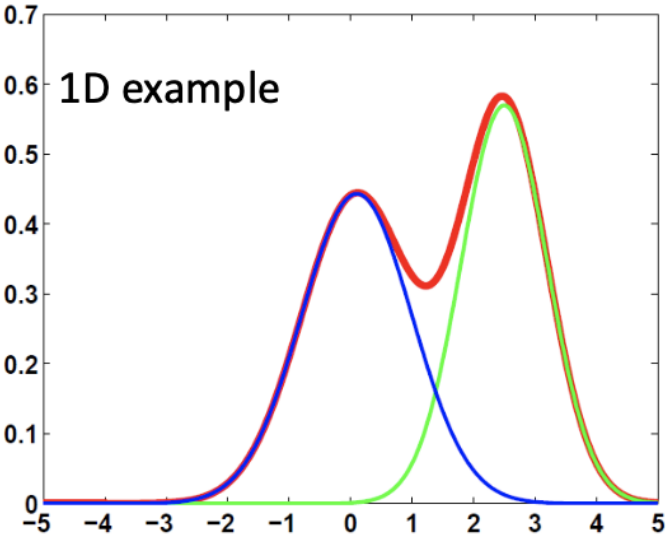
Lecture 18: Gaussian Mixture Model, Expectation Maximization

Unsupervised learning

- Aim: explore the structure (pattern, regularities) of the data
- Tasks:
  - Clustering (e.g. GMM)
  - Dimensionality Reduction (e.g. PCA)
  - Learning parameters of probabilistic models
- Applications:
  - Market basket analysis
  - Outlier detection
  - Unsupervised tasks in (supervised) ML pipelines

Gaussian Mixture Model (GMM)

- A probabilistic view of clustering
- Requires the user to choose the number of clusters in advance
- Gives a power to express **uncertainty about the origin** ("weights") of each point
  - Each point originates from cluster c with probability w_c, $c = 1, ..., k$
- Still originats from one particular cluster, but not sure from which one
- Data points are samples from **a mixture of K distributions (components)**
  - In principle, we can adopt any probability distribution for the components
  - Howeer, normal distribution is a common modelling choice -> GMM
- (d-dimensional) Gaussian distribution
  - $N(x|\mu, \Sigma) = (2\pi)^{-\frac{d}{2}} |\Sigma|^{-\frac{1}{2}} \exp(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu))$
- Gaussian Mixture Distribution: (for each data point)
  - $P(x) = \Sigma_{j=1}^k w_j N(x|\mu_j, \Sigma_j) = \Sigma_{j=1}^k P(C_j) P(x|C_j)$
  - $P(x|C_j)$ is **conditional density** for component j
  - Here $P(C_j) \geq 0$ and $\Sigma_{j=1}^k P(C_j) = 1$
  - (Unkown) params of the model are:
    - $P(C_j), \mu_j, \Sigma_j$ for $j = 1, ..., k$



Mixture and individual component densities
are re-scaled for visualisation purposes
Figure: Bishop

Clustering as model estimation

- Clustering now amounts to **finding parameters** of the GMM that "best explain" the observed data
  - -> **MLE** that maximise $p(x_1, ..., x_n)$

Fitting the GMM

- Aim: find parameters that maximise $p(x_1, ..., x_n)$
- Cannot solve analytically by taking (first) derivative!
  - Solution: Use **Expectation-Maximisation (EM)**

Expectation Maximisation (EM) algorithm

- Motivation:
  1. Sometimes we **don't observe** some of the variables needed to compute the log-likelihood
     - Hidden variables
  2. Sometimes the form of log-likelihood is inconvenient to work with
     - (No closed form solution...)
- EM is an algorithm
  - A way to **solve the problem posed by MLE**
  - Especially **convenient** under unobserved latent variables
- MLE can be found by other methods
  - E.g. Gradient Descent

Algorithm (Simple version)

1. Initialisation K clusters and their parameters
2. Iteration Step:
   - E-step:

        - Estimate the cluster of each data point
    - M-step:
        - Re-estimate the cluster parameters
            - $(\mu_j, \Sigma_j), p(C_j)$ for each cluster j

EM for GMM and generally

- EM is a general tool
    - Purpose: implement MLE under latent (missing) variables Z
- Variables and params in GMM
    - Variables:
        - Observed: Point locations X
        - Hidden: Cluster assignments Z
    - Parameters:
        - θ: cluster locations and scales (and $p(C_j)'s$)
- What EM is really doing:
    - Coordinate ascent on **lower-bound on the log-likelihood**
        - M-step: ascent in modelled parameter θ
        - E-step: ascent in marginal likelihood $P(Z)$
        - Each step moves towards a local optimum
        - Can get stuck (at local optima)
            - Need random restarts

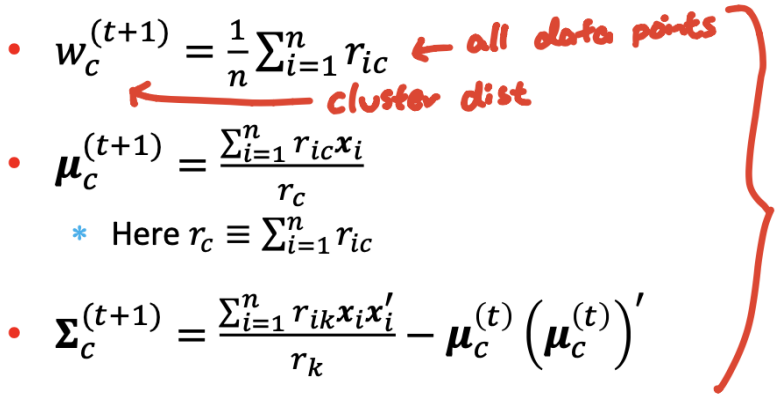
Not-Examinable Part

- Log is a convex function (can use Jensen's inequality)
- Maximise $\log p(X|\theta)$ difficult
    - Maximise $\log p(X, Z|\theta)$ (log complete likelihood) instead
- Marginalise and use Jensen's Inequality to get lower-bound $E_Z[\log \frac{p(x,z|\theta)}{p(z)}]$
    - Note: $p(z) = p(z|x, \theta)$
- Maximising lowerbound:
    - **Equivalent** to maximising original incomplete likelihood
    - Since $p(z) = p(z|x, \theta)$ makes the lower bound tight
- Resulting EM algorithm:
    1. Initialisation: choose random initial values of $\theta^{(1)}$
    2. Update:
        - E-step: compute $Q(\theta, \theta^{(t)}) = E_{Z|X,\theta^{(t)}}[\log p(X, Z|\theta)]$
    3. Termination: If no change then stop
    4. Go to step 2
- The algorithm could results in local maximum

Estimating Parameters of GMM

- Can't compute the complete likelihood because we don't know z
- EM handles this by replacing $\log p(X, z|\theta)$ with $E_{Z|X,\theta^{(t)}}[\log p(X,z|\theta)]$
    - Requires: $p(z|X, \theta^{(t)})$
    - Assuming z_i are pairwise independent, we need $P(z_i = c|x_i, \theta^{(t)})$
- E-step: calculating **cluster responsibility** (weights)

    - Use Bayes rule: $r_{ic} = P(z_i = c|x_i, \theta^{(t)}) = \frac{w_c N(x_i|\mu_c, \Sigma_c)}{\Sigma_{l=1}^{k} w_l N(x_i|\mu_l, \Sigma_l)}$
    - That (posterior) probability: responsibility that cluster c takes for data point i
- M-step:
    - Take partial derivatives of $Q(\theta, \theta^{(t)})$ with respect to each of the parameters and set the derivatives to 0
    - Obtain new parameter estimates:



    - (Estimates for step (t+1))

K-means as a EM for a restricted GMM

- Consider GMM in which:
    - All components have the same fixed probability: $w_c = 1/k$
    - Each Gaussian has the fixed covariance matrix $\Sigma_c = \sigma^2 I$
    - **Only component centroids μ_c need to be estimated**
- Approximate cluster responsibility:
    - Deterministic assignment:
        - $r_i c = 1$ if centroid $\mu_c^{(t))}$ is closest to point x_i
        - $r_i c = 0$ otherwise
- Results in E-step: μ_c should be set as a centroid of points assigned to cluster c
- => k-means algorithm