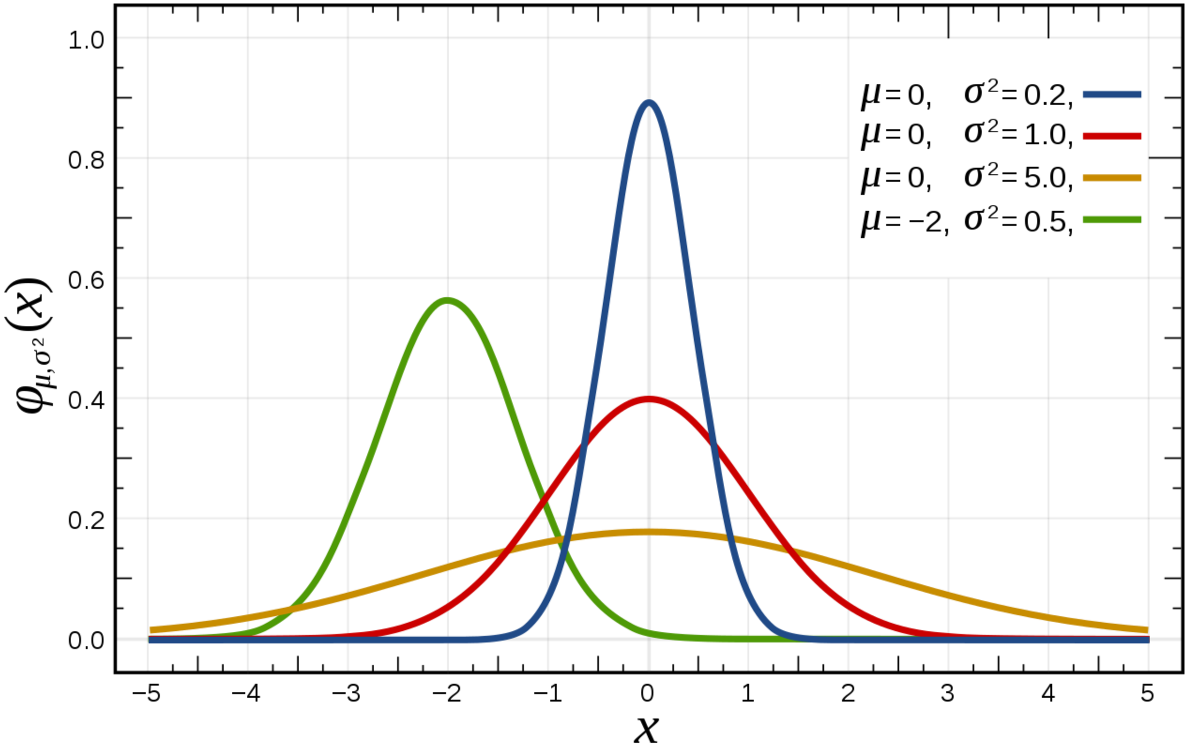
Mixture models – thinking generatively



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

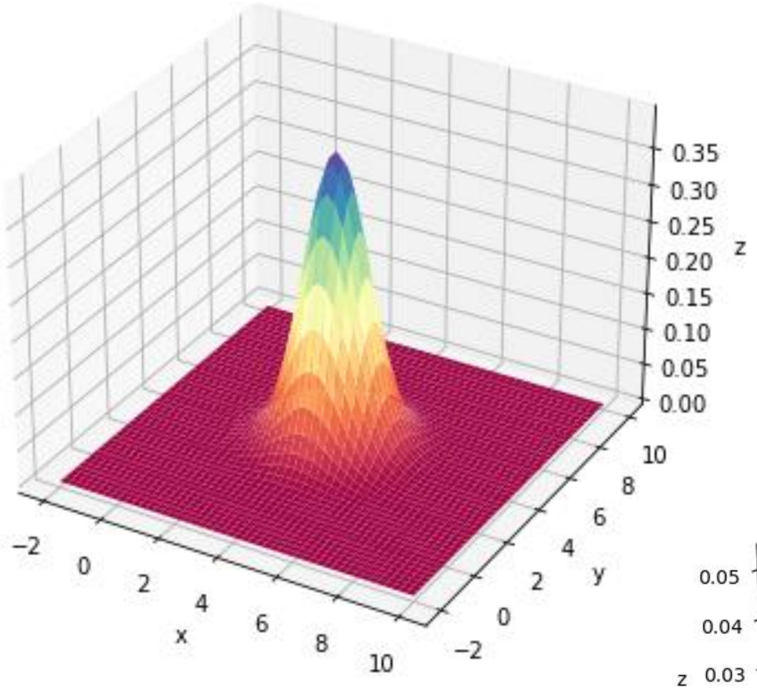
Mixture models – Gaussian Distribution

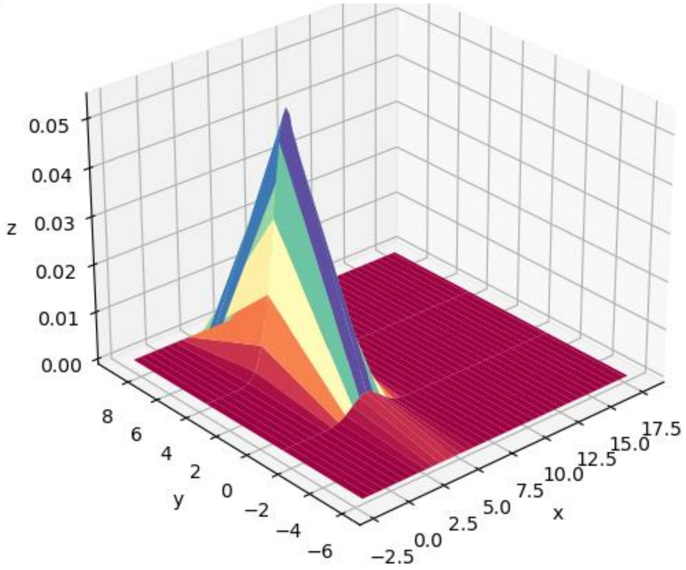


$$f(X) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{X-\mu}{\sigma}\right)^2}$$

$$\mathrm{p}(X|\mu,\sigma) \sim N(\mu,\sigma)$$

Mixture models – Gaussian Distribution in 2D





$$p(\boldsymbol{X}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{n/2}|\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\boldsymbol{X}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{X}-\boldsymbol{\mu})}$$

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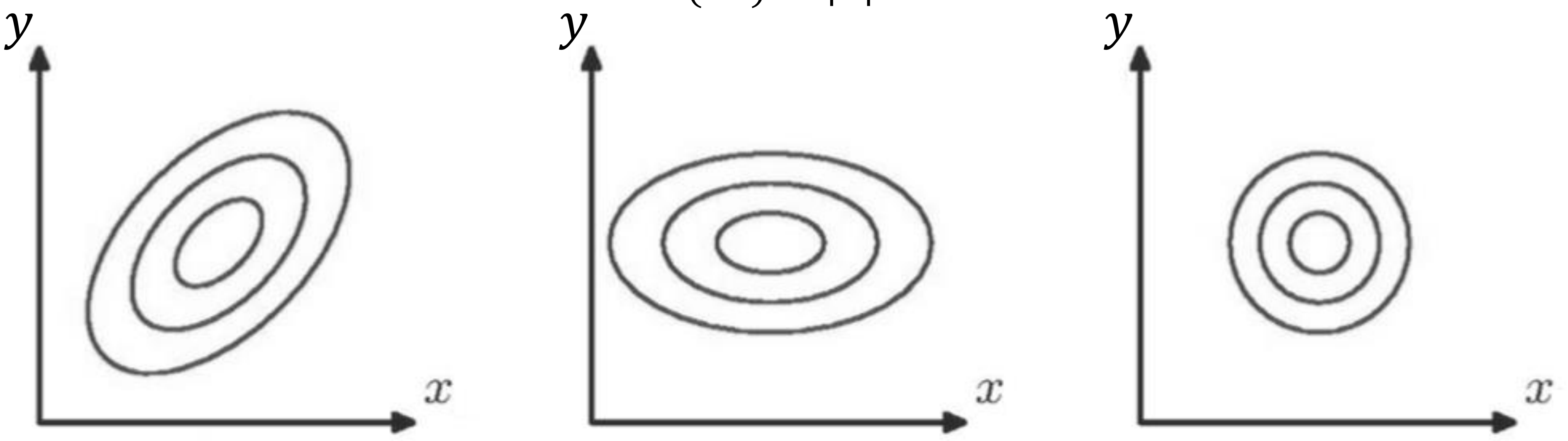
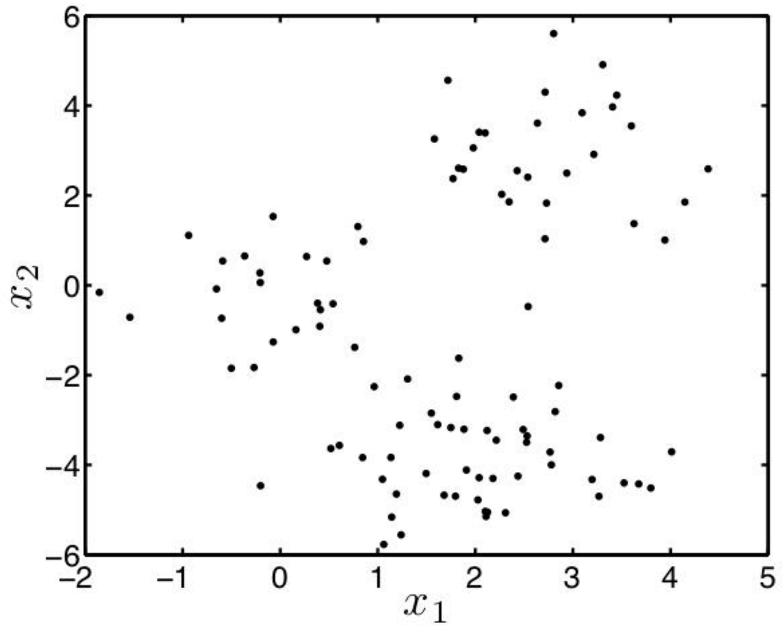


$$\boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{1,1} & \Sigma_{1,2} \\ \Sigma_{2,1} & \Sigma_{2,2} \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{1,1} & 0 \\ 0 & \Sigma_{2,2} \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \boldsymbol{\sigma}^2 \begin{bmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{bmatrix} = \boldsymbol{\sigma}^2 \mathbf{I}$$

Mixture models – thinking generatively



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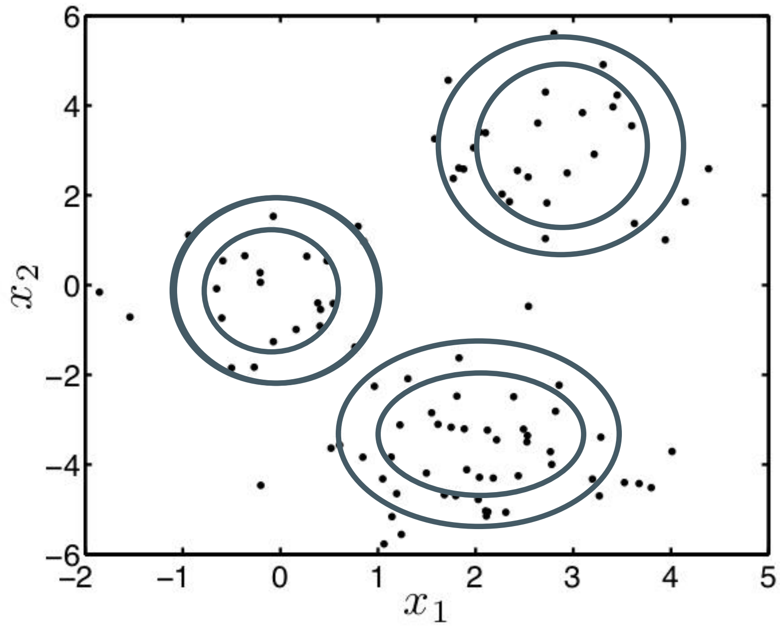
Mixture models – thinking generatively



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A generative model

- Assumption:Each $\mathbf{x}_n$ comes from one of different K distributions.
- To generate $\mathbf{X}$:
- For each n:
  1. Pick one of the K components.
  2. Sample $\mathbf{x}_n$ from this distribution.

- We already have $\mathbf{X}$
- Define parameters of all these distributions as Δ.
- We'd like to reverse-engineer this process learn Δ which we can then use to find which component each point came from.
- Maximise the likelihood!

Gaussian mixture model

- Assume component distributions are Gaussians with diagonal covariance:

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

- We need to be able to estimate the prior of assignment. Let

$$\pi_k = p(z_{nk} = 1|\Delta)$$

- We also want to estimate the probability to assign data to each component

$$q_{nk} = \frac{\pi_k p(\mathbf{x}_n|z_{nk} = 1, \boldsymbol{\mu}_k, \sigma_k^2)}{\sum_{j=1}^{K} \pi_j p(\mathbf{x}_n|z_{nj} = 1, \boldsymbol{\mu}_j, \sigma_j^2)}$$

Mixture model optimisation – the Expectation-Maximization (EM) algorithm

–

- Following optimisation algorithm:
  1. Guess $\boldsymbol{\mu}_k, \sigma_k^2, \pi_k$
  2. **(E)**xpectation-step: Compute q_{nk}
  3. **(M)**aximization-step: Update $\boldsymbol{\mu}_k, \sigma_k^2, \pi_k$
  4. Return to 2 unless parameters are unchanged.
- Guaranteed to converge to a local maximum of the lower bound.
- Note the similarity with kmeans.

Mixture model optimisation – the Expectation-Maximization (EM) algorithm

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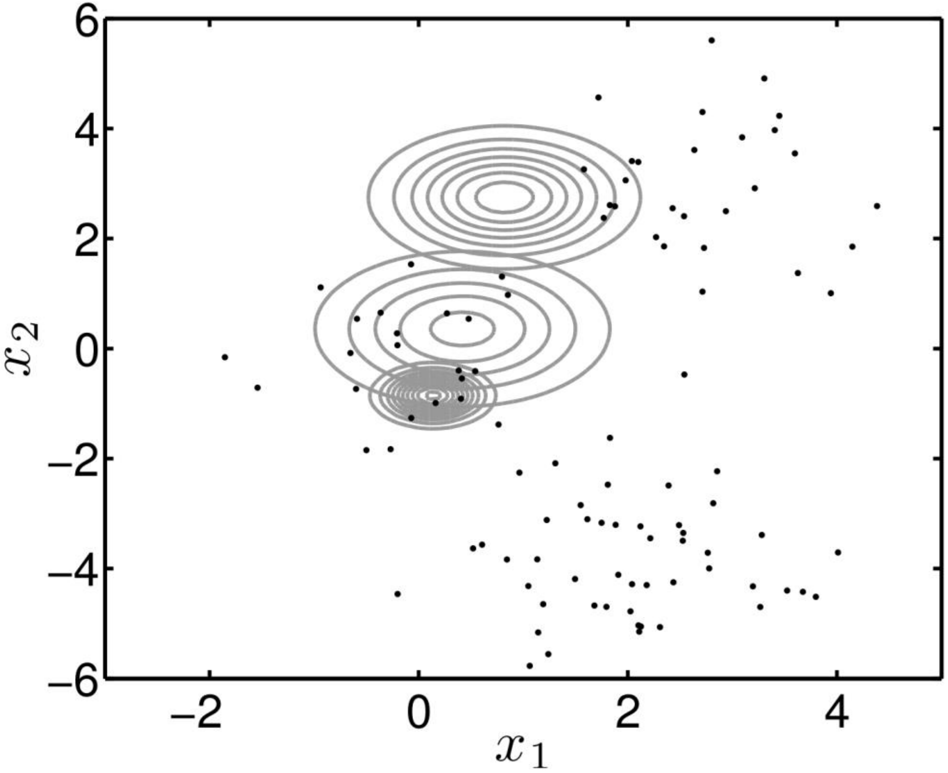
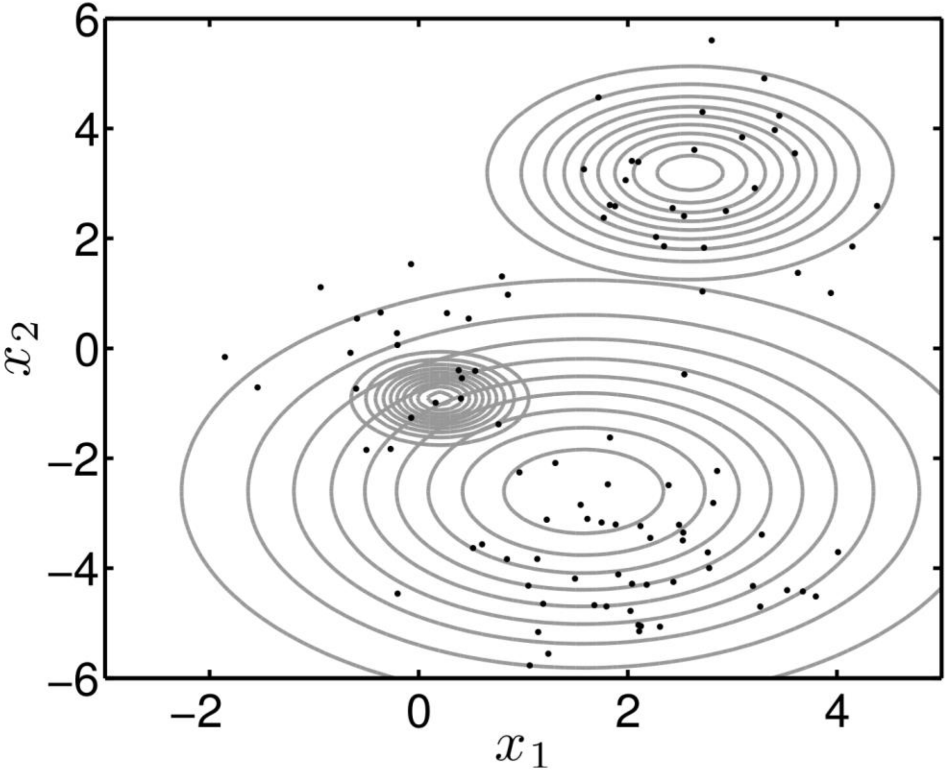
$$\widehat{N}_k = \sum_{i=1}^{N} q_{ik} \quad \hat{\mu}_k = \frac{1}{\widehat{N}_k} \sum_{i=1}^{N} q_{ik} x_i \quad \widehat{\boldsymbol{\Sigma}}_k = \frac{1}{\widehat{N}_k} \sum_{i=1}^{N} q_{ik} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

Algorithm in operation



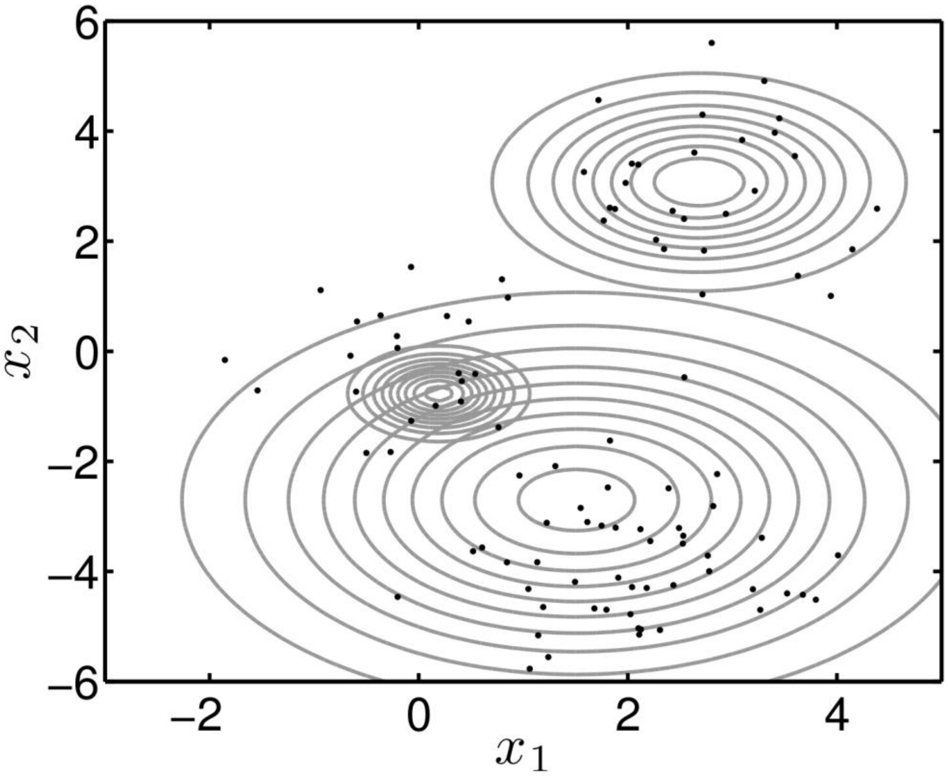
Initial guess

Algorithm in operation



Update q_nk and then other parameters.

Algorithm in operation



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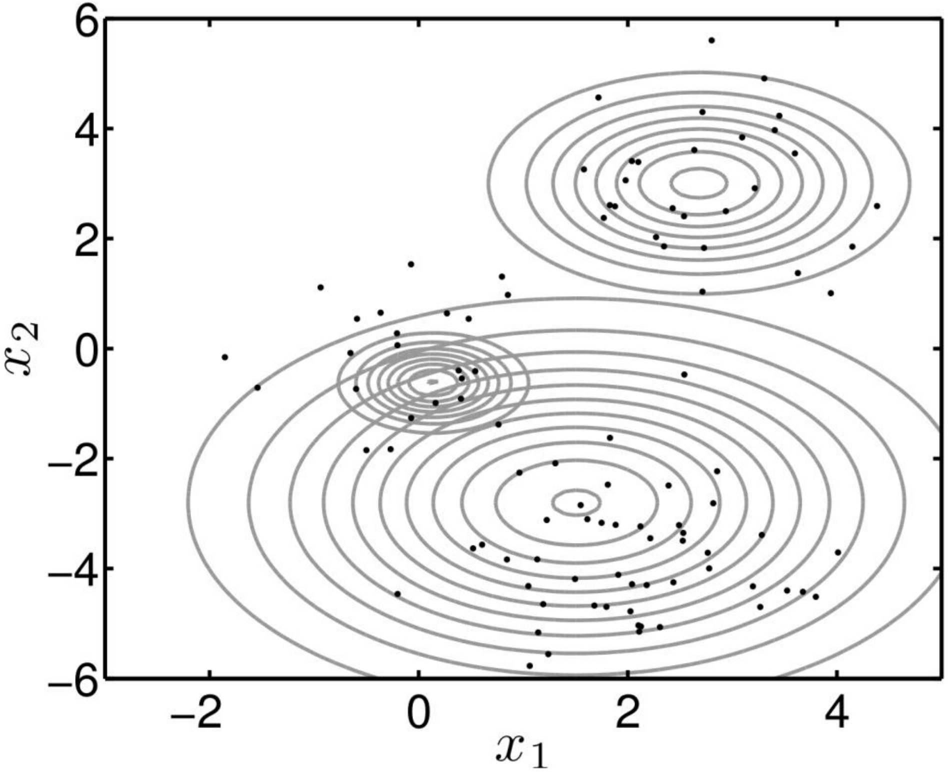

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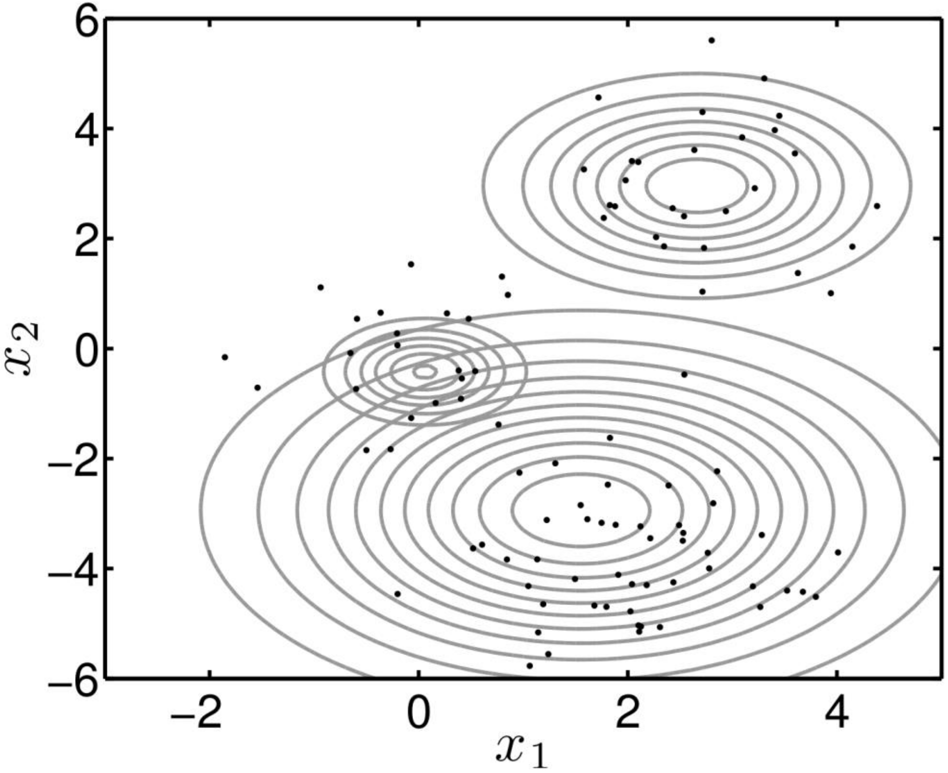

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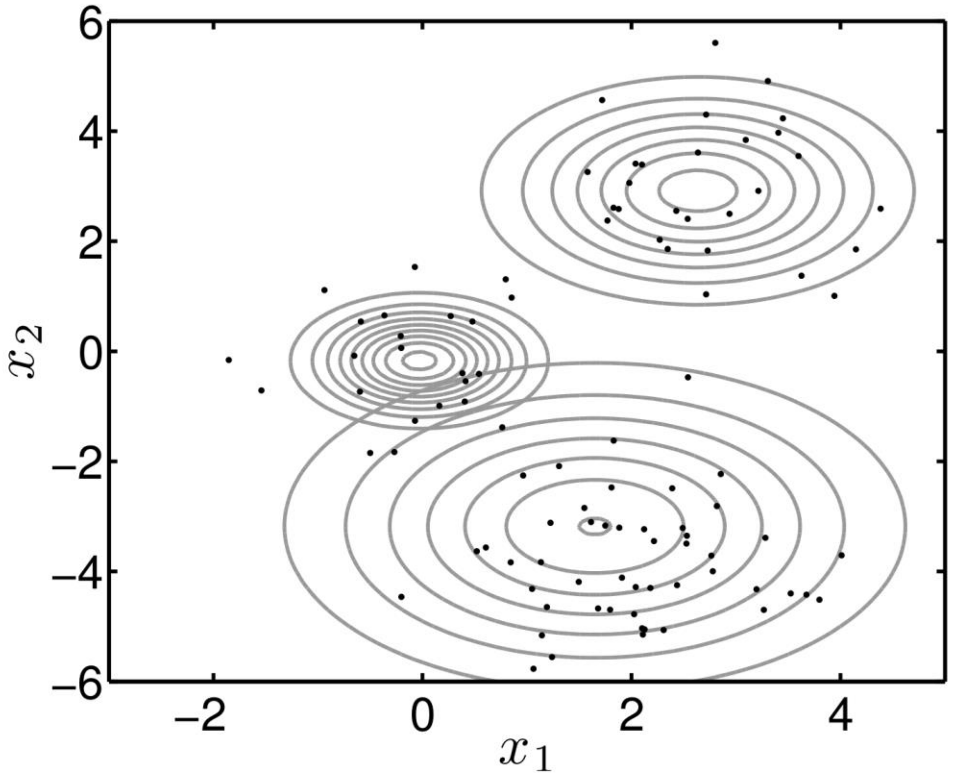

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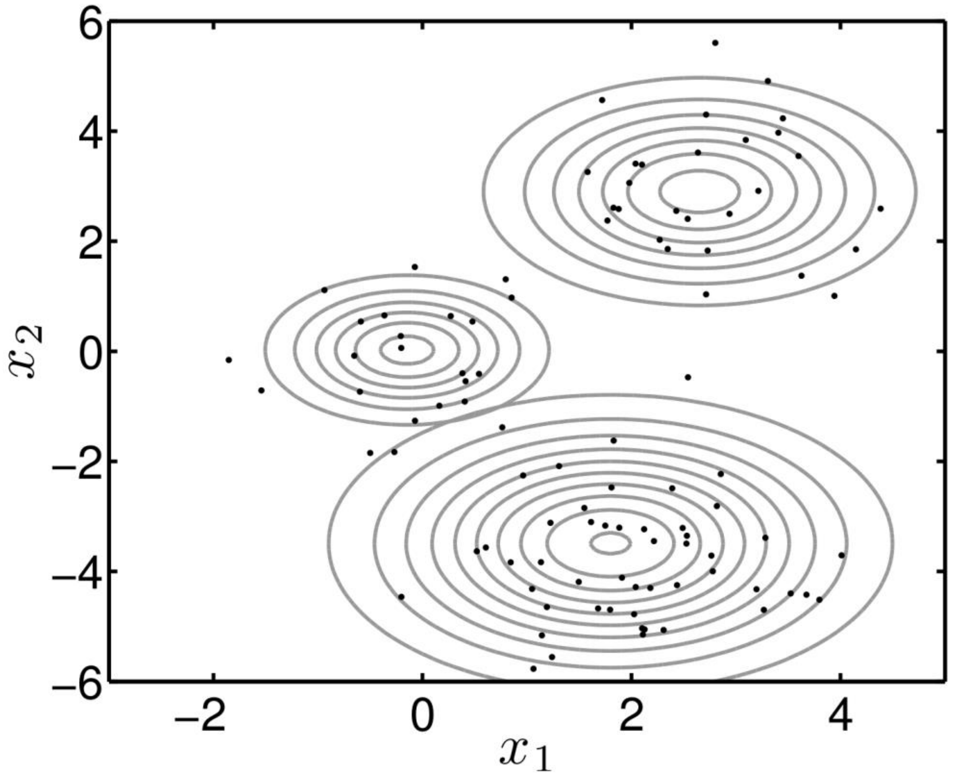

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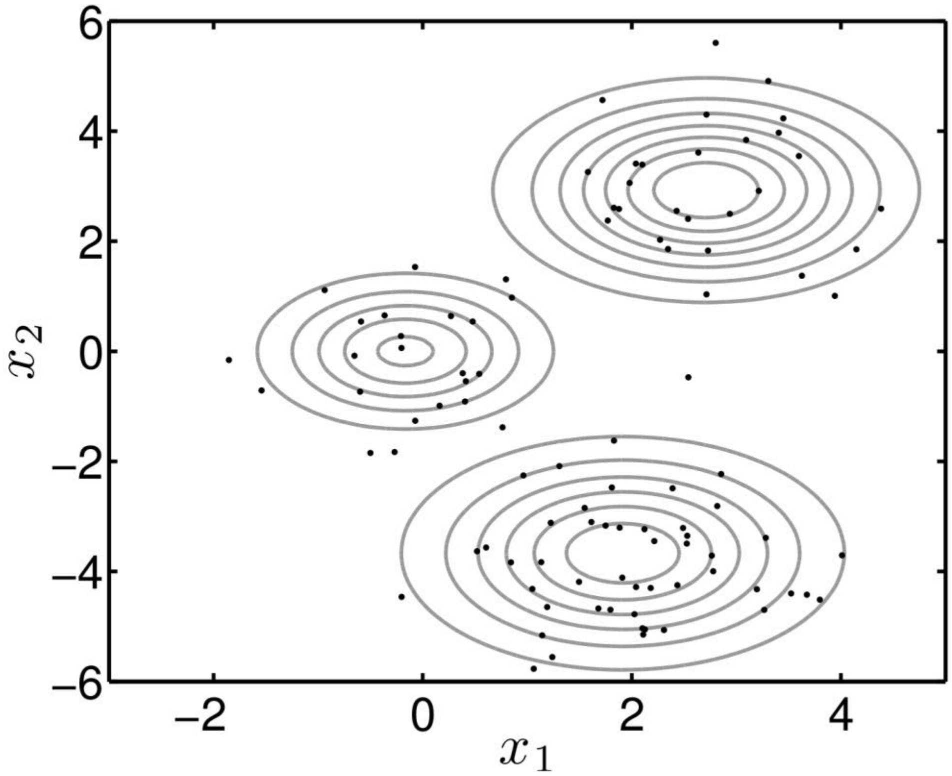

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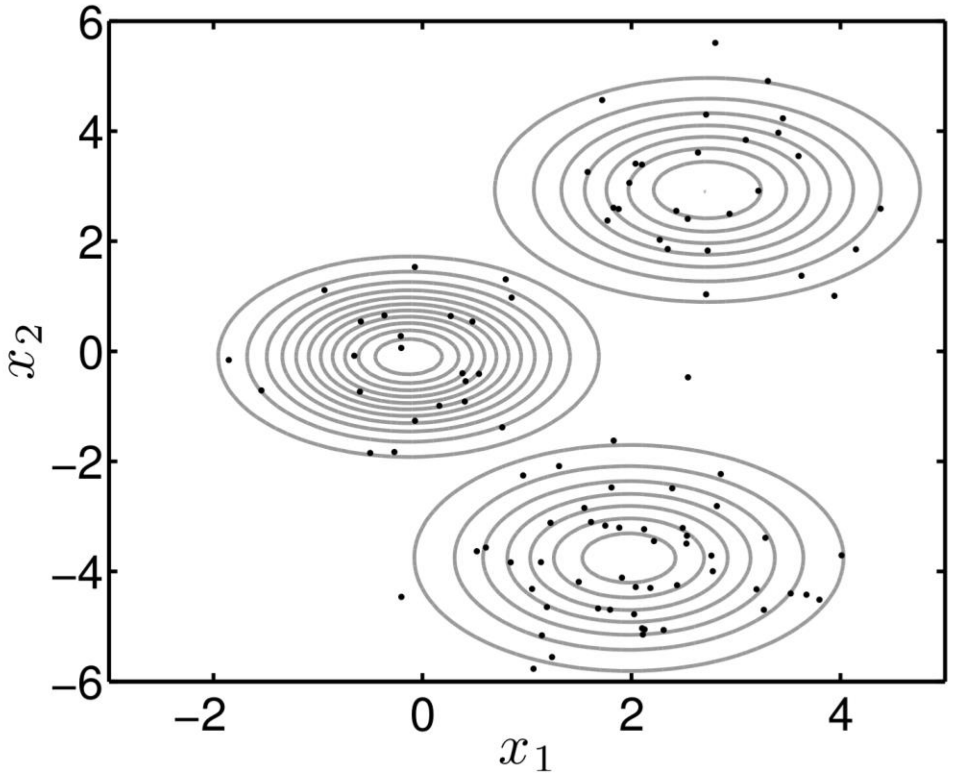

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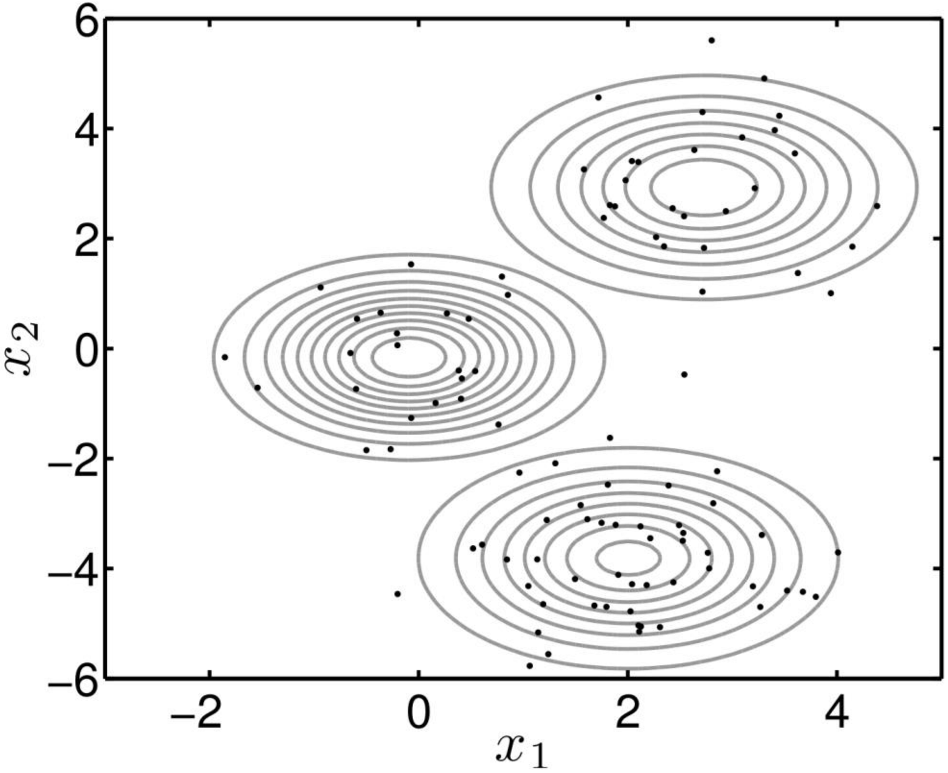

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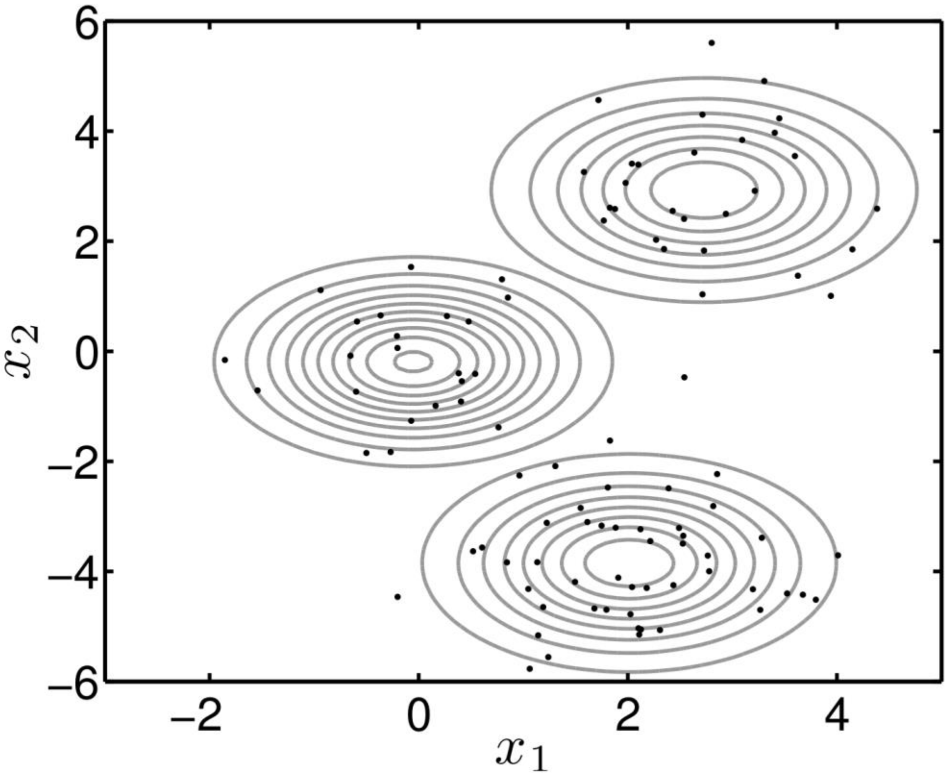

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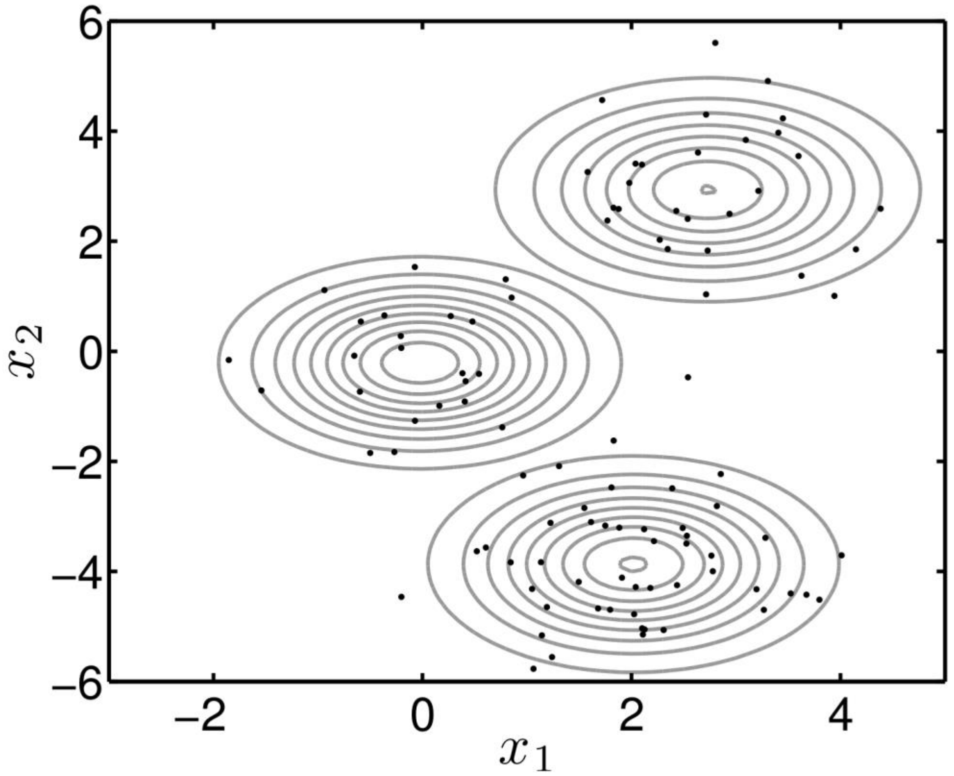

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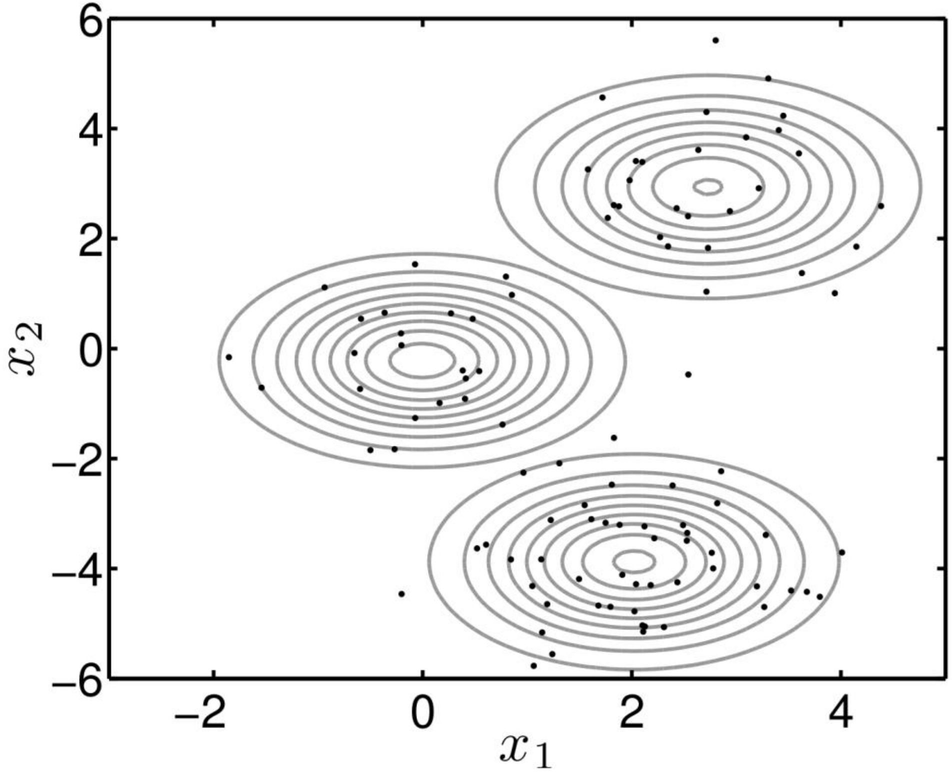

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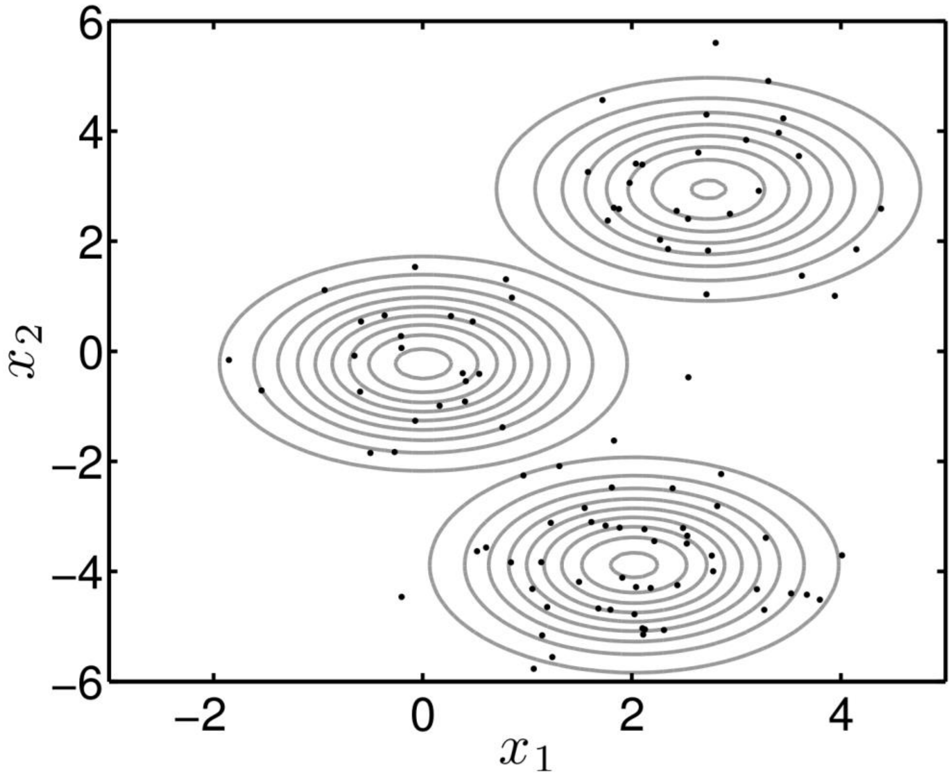

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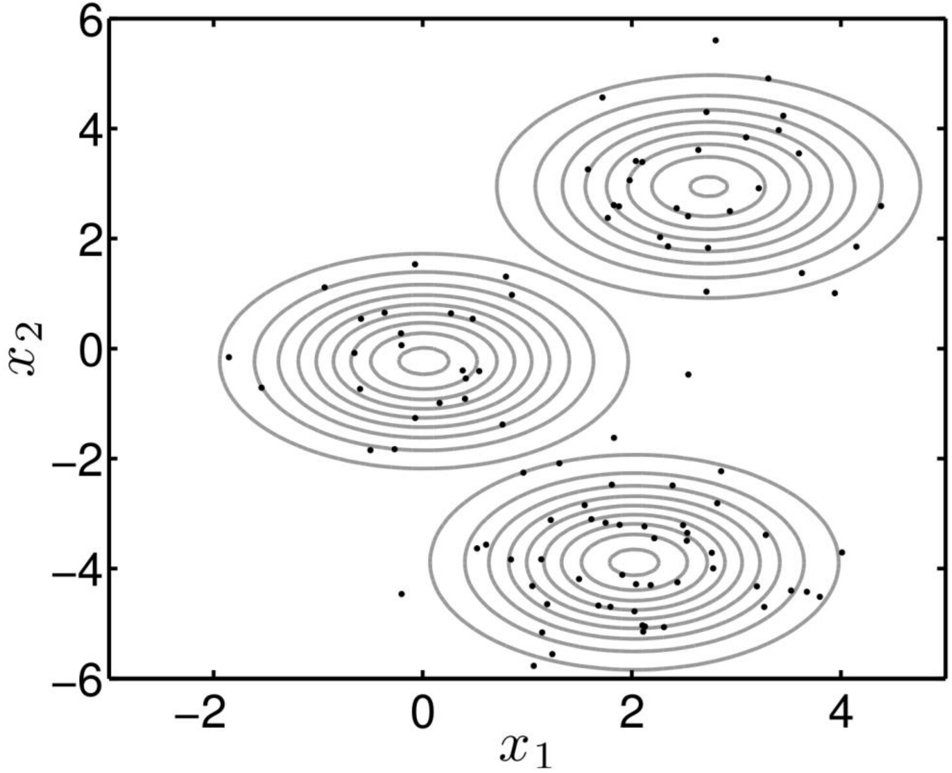

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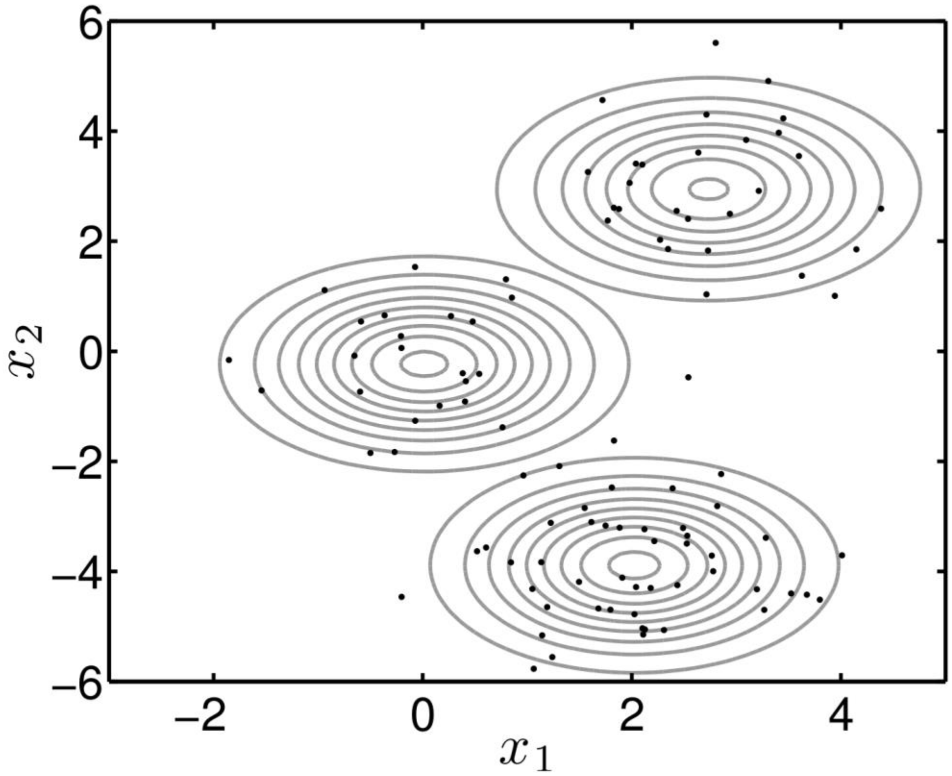


Solution at convergence

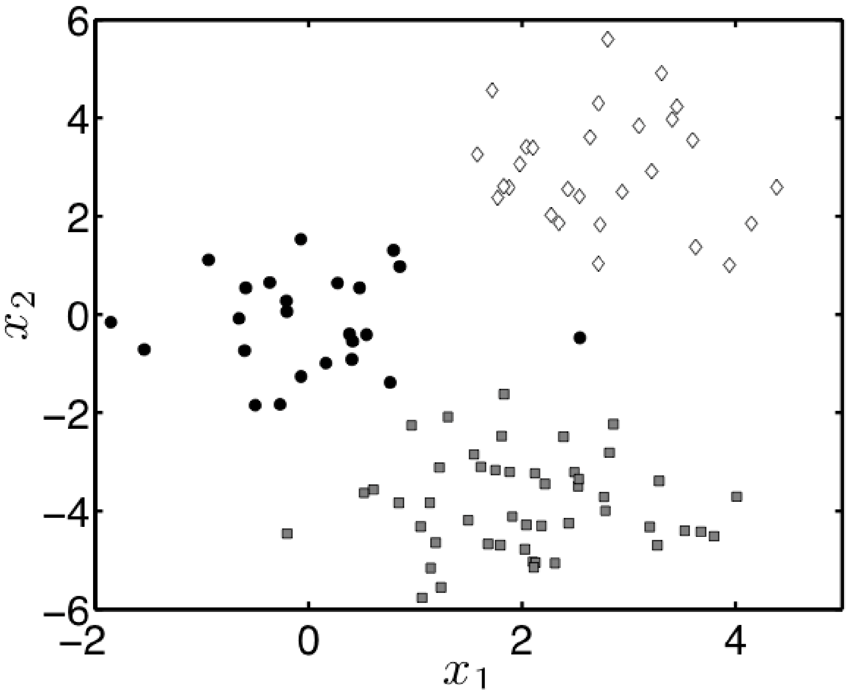
Mixture model clustering

- So, we've got the parameters, but what about the assignments?
- Which points came from which distributions?
- q_{nk} is the probability that $\mathbf{x}_n$ came from distribution k.

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

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

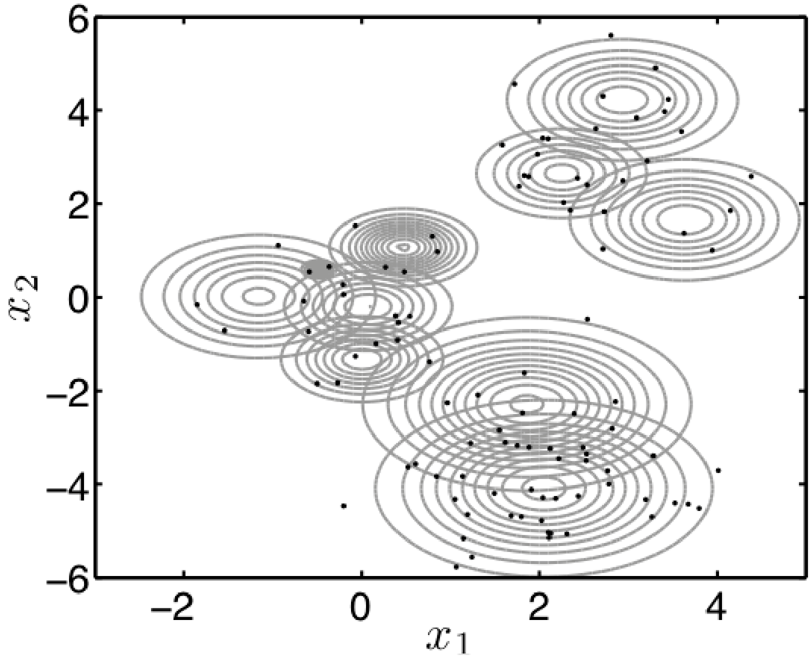
Mixture model clustering



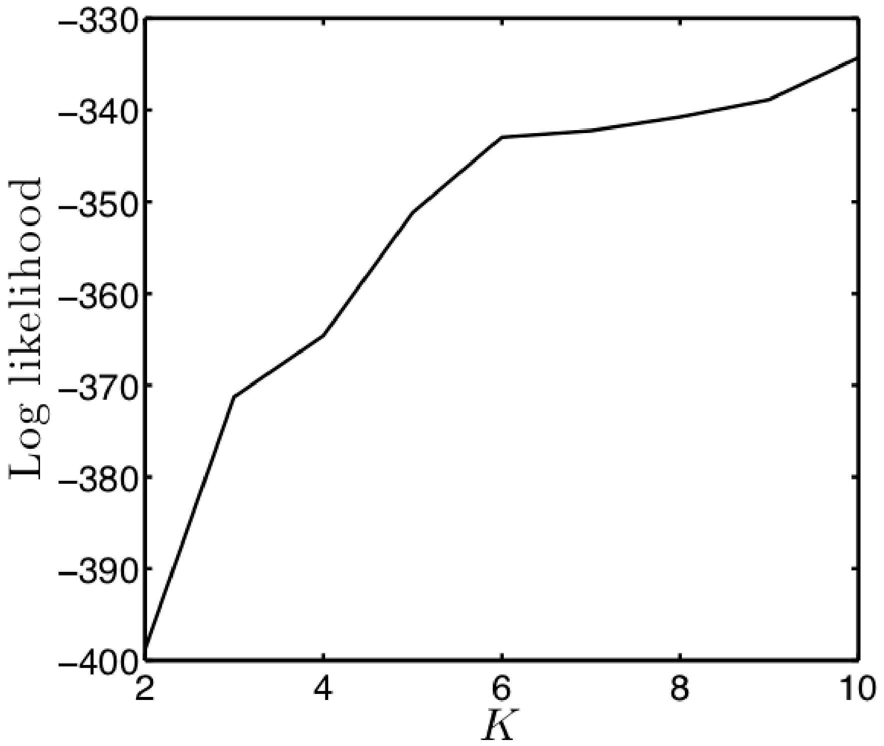
- Points assigned to the cluster with the highest q_{nk} value.

Mixture model – issues

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



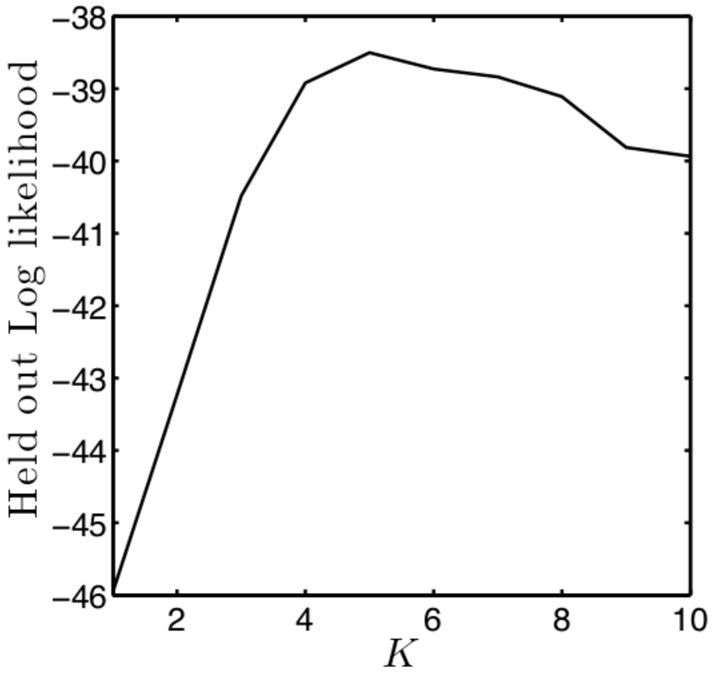
Likelihood increase



- Likelihood always increases as σ_k^2 decreases.

What can we do?

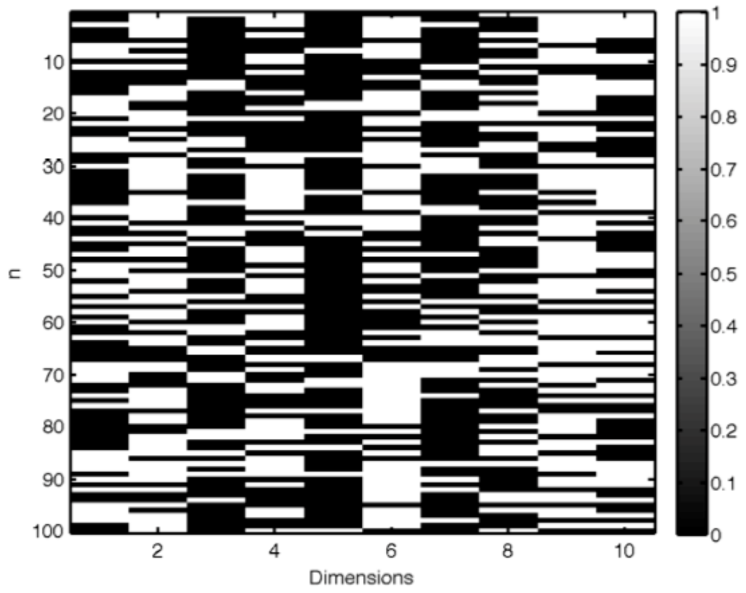
- What can we do?
- Cross-validation...



- 10-fold CV. Maximum is close to true value (3)
- 5 might be better for this data....

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:



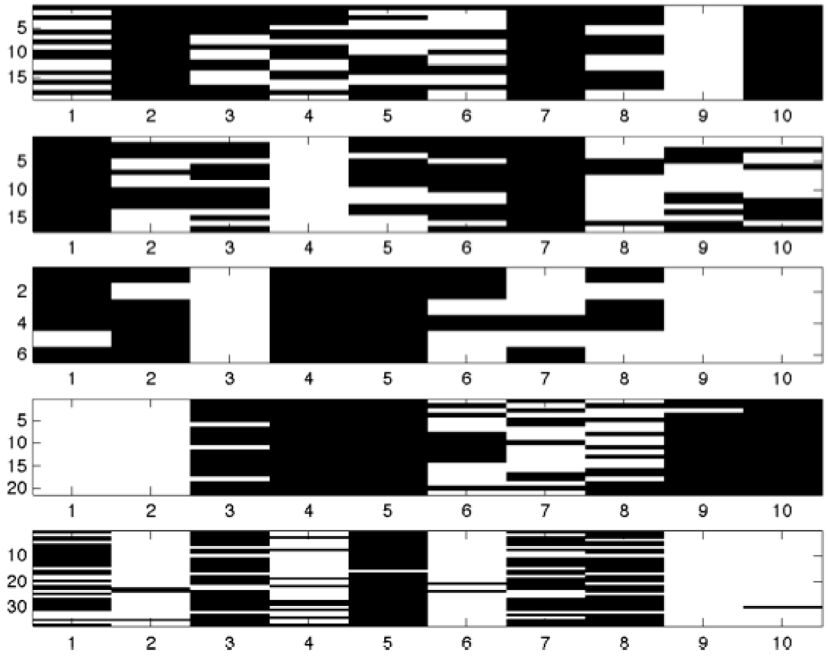
Binary example

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

$$p_{kd} = \frac{\sum_n q_{nk} x_{nd}}{\sum_n q_{nk}}$$

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

Binary example



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

Summary

- Introduced two clustering methods.
- K-means
  - Very simple.
  - Iterative scheme.
  - Can be kernelised.
  - 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.