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- We have studied maximum likelihood estimation and Bayesian estimation of density functions.
- Given estimated densities, we can implement Bayes classifier.
- We have also discussed the exponential family of densities and role of sufficient statistics in estimation.

Mixture densities

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Mixture densities

- The last topic we consider under parametric estimation is that of mixture densities.
- In many cases we may not be able to capture the class conditional density using any standard density model.
- In such cases, often, modelling the class conditional density as a mixture of densities is helpful.
- We look at this and a special technique, called the EM algorithm, for ML estimation of mixture densities in this class.

Mixture density model

- Consider a density model

$$f(x) = \sum_{k=1}^{K} \lambda_k f_k(x), \quad \lambda_k \geq 0, \text{ and } \sum_{k=1}^{K} \lambda_k = 1$$

where each f_k is a density function.

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  where each f_k is a density function.
- Since each f_k is a density, given the conditions on λ_k, f is a convex combination of densities and hence is itself a density.
- Mixture densities are useful when data distribution is multimodal.

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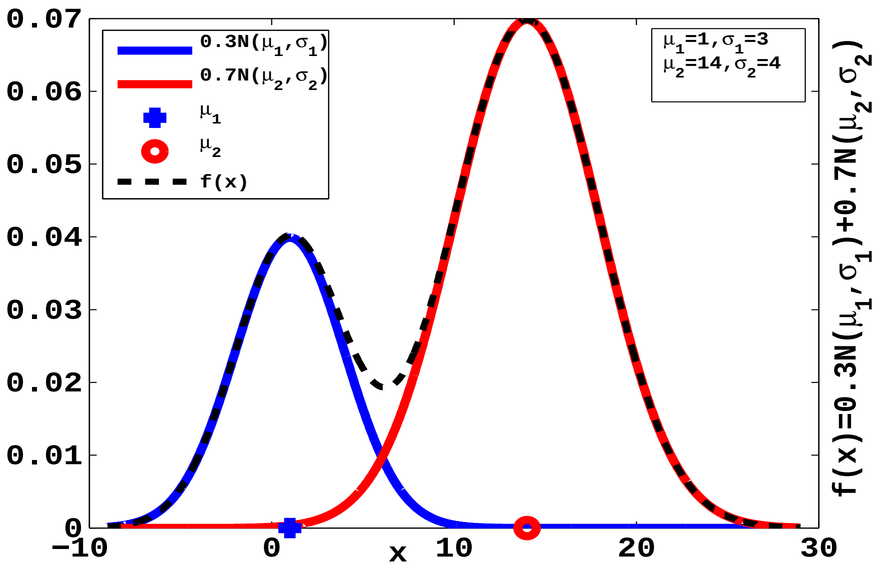
- For example, consider the normal density.



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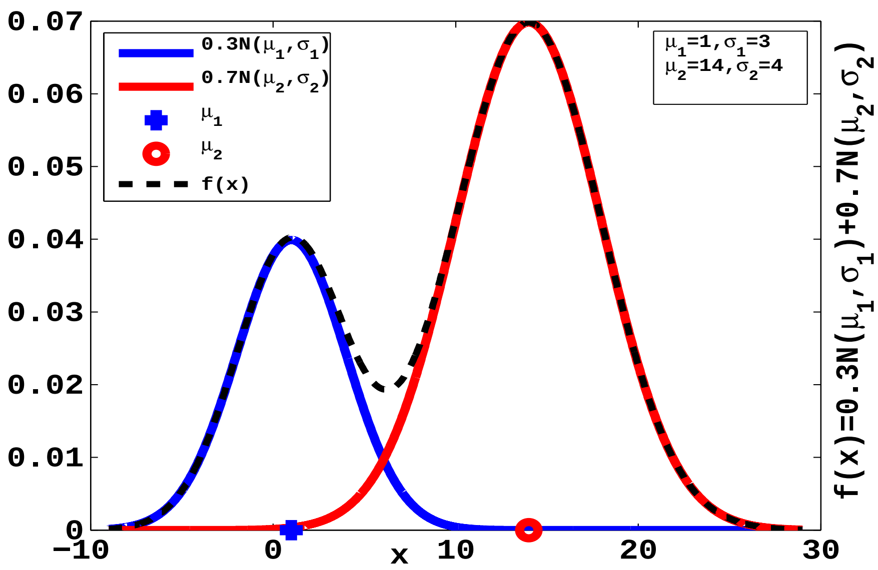

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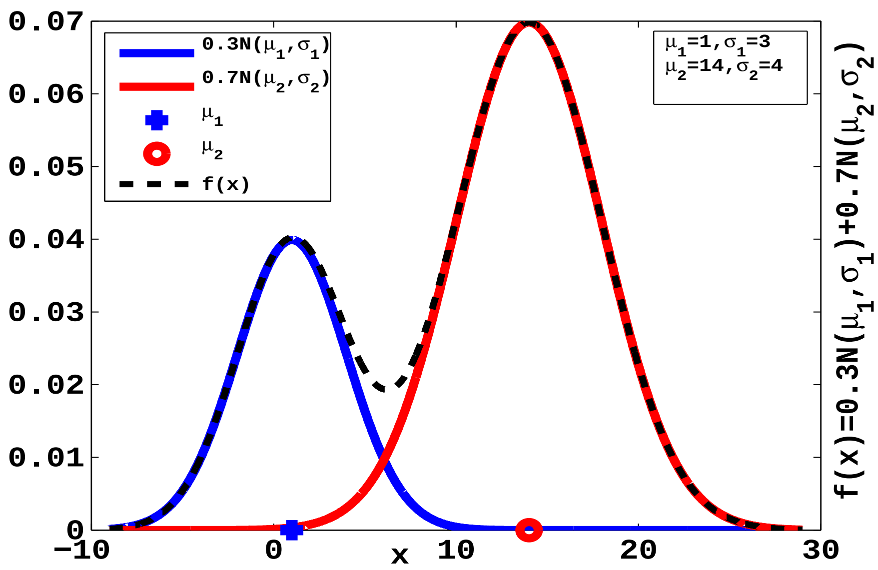

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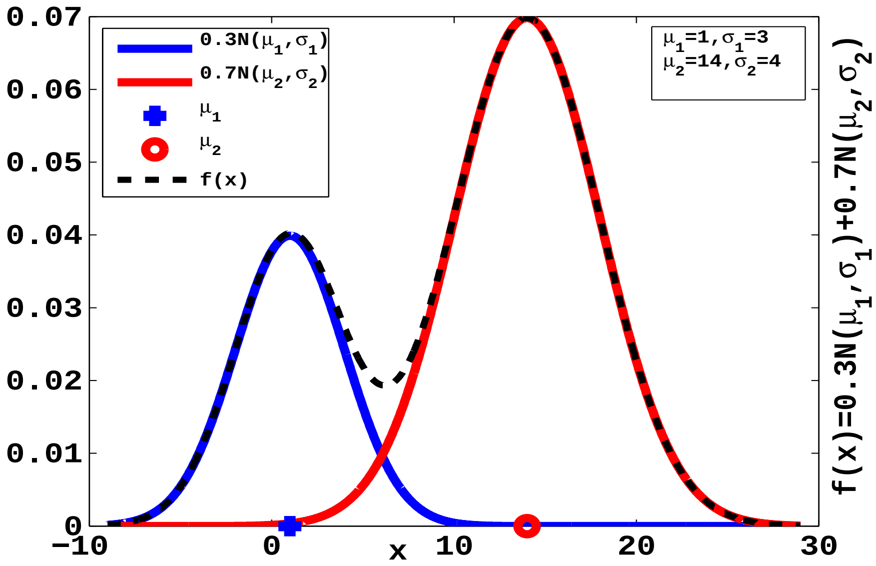

- This is a multimodal density
- When data density is multi-modal, we can often approximate it with mixture of gaussians.

ML estimation of mixture models

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$$f(x \mid \theta) = \sum_{k=1}^{K} \lambda_k \, f_k(x)$$

where each f_k is $\mathcal{N}(\mu_k, \, \Sigma_k)$.

ML estimation of mixture models

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  where each f_k is $\mathcal{N}(\mu_k,\ \Sigma_k)$.

- The parameter vector, θ, consists of all λ_k, which are called mixing coefficients, and all the parameters of the constituent densities, namely, $\mu_k,\ \Sigma_k$, $k = 1, \cdots, K$.

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- Then the likelihood function is

$$L(\theta \mid \mathcal{D}) = \prod_{i=1}^{n} \left[\sum_{k=1}^{K} \lambda_k \, f_k(x_i) \right]$$

- The log likelihood is given by

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- Since there is a sum inside the log function, the densities f_k being from exponential family, does not simplify log likelihood.
- Maximizing log likelihood could become a difficult optimization problem.

Mixture of two one dimensional densities

- Consider one dimensional case with $K = 2$. Let, for $j = 1, 2$,

$$\phi(x \,|\, \theta_j) = \frac{1}{\sigma_j \sqrt{2\pi}} \exp\left(- \frac{(x - \mu_j)^2}{2\sigma_j^2} \right), \quad \theta_j = (\mu_j, \sigma_j)$$

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- The density model is

$$f(x \mid \theta) = \lambda_1 \, \phi(x \mid \theta_1) + \lambda_2 \, \phi(x \mid \theta_2)$$

where $\theta = (\theta_1, \ \theta_2, \ \lambda_1, \ \lambda_2)$

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- First note that

$$\frac{\partial\, \phi(x \mid \theta_j)}{\partial \mu_s} = \frac{\partial\, \phi(x \mid \theta_j)}{\partial \sigma_s} = 0, \quad \text{if} \;\; j \neq s.$$

By differentiation we get, for $j = 1, 2$,

$$\frac{\partial\, \phi(x \mid \theta_j)}{\partial \mu_j} = \phi(x \mid \theta_j)\, \frac{(x - \mu_j)}{\sigma_j^2}$$

$$\frac{\partial\, \phi(x \mid \theta_j)}{\partial \sigma_j} = \phi(x \mid \theta_j) \left[\frac{(x - \mu_j)^2}{\sigma_j^3} - \frac{1}{\sigma_j} \right]$$

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\end{aligned}
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Now we have

$$
\frac{\partial\, l(\mathcal{D} \mid \theta)}{\partial \mu_j} = \sum_{i=1}^{n} \frac{\lambda_j\, \phi(x_i \mid \theta_j)\, \frac{(x_i - \mu_j)}{\sigma_j^2}}{\lambda_1\, \phi(x_i \mid \theta_1) \; + \; \lambda_2 \phi(x_i \mid \theta_2)}
$$

- Define γ_{ij}, $i = 1, \cdots, n$, $j = 1, 2$,

$$\gamma_{ij} = \frac{\lambda_j \, \phi(x_i \mid \theta_j)}{\lambda_1 \, \phi(x_i \mid \theta_1) \; + \; \lambda_2 \phi(x_i \mid \theta_2)}$$

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- Then we get

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- Hence the ML estimates satisfy, for $j = 1, 2$,

$$\hat{\mu}_j = \frac{\sum_{i=1}^{n} \gamma_{ij} \, x_i}{\sum_{i=1}^{n} \gamma_{ij}}$$

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- However, there is an interesting structure here.

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- It is a sample mean with ‘weight’ γ_{ij} for x_i.
  γ_{ij} are sometimes called responsibility coefficients.
- If there is only one component in the mixture, these become the usual ML estimates.

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- So, we need to equate to zero, the partial derivatives of
$$l(\mathcal{D} \mid \theta) + \eta(\lambda_1 + \lambda_2 - 1)$$
where η is the Lagrange multiplier.
- By equating to zero the partial derivative of the above with respect to λ_1, we get

$$\sum_{i=1}^{n} \frac{\phi(x_i \mid \theta_1)}{\lambda_1 \, \phi(x_i \mid \theta_1) + \lambda_2 \phi(x_i \mid \theta_2)} + \eta = 0$$

or

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- we get a similar equation for derivetive w.r.t. λ_2.
- Now, using $\lambda_1 + \lambda_2 = 1$, we get

$$\eta = \eta(\lambda_1 + \lambda_2) = -\sum_{i=1}^{n} (\gamma_{i1} + \gamma_{i2}) = -n$$

- Hence, the ML estimates for λ_j satisfy

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- Putting all these together we get

- The ML estimates for $\mu_j, \sigma_j, \lambda_j$, $j = 1, 2$, satisfy

$$\hat{\mu}_j = \frac{\sum_{i=1}^{n} \gamma_{ij}\, x_i}{\sum_{i=1}^{n} \gamma_{ij}}, \quad \hat{\lambda}_j = \frac{1}{n} \sum_{i=1}^{n} \gamma_{ij}$$

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- The structure of equations is interesting.
- These are not expressions for estimates.
- However, we can solve for estimates using, e.g., Gauss-Siedel iteration.

$$
\begin{aligned}
\mu_j^{(k+1)} &= \frac{\sum_{i=1}^n \gamma_{ij}^{(k)} \; x_i}{\sum_{i=1}^n \gamma_{ij}^{(k)}}, \quad \lambda_j^{(k+1)} = \frac{1}{n} \sum_{i=1}^{n} \gamma_{ij}^{(k)} \\
(\sigma_j^2)^{(k+1)} &= \frac{\sum_{i=1}^n \gamma_{ij}^{(k)} \, (x_i - \mu_j^{(k)})^2}{\sum_{i=1}^n \gamma_{ij}^{(k)}} \\
\gamma_{ij}^{(k+1)} &= \frac{\lambda_j^{(k+1)} \, \phi(x_i \mid \theta_j^{(k+1)})}{\sum_{j=1}^2 \lambda_j^{(k+1)} \, \phi(x_i \mid \theta_j^{(k+1)})}
\end{aligned}
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- It is easy to generalize this to mixture of K Gaussians.

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- In many cases the ML estimation of mixture of densities gives rise to such an iterative optimization procedure.
- We now look at this general procedure.

- Our density model was

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- In our sample each x_i is drawn *iid* according to this distribution.

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- If we knew which x_i are generated from which component density, then the estimation of all parameters is very easy.
- Let us first formalize this notion.

Missing Information

- Let random variables Z_{ij}, $i = 1, \cdots, n$, $j = 1, 2$, denote the information of which component density each sample comes from.

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We can think of Z_{ij} as the 'missing information'.

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- Then estimation is easy. For example,

$$\hat{\mu}_1 = \frac{\sum_{i=1}^{n} Z_{i1}\, x_i}{\sum_{i=1}^{n} Z_{i1}}, \quad \hat{\mu}_2 = \frac{\sum_{i=1}^{n} Z_{i2}\, x_i}{\sum_{i=1}^{n} Z_{i2}}$$

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- These are very similar to earlier equations.

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- This is because of some ‘hidden’ or ‘missing’ data.
- If we are given the complete data then ML estimation is easy.
- In our example, x_i is the incomplete data.
- (x_i, Z_i) constitutes the complete data and Z_i constitute the missing or hidden data/variables.

The EM Algorithm

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- Hence the name of the algorithm.
- As per our notation, x_i, $i = 1, \cdots, n$ is the incomplete data and (x_i, Z_i), $i = 1, \cdots, n$ is the complete data.

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- The Z_{ij}, $i = 1, \cdots, n$, $j = 1, 2$, that we defined earlier are the hidden variables or the missing data.
- Recall that Z_{ij} is the indicator whether or not x_i came from the j^{th} component of the mixture.

- By definition of Z_{ij}, we have

$$P[Z_{ij} = 1] = \lambda_j, \ \forall i; \quad \text{and} \quad f(x_i \mid Z_{ij} = 1) = \phi(x_i \mid \theta_j)$$

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- Recall $Z_i = (Z_{i1}, \ Z_{i2})$. Hence

$$f(Z_i|\theta) = \prod_{j=1}^{2} (\lambda_j)^{Z_{ij}}, \quad \text{and} \quad f(x_i|Z_i, \theta) = \prod_{j=1}^{2} (\phi(x_i|\theta_j))^{Z_{ij}}$$

- Hence density of complete data is

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$$f(\mathbf{x},\ \mathbf{Z} \mid \theta) = \prod_{i=1}^{n} \left[\prod_{j=1}^{2} (\lambda_j\ \phi(x_i \mid \theta_j))^{Z_{ij}} \right]$$

- The complete data log likelihood is

$$\ln(f(\mathbf{x}, \mathbf{Z} \mid \theta)) = \sum_{i=1}^{n} \left[\sum_{j=1}^{2} Z_{ij} \ln(\lambda_j \, \phi(x_i \mid \theta_j)) \right]$$

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- It is easy to see how knowledge of the ‘hidden’ variables makes the ML estimation easy.

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&= \frac{f(x_i \mid Z_{ij} = 1,\ \theta')\ P[Z_{ij} = 1]}{\sum_{j=1}^{2} f(x_i \mid Z_{ij} = 1,\ \theta')\ P[Z_{ij} = 1]}
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$$\begin{aligned} E[Z_{ij} \mid \mathbf{x}, \theta'] &= P[Z_{ij} = 1 \mid \mathbf{x},\ \theta'] = P[Z_{ij} = 1 \mid x_i,\ \theta'] \\ &= \frac{f(x_i \mid Z_{ij} = 1,\ \theta')\ P[Z_{ij} = 1]}{\sum_{j=1}^{2}\ f(x_i \mid Z_{ij} = 1,\ \theta')\ P[Z_{ij} = 1]} \\ &= \frac{\lambda_j\ \phi(x_i \mid \theta'_j)}{\sum_{j=1}^{2}\ \lambda_j\ \phi(x_i \mid \theta'_j)} \end{aligned}$$

- Thus, $E[Z_{ij} \mid \mathbf{x}, \theta'] = \gamma_{ij}(\theta')$ where

$$\gamma_{ij}(\theta') = \frac{\lambda_j \, \phi(x_i \mid \theta'_j)}{\sum_{j=1}^{2} \lambda_j \, \phi(x_i \mid \theta'_j)}$$

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- This is the same γ_{ij} that we defined earlier.
- This notation emphasizes the fact that the value of γ_{ij} depends on the parameter vector.
- Now we need to do this expectation on the complete data log likelihood which is

$$\ln(f(\mathbf{x}, \mathbf{Z} \mid \theta)) = \sum_{i=1}^{n} \left[\sum_{j=1}^{2} Z_{ij} \ln(\lambda_j \, \phi(x_i \mid \theta_j)) \right]$$

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- Thus, under the E-step, we get

$$Q(\theta,\ \theta^{(k)}) \ = \ \sum_{i=1}^{n} \left[\sum_{j=1}^{2} E[Z_{ij} \mid \mathbf{x},\ \theta^{(k)}] \ln(\lambda_j \, \phi(x_i \mid \theta_j)) \right]$$

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$$\begin{aligned} Q(\theta,\ \theta^{(k)}) &= \sum_{i=1}^{n} \left[\sum_{j=1}^{2} E[Z_{ij} \mid \mathbf{x},\ \theta^{(k)}] \ln(\lambda_j \, \phi(x_i \mid \theta_j)) \right] \\ &= \sum_{i=1}^{n} \left[\sum_{j=1}^{2} \gamma_{ij}(\theta^{(k)}) \ \ln(\lambda_j \, \phi(x_i \mid \theta_j)) \right] \end{aligned}$$

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- This is now a simple optimization problem.

- For example, $\frac{\partial Q}{\partial \mu_1} = 0$ gives us

$$\sum_{i=1}^{n} \gamma_{i1}(\theta^k) \, \frac{(x_i - \mu_1)}{\sigma_1^2} = 0$$

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$$\mu_1^{k+1} = \frac{\sum_{i=1}^{n} \gamma_{i1}(\theta^{(k)}) \, x_i}{\sum_{i=1}^{n} \gamma_{i1}(\theta^k)}$$

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- This is same as the iterative algorithm we derived earlier.

- Similarly, $\frac{\partial Q}{\partial \sigma_1} = 0$ gives

$$\sum_{i=1}^{n} \gamma_{i1}(\theta^{(k)}) \left[- \frac{1}{\sigma_1} + \frac{(x_i - \mu_1)^2}{\sigma_1^3}\right] = 0$$

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- Once again same as earlier algorithm.

$$\mu_j^{(k+1)} = \frac{\sum_{i=1}^n \gamma_{ij}^{(k)} x_i}{\sum_{i=1}^n \gamma_{ij}^{(k)}}, \quad \lambda_j^{(k+1)} = \frac{1}{n} \sum_{i=1}^n \gamma_{ij}^{(k)}$$

$$(\sigma_j^2)^{(k+1)} = \frac{\sum_{i=1}^n \gamma_{ij}^{(k)} (x_i - \mu_j^{(k)})^2}{\sum_{i=1}^n \gamma_{ij}^{(k)}}$$

$$\gamma_{ij}^{(k+1)} = \frac{\lambda_j^{(k+1)} \phi(x_i \mid \theta_j^{(k+1)})}{\sum_{j=1}^2 \lambda_j^{(k+1)} \phi(x_i \mid \theta_j^{(k+1)})} = \gamma_{ij}(\theta^{(k+1)})$$

- So, this is actually the EM algorithm.