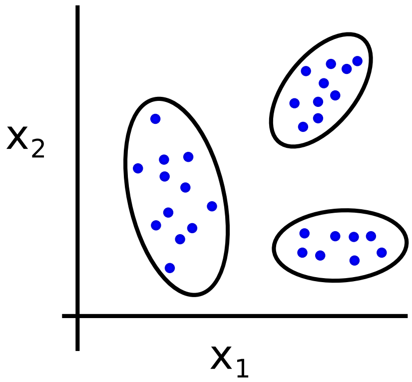
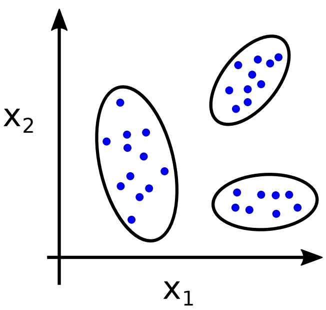
Clustering and the EM algorithm

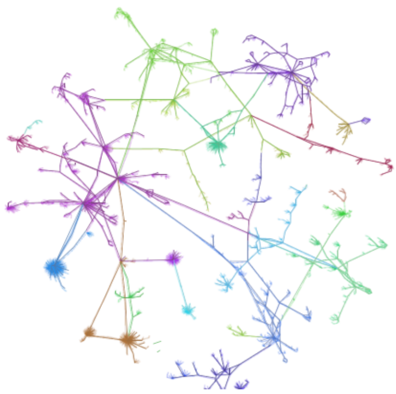
Rich Turner and José Miguel Hernández-Lobato



What is clustering?

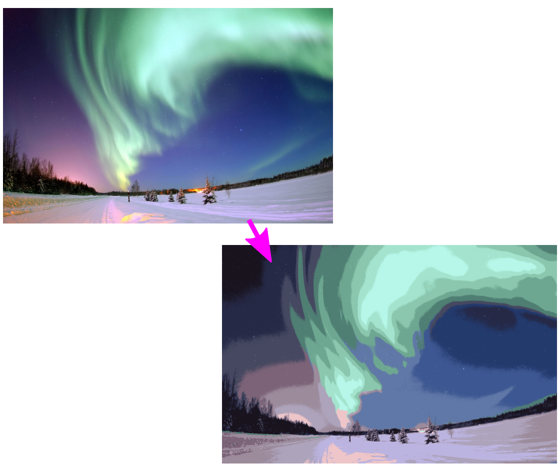


network community detection



Campbell et al Social Network Analysis

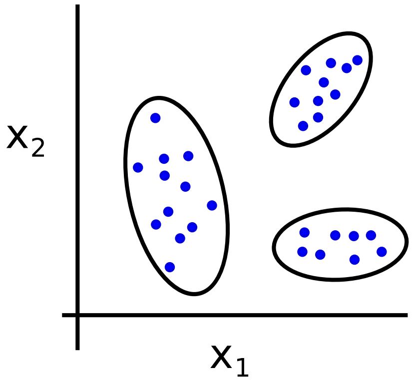
image segmentation



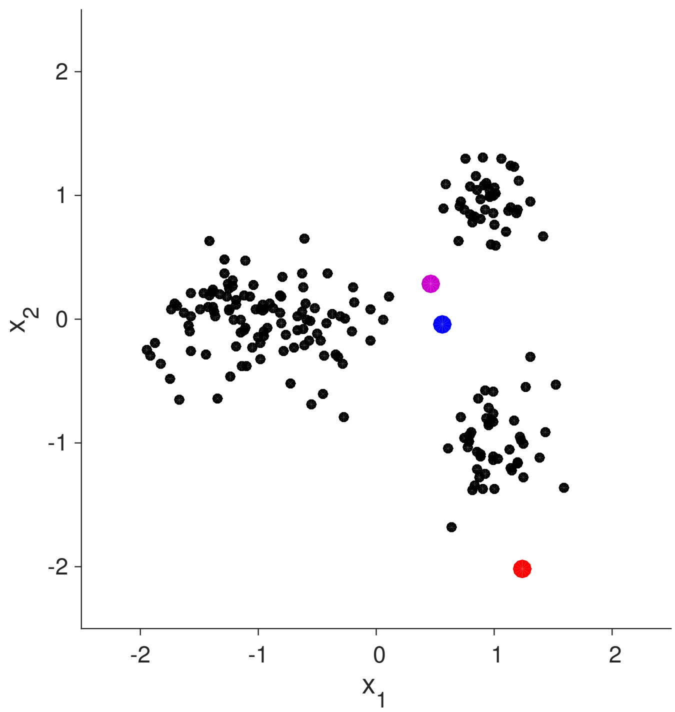
vector quantisation
genetic clustering
anomaly detection
crime analysis

What is clustering?

- Roughly speaking, two points belonging to the same cluster are generally more similar to each other or closer to each other than two points belonging to different clusters.
- $\mathcal{D} = \{\mathrm{x}_1 \dots \mathrm{x}_N\} \rightarrow \boldsymbol{s} = \{s_1 \dots s_N\}$
- Unsupervised learning problem (no labels or rewards)



A first clustering algorithm: k-means



input: $\mathcal{D} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$, $\boldsymbol{x}_n \in \mathbb{R}^D$

initialise: $\boldsymbol{m}_k \in \mathbb{R}^D$ for $k = 1 \dots K$

repeat

  for $n = 1 \dots N$

$$s_n = \arg\min_k ||\boldsymbol{x}_n - \boldsymbol{m}_k||$$

  endfor

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  endfor

until convergence (s_n fixed)

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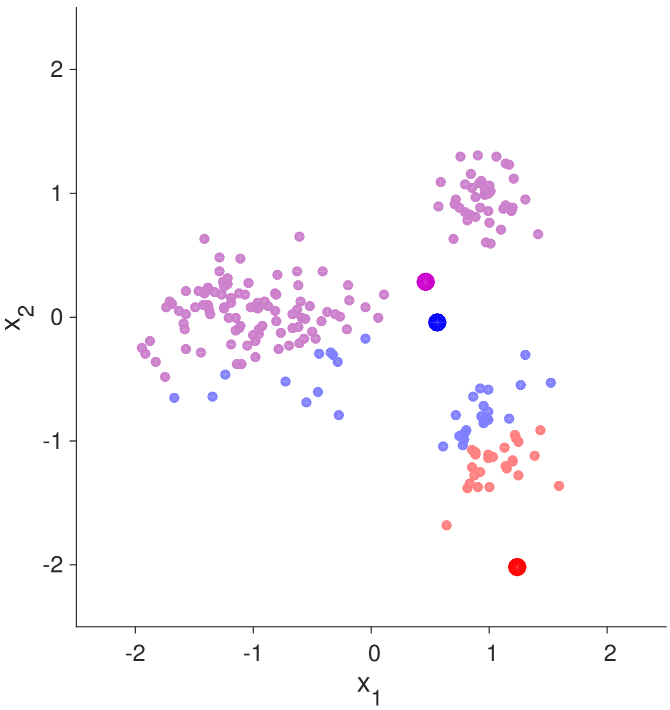

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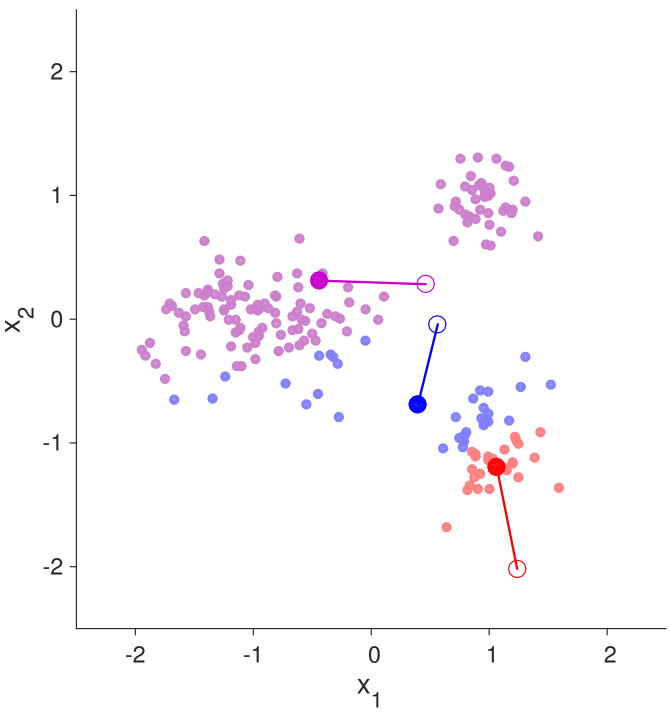

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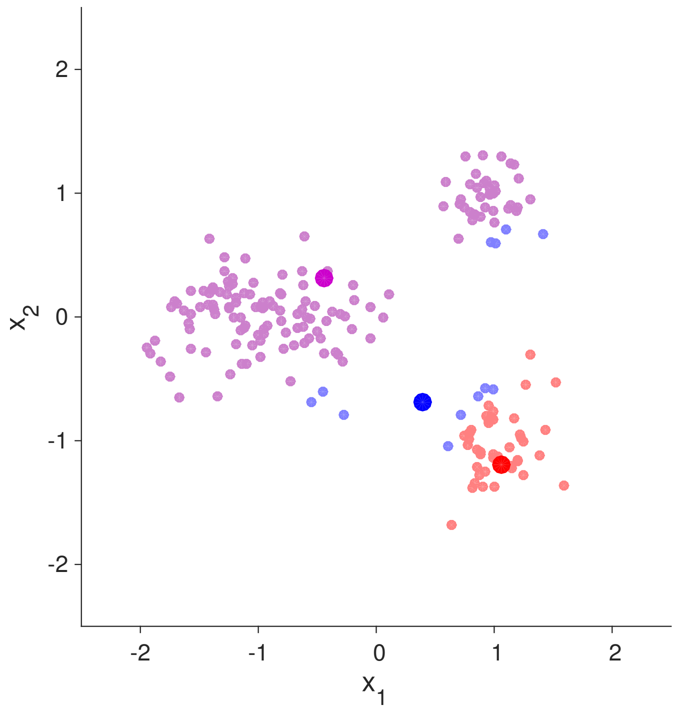

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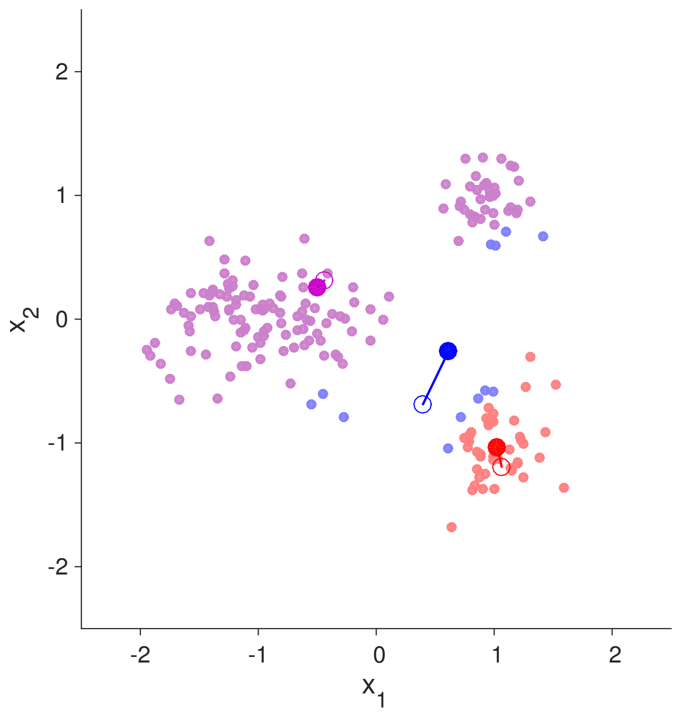

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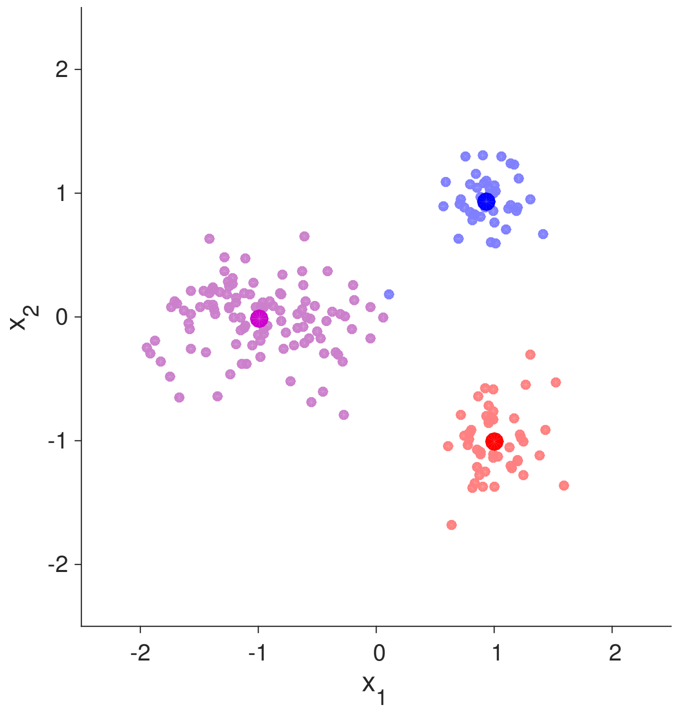
Question: is K-means guaranteed to converge for any dataset $\mathcal{D}$?

could one or more of the cluster centres diverge or oscillate?



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K-means as optimisation

Let $s_{n,k} = 1$ if data point n is assigned to cluster k and zero otherwise

Note: $\sum_{k=1}^K s_{n,k} = 1$

Cost:

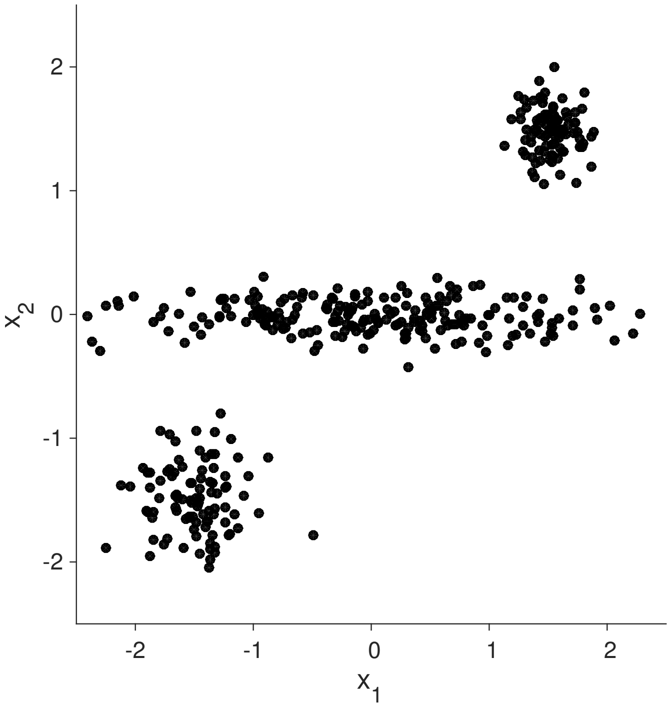
$$\mathcal{C}(\{s_{n,k}\}, \{\boldsymbol{m}_k\}) = \sum_{n=1}^N \sum_{k=1}^K s_{n,k} ||\boldsymbol{x}_n - \boldsymbol{m}_k||^2$$

K-means tries to minimise the cost function $\mathcal{C}$ with respect to $\{s_{n,k}\}$ and $\{\boldsymbol{m}_k\}$, subject to $\sum_k s_{n,k} = 1$ and $s_{n,k} \in \{0, 1\}$

K-means sequentially:

- minimises $\mathcal{C}$ with respect to $\{s_{n,k}\}$, holding $\{\boldsymbol{m}_k\}$ fixed.
- minimises $\mathcal{C}$ with respect to $\{\boldsymbol{m}_k\}$, holding $\{s_{n,k}\}$ fixed.

Where will K-means converge to when run on these data?



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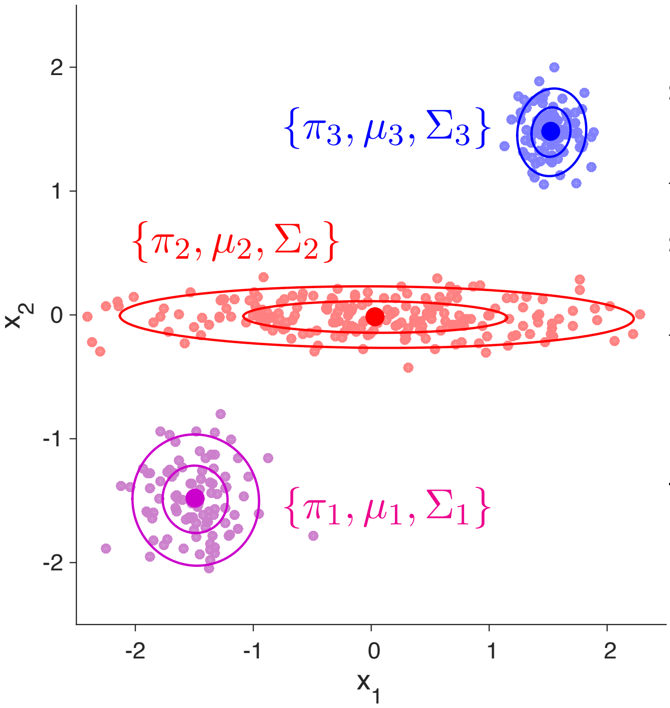
Mixture of Gaussians: Generative Model



For each data point $1 \ldots N$

sample cluster membership:

$p(s_n = k|\theta) = \pi_k$ note $\sum_{k=1}^K \pi_k = 1$

sample data-value given cluster mem.:

$p(\boldsymbol{x}_n|s_n = k, \theta) = \mathcal{N}(\boldsymbol{x}_n; \boldsymbol{m}_k, \Sigma_k)$

How can we learn the parameters of this model from data using maximum-likelihood?

$$\theta_{\text{ML}} = \arg\max_\theta \log p(\{\boldsymbol{x}_n\}_{n=1}^N|\theta)$$

A lower bound on the log-likelihood $\log p(\boldsymbol{x}|\theta)$

arbitrary distribution over class memberships

posterior distribution over class memberships

$$\underbrace{\mathcal{F}(q(\boldsymbol{s}),\theta)}_{\text{free-energy}} = \underbrace{\log p(\boldsymbol{x}|\theta)}_{\text{log-likelihood}} - \underbrace{\sum_{\boldsymbol{s}} q(\boldsymbol{s}) \log \frac{q(\boldsymbol{s})}{p(\boldsymbol{s}|\boldsymbol{x},\theta)}}_{\substack{\text{KL-Divergence} \\ \mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x}\ \theta))}}$$

A brief introduction to the Kullback-Leibler divergence

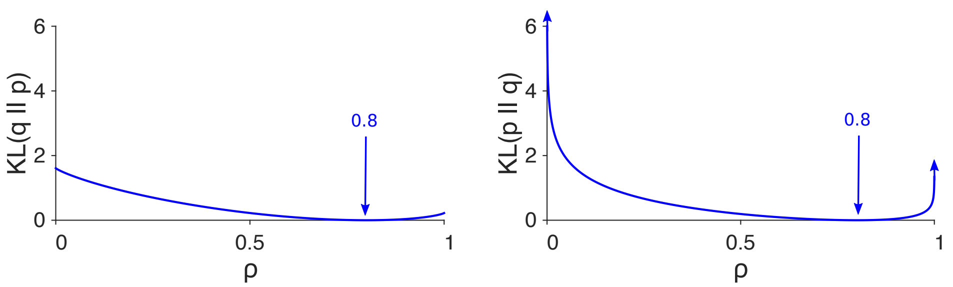
$$\mathcal{KL}(p_1(z)||p_2(z)) = \sum_z p_1(z) \log \frac{p_1(z)}{p_2(z)}$$

Important properties:

- Gibb's inequality: $\mathcal{KL}(p_1(z)|p_2(z)) \geq 0$, equality at $p_1(z) = p_2(z)$
  - proof via Jensen's inequality or differentiation (see MacKay pg. 35)
- Non-symmetric: $\mathcal{KL}(p_1(z)|p_2(z)) \neq \mathcal{KL}(p_2(z)|p_1(z))$
  - hence named *divergence* and not *distance*

Example:

- binary variables $z \in \{0, 1\}$
- $p(z = 1) = 0.8$ and $q(z = 1) = \rho$



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$$\mathcal{F}(q(\boldsymbol{s}),\theta) = \sum_{\boldsymbol{s}} q(\boldsymbol{s}) \log \frac{p(\boldsymbol{x}|\boldsymbol{s},\theta)p(\boldsymbol{s}|\theta)}{q(\boldsymbol{s})} \Rightarrow \text{simple to compute}$$

Non-negativity of KL-Divergence

Free-energy is lower bound on log-likelihood

$$\mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x},\theta)) \geq 0 \implies \mathcal{F}(q(\boldsymbol{s}),\theta) \leq \log p(\boldsymbol{x}|\theta)$$

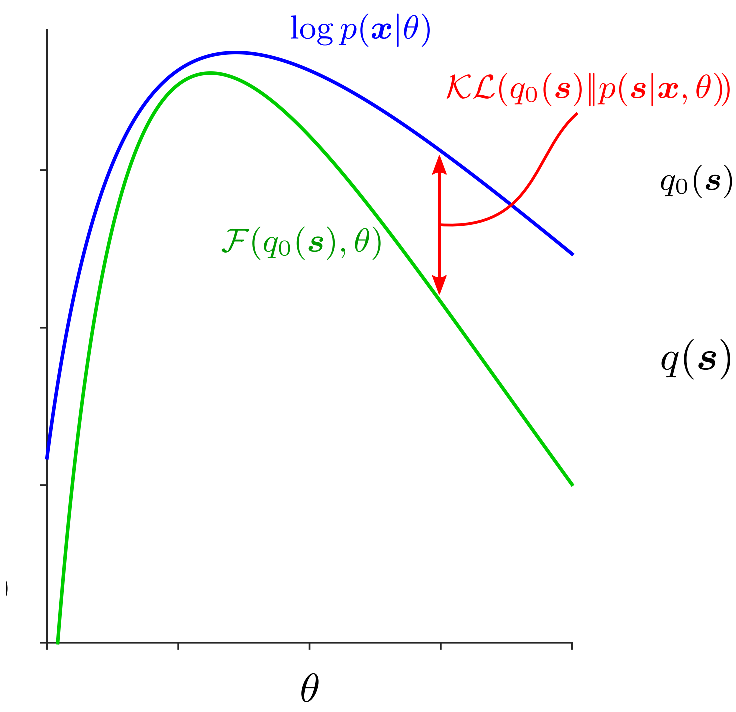
KL-Divergence equal to 0 when $q(\boldsymbol{s}) = p(\boldsymbol{s}|\boldsymbol{x},\theta)$

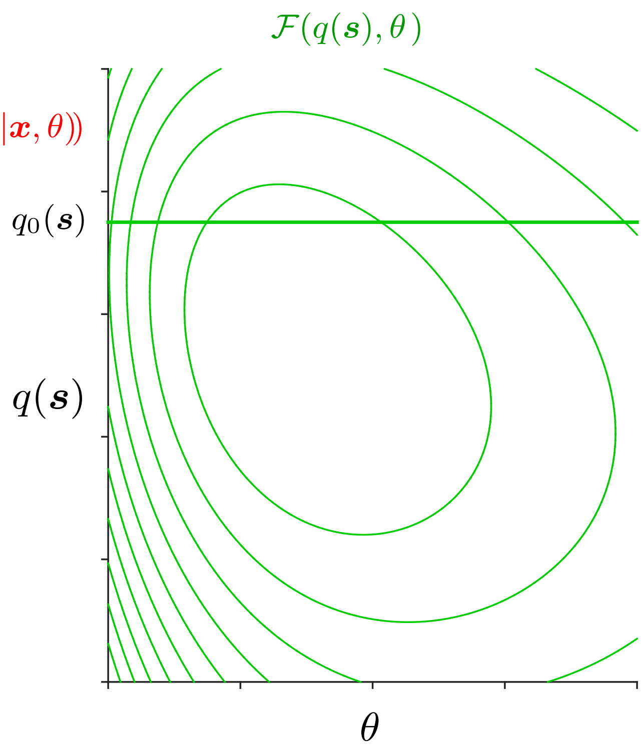
Free-energy equal to log-likelihood when $q(\boldsymbol{s}) = p(\boldsymbol{s}|\boldsymbol{x},\theta)$

$$\mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x},\theta)) = 0 \implies \mathcal{F}(q(\boldsymbol{s}),\theta) = \log p(\boldsymbol{x}|\theta)$$

Visualising the free-energy lower bound

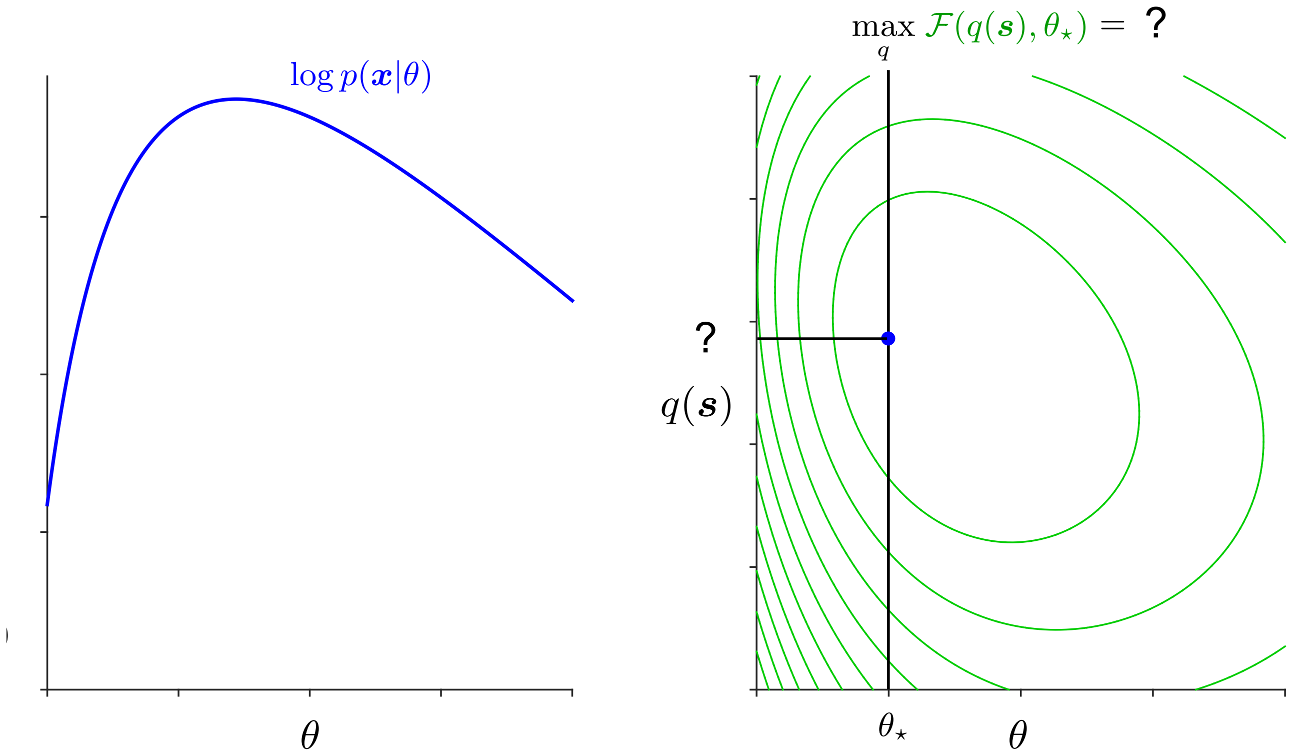
$$\mathcal{F}(q(\boldsymbol{s}),\theta) = \log p(\boldsymbol{x}|\theta) - \mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x},\theta))$$





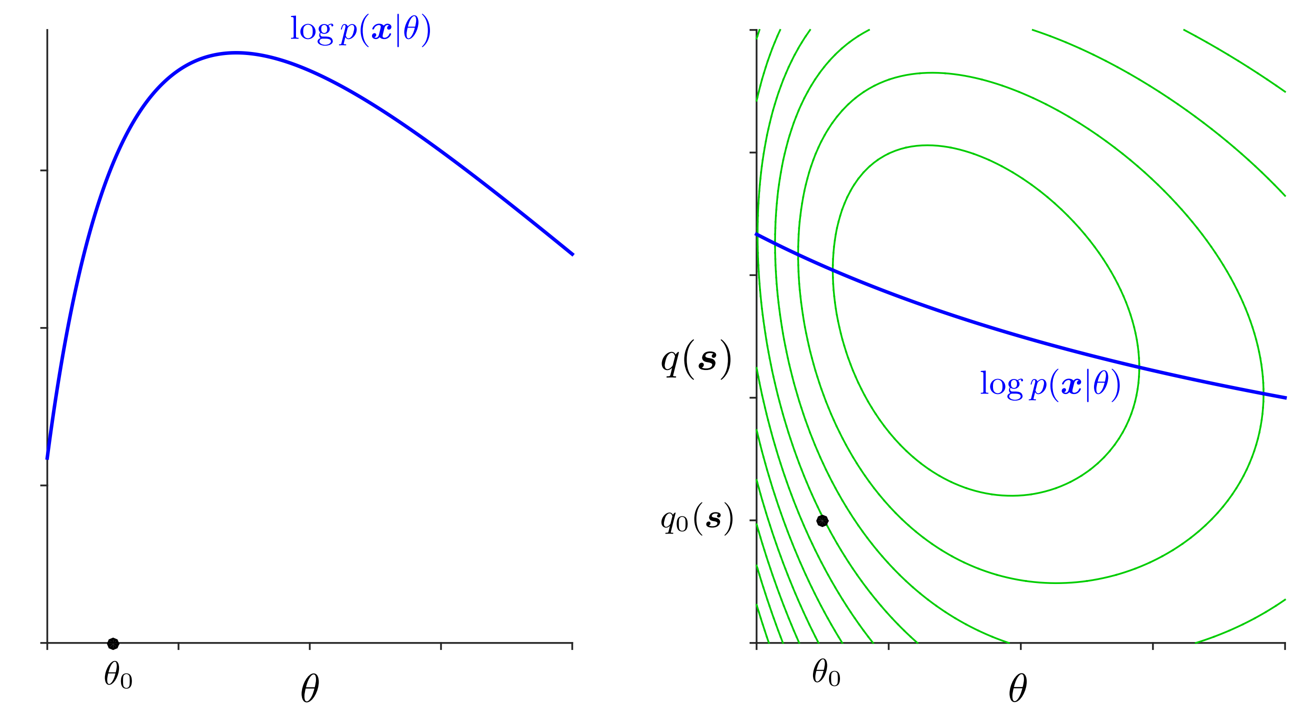
What is the maximal value of the free-energy along this vertical slice?

$$\mathcal{F}(q(\boldsymbol{s}),\theta) \;= \log p(\boldsymbol{x}|\theta) - \mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x},\theta))$$



The Expectation Maximisation (EM) algorithm

$$\mathcal{F}(q(\boldsymbol{s}),\theta) \;= \log p(\boldsymbol{x}|\theta) - \mathcal{KL}(q(\boldsymbol{s})\|p(\boldsymbol{s}|\boldsymbol{x},\theta))$$



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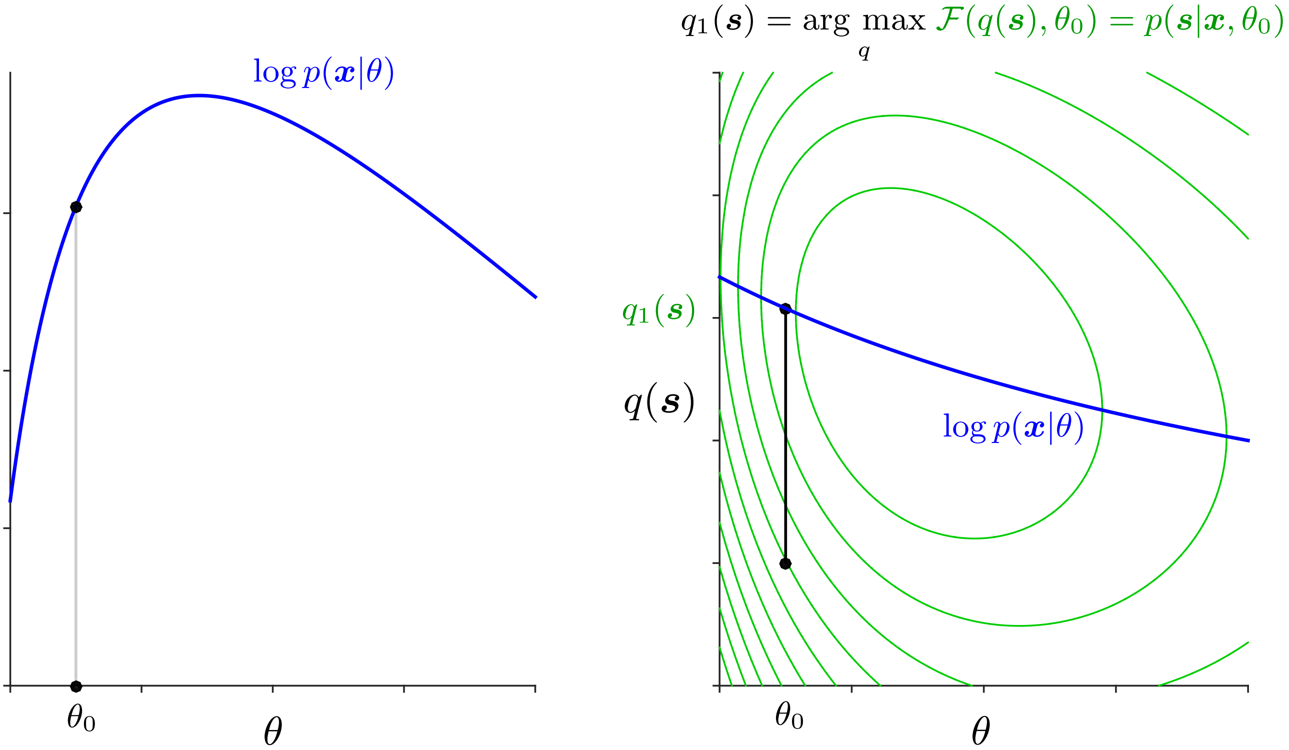

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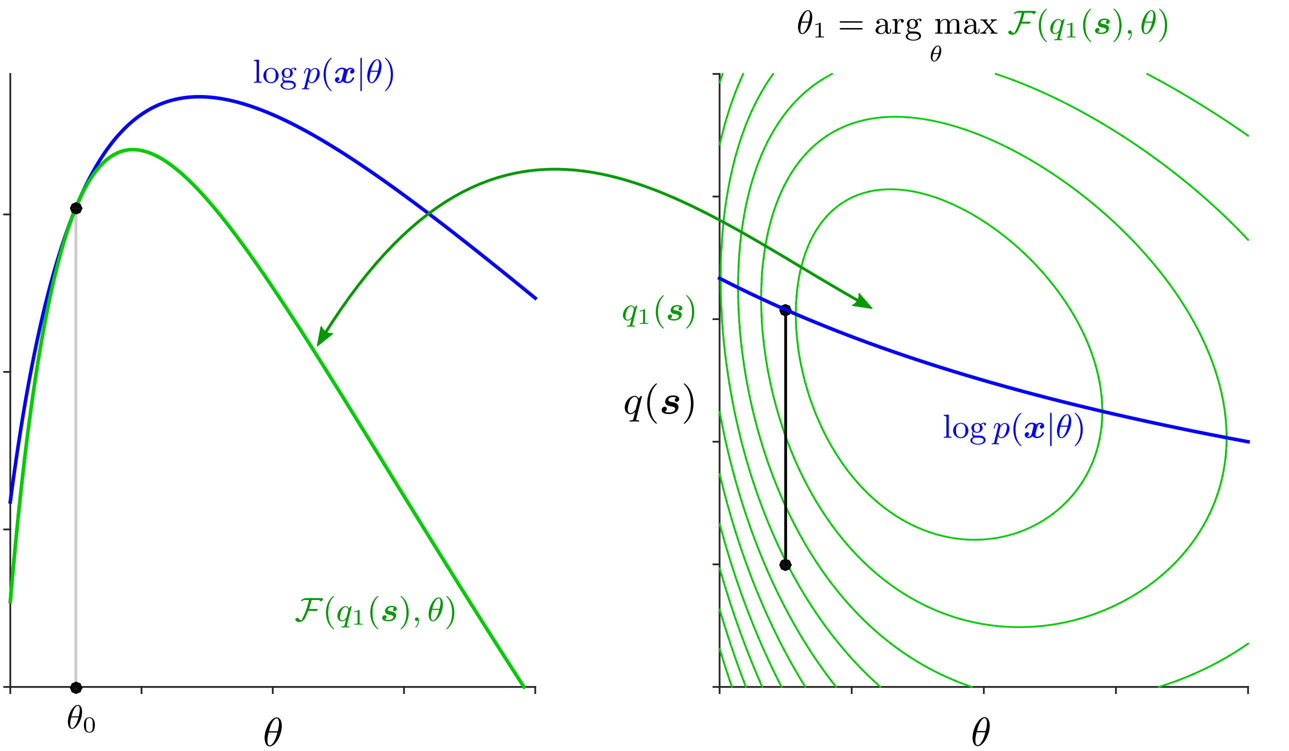

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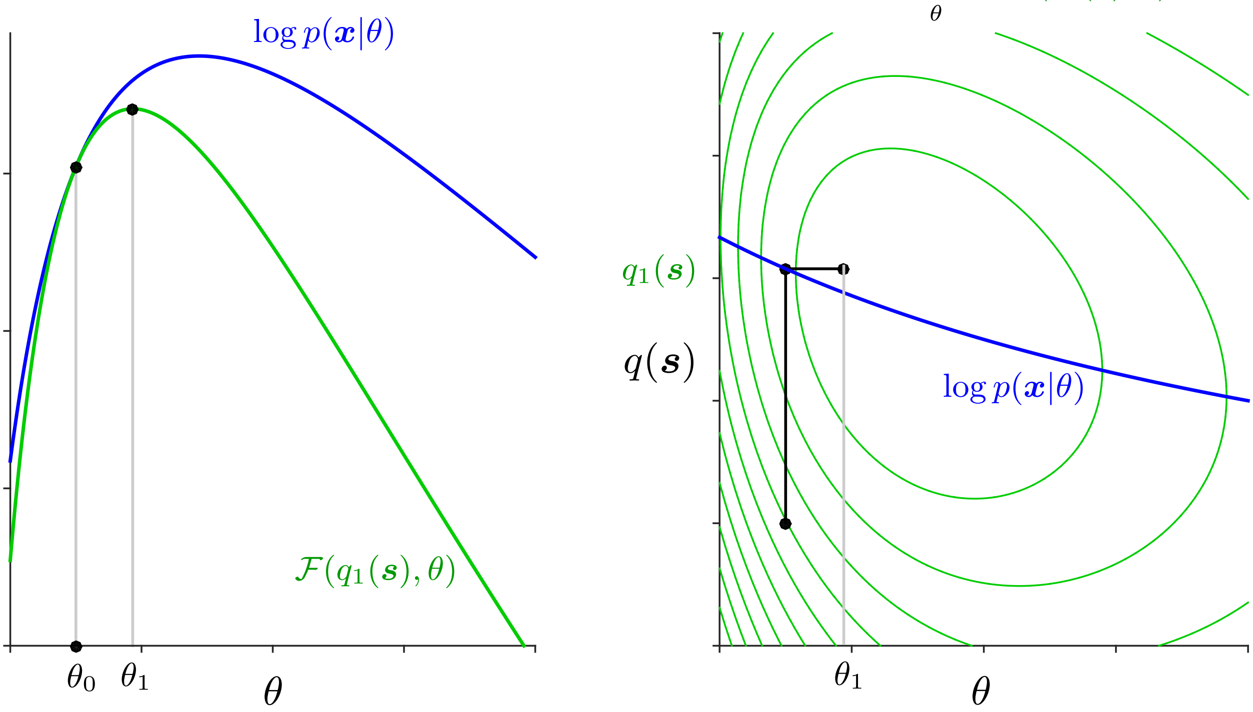

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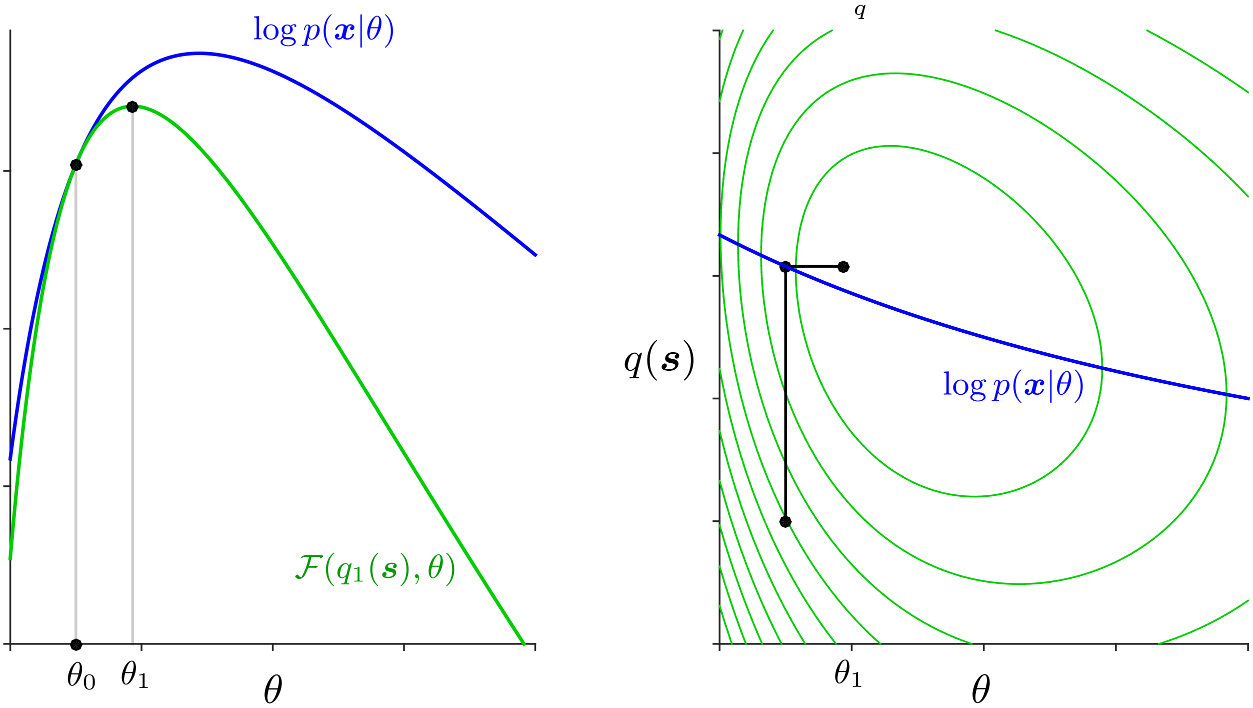
$$q_2(\boldsymbol{s}) = \arg\max_{q} \mathcal{F}(q(\boldsymbol{s}),\theta_1) = p(\boldsymbol{s}|\boldsymbol{x},\theta_1)$$



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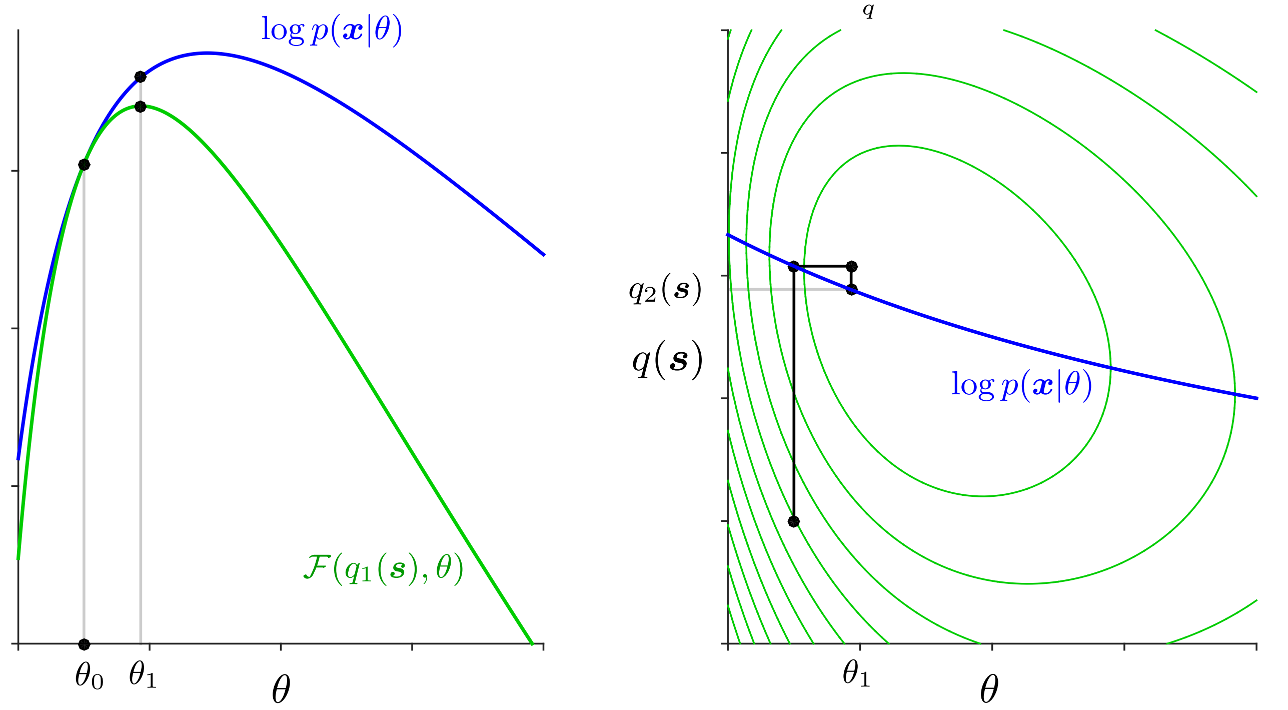

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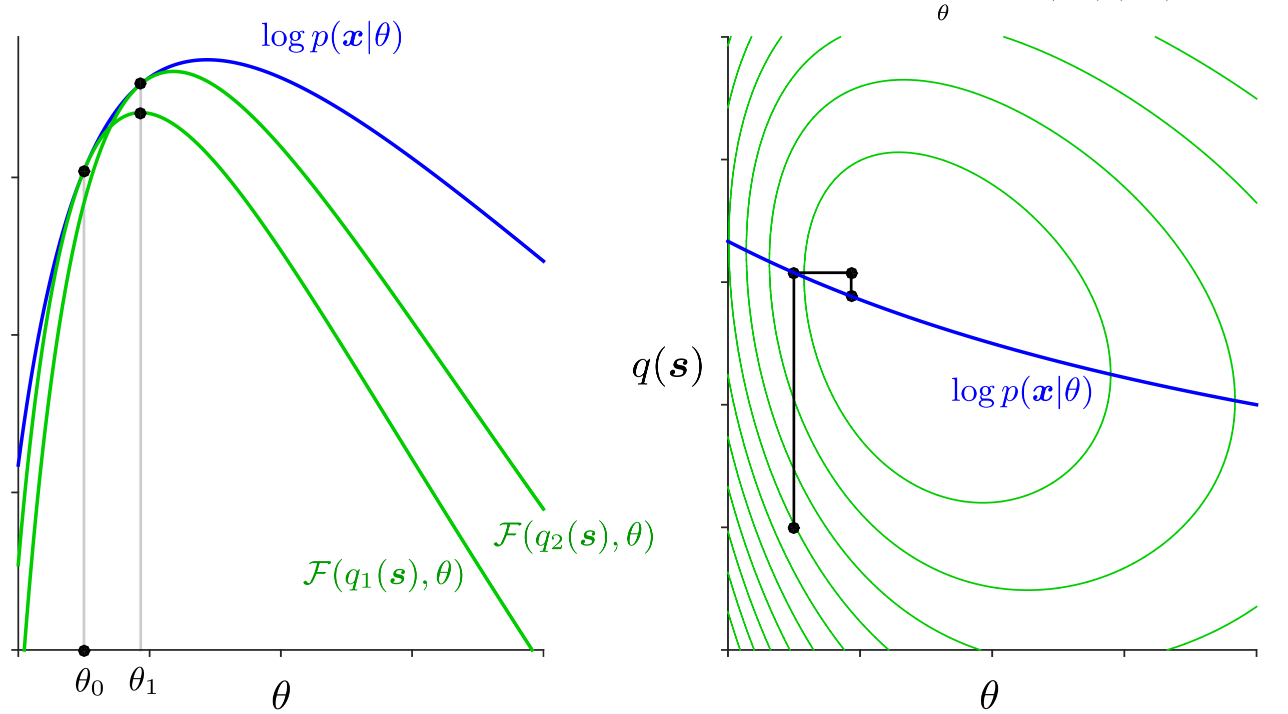

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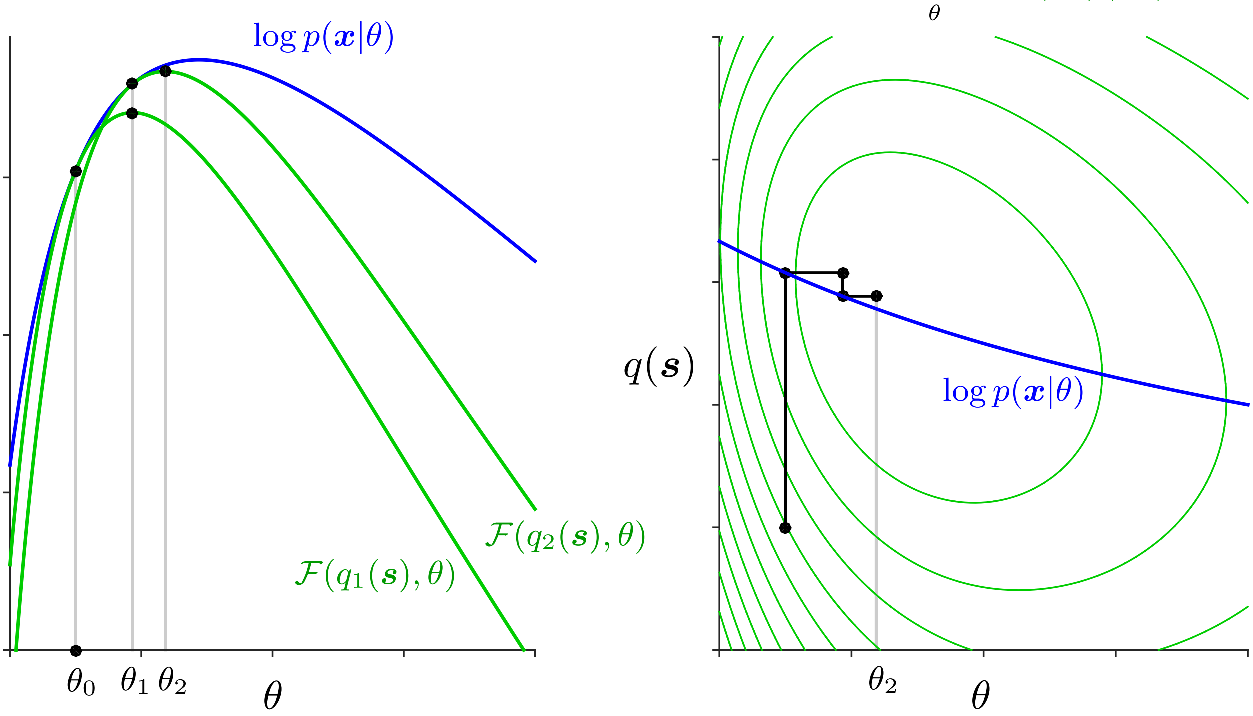

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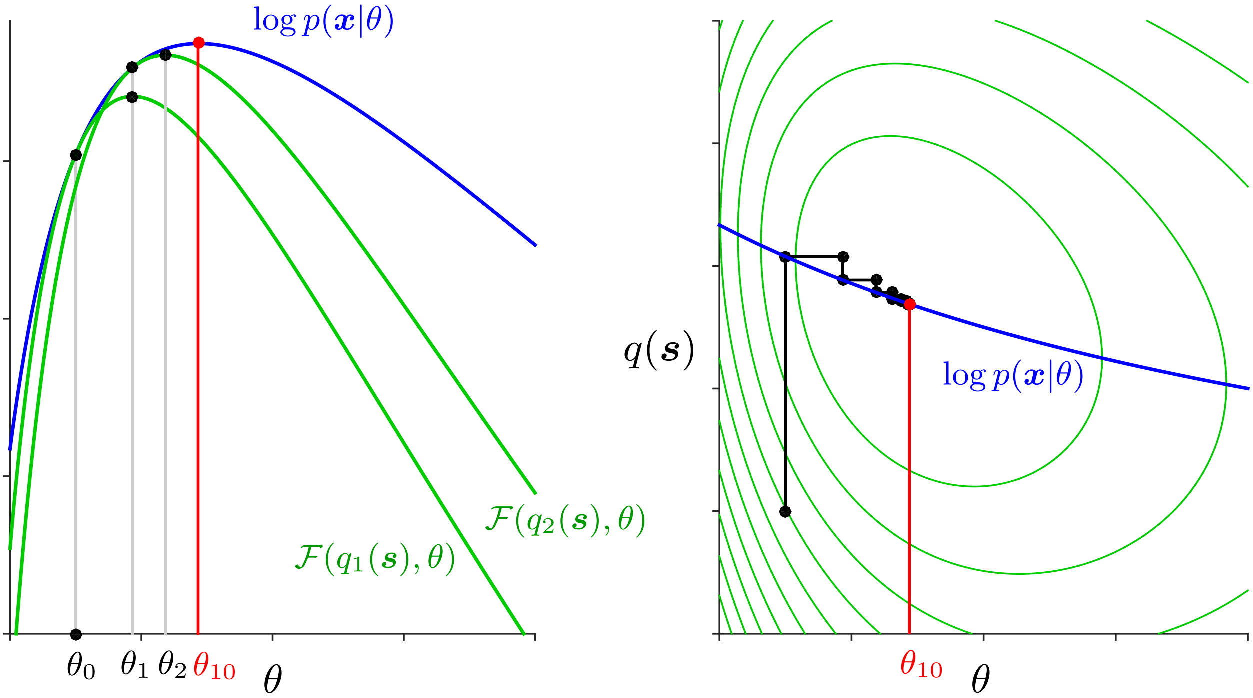


The Expectation Maximisation (EM) algorithm

From initial (random) parameters θ_0 iterate $t = 1, \ldots, T$ the two steps:

E step: for fixed θ_{t-1}, maximize lower bound $\mathcal{F}(q(\boldsymbol{s}), \theta_{t-1})$ wrt $q(\boldsymbol{s})$. As log likelihood $\log p(\boldsymbol{x}|\theta)$ is independent of $q(\boldsymbol{s})$ this is equivalent to minimizing $\mathcal{KL}(q(\boldsymbol{s})||p(\boldsymbol{s}|\boldsymbol{x}, \theta_{t-1}))$, so $q_t(\boldsymbol{s}) = p(\boldsymbol{s}|\boldsymbol{x}, \theta_{t-1})$.

M step: for fixed $q_t(\boldsymbol{s})$ maximize the lower bound $\mathcal{F}(q_t(\boldsymbol{s}), \theta)$ wrt θ.

$$\mathcal{F}(q(\boldsymbol{s}), \theta) \;=\; \sum_{\boldsymbol{s}} q(\boldsymbol{s}) \log \big(p(\boldsymbol{x}|\boldsymbol{s}, \theta) p(\boldsymbol{s}|\theta)\big) - \sum_{\boldsymbol{s}} q(\boldsymbol{s}) \log q(\boldsymbol{s}),$$

the second term is the entropy of $q(\boldsymbol{s})$, independent of θ, so the M step is

$$\theta_t \;=\; \operatorname*{argmax}_{\theta} \sum_{\boldsymbol{s}} q_t(\boldsymbol{s}) \log \big(p(\boldsymbol{x}|\boldsymbol{s}, \theta) p(\boldsymbol{s}|\theta)\big).$$

Although the steps work with the lower bound (Lyupanov* function), each iteration cannot decrease the log likelihood as

$$\log p(\boldsymbol{s}|\theta_{t-1}) \;\overset{\text{E step}}{=}\; \mathcal{F}(q_t(\boldsymbol{s}), \theta_{t-1}) \;\overset{\text{M step}}{\leq}\; \mathcal{F}(q_t(\boldsymbol{s}), \theta_t) \;\overset{\text{lower bound}}{\leq}\; \log p(\boldsymbol{x}|\theta_t)$$

Application of EM to Mixture of Gaussians (E Step)

- Assume $D = 1$ dimensional data for x simplicity
- Gaussian mixture model parameters: $\theta = \{\mu_k, \sigma_k^2, \pi_k\}_{k=1\ldots K}$
- One latent variable per datapoint $s_n, n = 1 \ldots N$ takes values $1 \ldots K$.

Probability of the observations given the latent variables and the parameters, and the prior on latent variables are:

$$p(x_n|s_n = k, \theta) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \mathrm{e}^{-\frac{1}{2\sigma_k^2}(x_n - \mu_k)^2} \qquad\qquad p(s_n = k|\theta) = \pi_k$$

so the E step becomes:

$$q(s_n = k) = p(s_n = k|x_n, \theta) \propto p(x_n, s_n = k|\theta) = \frac{\pi_k}{\sqrt{2\pi\sigma_k^2}} \mathrm{e}^{-\frac{1}{2\sigma_k^2}(x_n - \mu_k)^2} = u_{nk}$$

That is: $q(s_n = k) = r_{nk} = \frac{u_{nk}}{u_n}$ where $u_n = \sum_{k=1}^{K} u_{nk}$

Posterior for each latent variable, s_n follows a categorical distribution with probability given by the product of the prior and likelihood, renormalised. r_{nk} is called the *responsibility* that component k takes for data point n.

Application of EM to Mixture of Gaussians (M Step)

The lower bound is

$$\mathcal{F}(q(\boldsymbol{s}),\theta) = \sum_{n=1}^{N}\sum_{k=1}^{K} q(s_n=k)\left[\log(\pi_k) - \frac{1}{2\sigma_k^2}(x_n-\mu_k)^2 - \frac{1}{2}\log(\sigma_k^2)\right] + \text{const.}$$

The M step, optimizing $\mathcal{F}(q(\boldsymbol{s}),\theta)$ wrt the parameters, θ

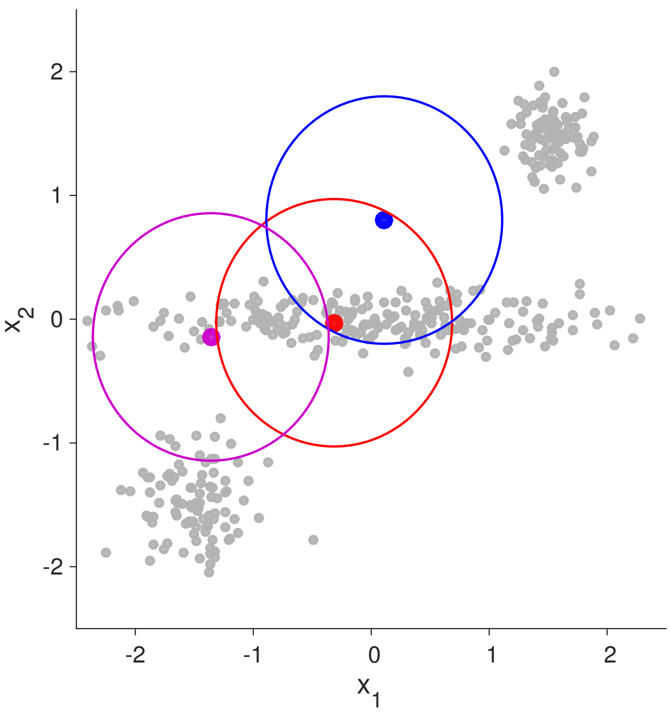
$$\frac{\partial \mathcal{F}}{\partial \mu_j} = \sum_{n=1}^{N} q(s_n=k)\frac{x_n-\mu_j}{\sigma_j^2} = 0 \Rightarrow \mu_j = \frac{\sum_{n=1}^{N} q(s_n=j)x_n}{\sum_{n=1}^{N} q(s_n=j)},$$

$$\frac{\partial \mathcal{F}}{\partial \sigma_j^2} = \sum_{n=1}^{N} q(s_n=j)\left[\frac{(x_n-\mu_j)^2}{2\sigma_j^4} - \frac{1}{2\sigma_j^2}\right] = 0 \Rightarrow \sigma_j^2 = \frac{\sum_{n=1}^{N} q(s_n=j)(x_n-\mu_j)^2}{\sum_{n=1}^{N} q(s_n=j)}$$

$$\frac{\partial[\mathcal{F} + \lambda(1-\sum_k \pi_k)]}{\partial \pi_j} = \sum_{n=1}^{N}\frac{q(s_n=j)}{\pi_j} - \lambda = 0 \Rightarrow \pi_j = \frac{1}{N}\sum_{n=1}^{N} q(s_n=j)$$

E step fills in the values of the hidden variables: M step just like performing **supervised learning** with known (soft) cluster assignments.

EM for MoGs: soft, non-axis aligned K-means



initialise: $\theta = \{\pi_k, \boldsymbol{m}_k, \Sigma_k\}_{k=1}^{K}$

repeat

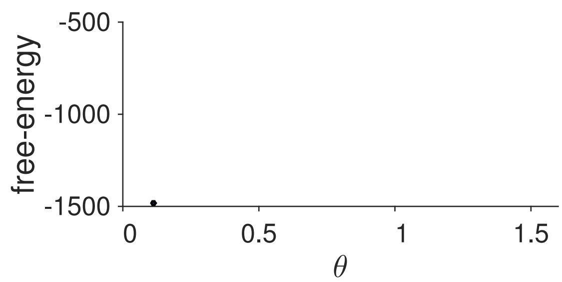
E-Step:

$r_{nk} = p(s_n = k|\boldsymbol{x}_n, \theta)$ for $n = 1 \ldots N$

M-Step:

$\arg\max_{\theta} \sum_{n,k} r_{nk}\log p(s_n = k, \boldsymbol{x}|\theta)$

until convergence



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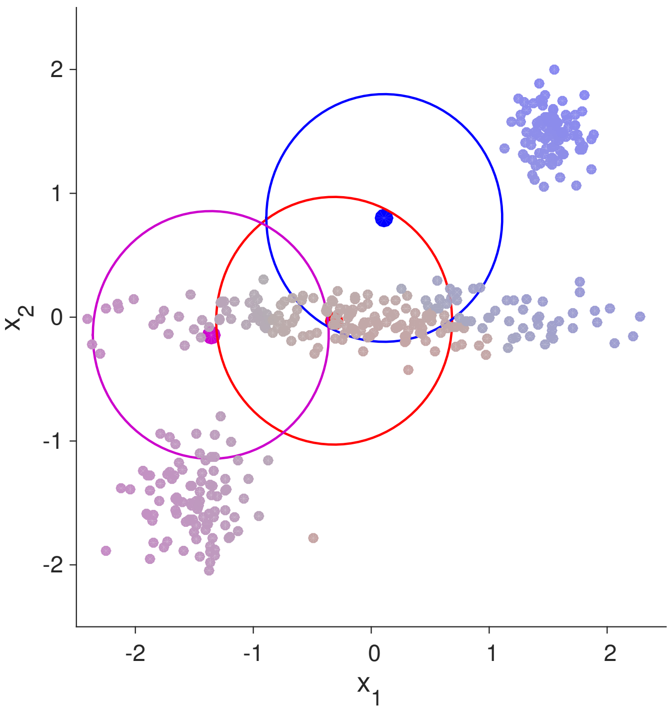


initialise: $\theta = \{\pi_k, \boldsymbol{m}_k, \Sigma_k\}_{k=1}^{K}$

repeat

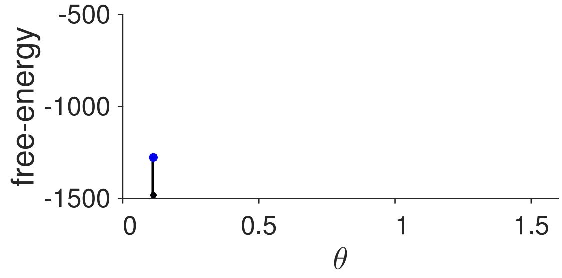
E-Step:

$r_{nk} = p(s_n = k|\boldsymbol{x}_n, \theta)$ for $n = 1 \ldots N$

M-Step:

$\arg\max_{\theta} \sum_{n,k} r_{nk} \log p(s_n = k, \boldsymbol{x}|\theta)$

until convergence



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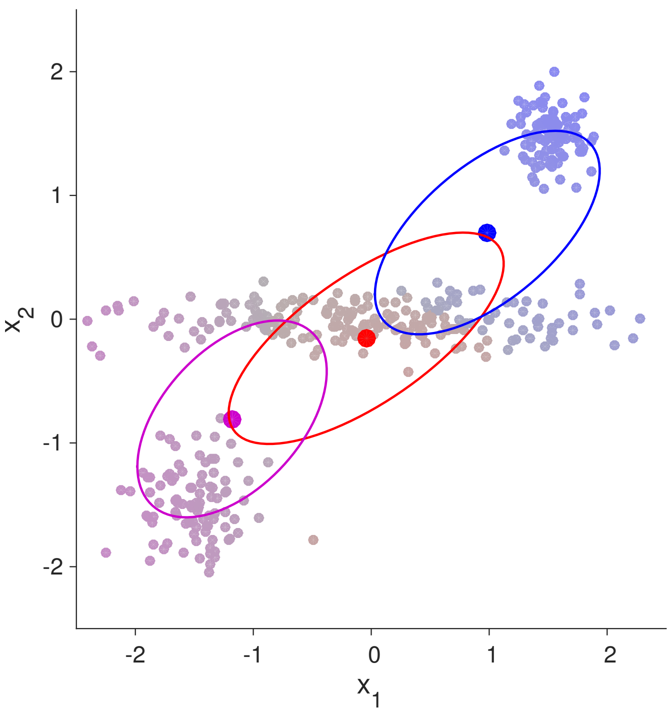

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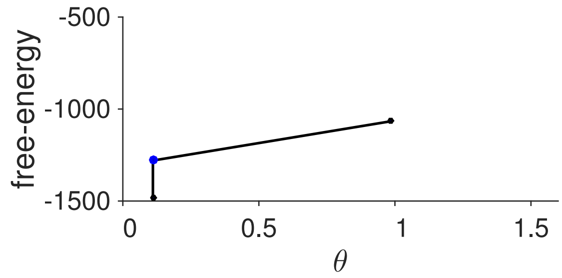

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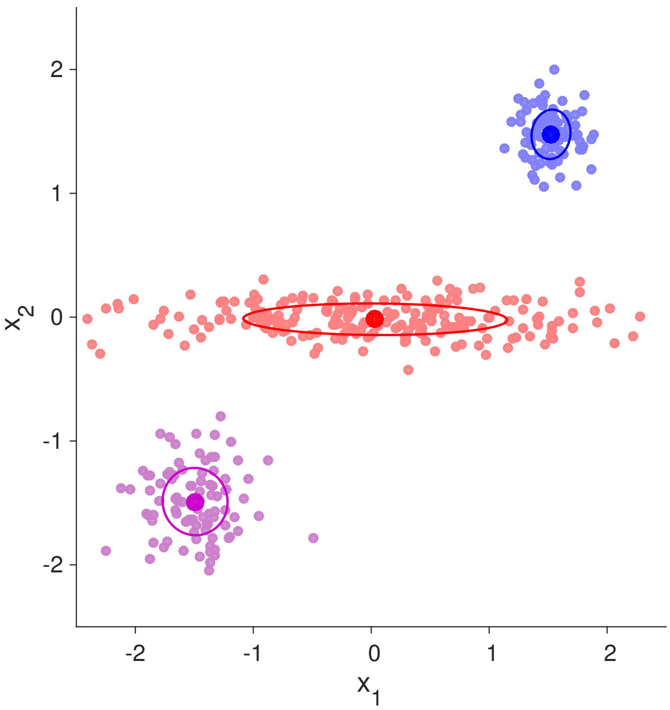

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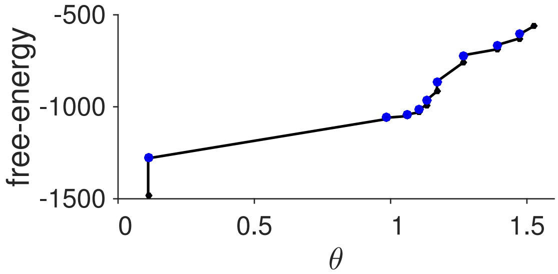
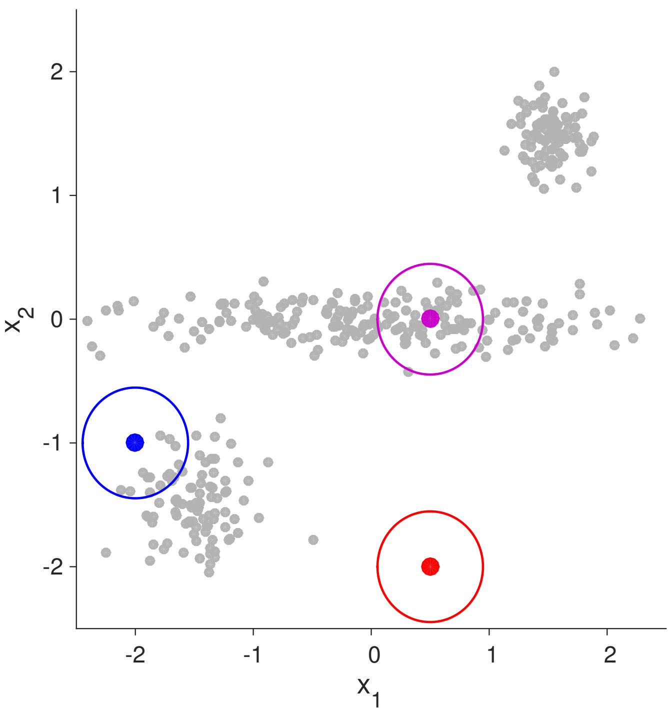


What will happen with this initialisation?



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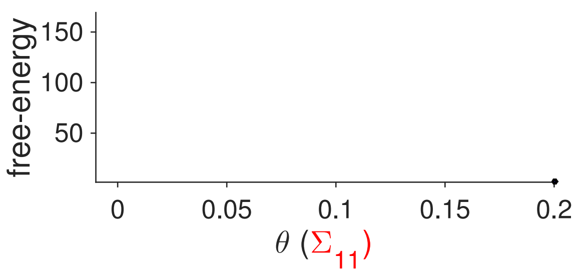

Summary

- MoG + EM algorithm = soft k-means clustering with non-axis aligned, non-equally weighted clusters
- EM can be used to fit **latent variable models** e.g. PCA, Factor analysis, MoGs, HMMs, ...
  - requires tractable posterior $p(\boldsymbol{s}|\boldsymbol{x},\theta)$ entropy and average log-joint $\mathbb{E}_{q(\boldsymbol{s}|\theta)}\left[\log p(\boldsymbol{s},\boldsymbol{x}|\theta)\right]$

Limitations

- MoG clusters still have simple shapes (ellipses)
  - a single real cluster might be described by many components
  - more complex cluster models have been developed
- maximum-likelihood can overfit
  - Bayesian approaches avoid overfitting $p(\theta, \boldsymbol{s}|\boldsymbol{x})$
- co-ordinate ascent is often slow to converge (lots of iterations required)
  - joint optimisation of $\mathcal{F}(q(\boldsymbol{s}), \theta)$ faster
  - direct optimisation of log-likelihood $\log p(\boldsymbol{x}|\theta)$

Appendix: proof of KL divergence properties

Minimise Kullback Leibler divergence (relative entropy) $\mathcal{KL}(q(x)||p(x))$: add Lagrange multiplier (enforce $q(x)$ normalises), take variational derivatives:

$$\frac{\delta}{\delta q(x)}\Big[\int q(x)\log\frac{q(x)}{p(x)}dx + \lambda(1-\int q(x)\,dx)\Big] \;=\; \log\frac{q(x)}{p(x)} + 1 - \lambda.$$

Find staionary point by setting the derivative to zero:

$q(x) \;=\; \exp(\lambda{-}1)p(x)$, normalization conditon $\lambda \;=\; 1$, so $q(x) \;=\; p(x)$,

which corresponds to a minimum, since the second derivative is positive:

$$\frac{\delta^2}{\delta q(x)\delta q(x)}\mathcal{KL}(q(x)||p(x)) \;=\; \frac{1}{q(x)} \;>\; 0.$$

The minimum value attained at $q(x) = p(x)$ is $\mathcal{KL}(p(x)||p(x)) = 0$, showing that $\mathcal{KL}(q(x)||p(x))$

- is non-negative
- attains its minimum 0 when $p(x)$ and $q(x)$ are equal