Expectation Maximization

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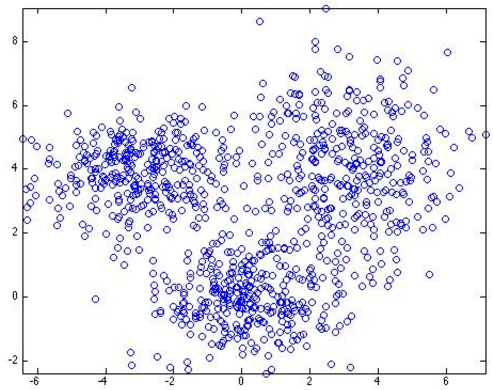
1 Motivation - Mixture Density models

When you have data that looks like:



Can you fit them using a single-mode Gaussian distribution, i.e.,:

$$
\begin{aligned}
p(X) &= \mathcal{N}(X|\mu, \Sigma) \\
&= (2\pi)^{-k/2}|\Sigma|^{-\frac{1}{2}} \exp^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}
\end{aligned} \tag{1}
$$

Clearly Not! This is typically modelling using Mixture Densities, in the case of Gaussian Mixture Model (k-mixture) (GMM):

$$
p(X) = \sum_{l=1}^{k} \alpha_l \mathcal{N}(X|\mu_l, \Sigma_l) \qquad \text{s.t.} \quad \sum_{l=1}^{k} \alpha_l = 1 \tag{2}
$$

1.1 Gaussian Mixture model result

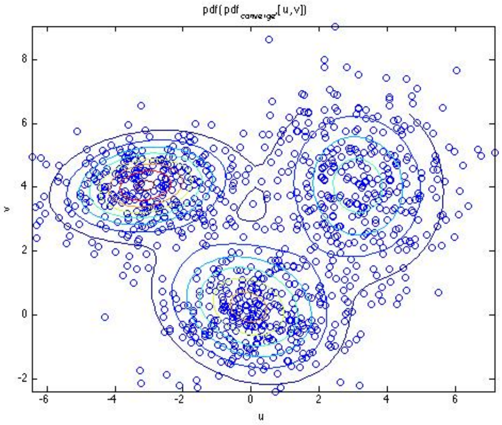


Figure 1: gmm fitting result

Let $\Theta = \{\alpha_1, \dots \alpha_k, \mu_1, \dots \mu_k, \Sigma_1, \dots \Sigma_k\}$

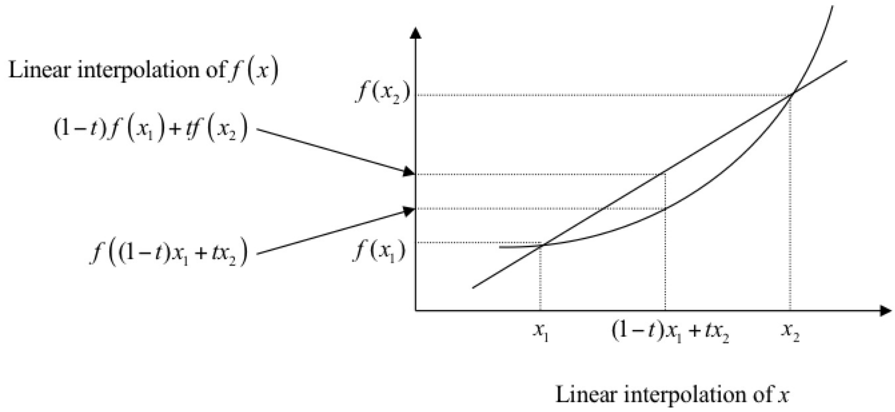
$$
\begin{aligned}
\Theta_{\text{MLE}} &= \arg\max_{\Theta} \mathcal{L}(\Theta|X) \\
&= \arg\max_{\Theta} \left(\sum_{i=1}^{n} \log \sum_{l=1}^{k} \alpha_l \mathcal{N}(X|\mu_l, \Sigma_l) \right) \qquad \sum_{l=1}^{k} \alpha_l = 1
\end{aligned} \tag{3}
$$

1. Unlike single mode Gaussian, we can't just take derivatives and let it equal zero easily, i.e., optimize it analytically.
2. In terms of optimizing its parameters: the problem is **non-concave**. So traditional gradient ascend is **not** suitable for it, i.e., many local maximums.

The **goal** is to find an iterative process that ensures that $\log(p(X|\Theta^{(g)}))$ remains non-decreasing for $g = 1, \dots$.
To do so, for data $X = \{x_1, \dots x_n\}$, we introduce "latent" variables $Z = \{z_1, \dots z_n\}$, each z_i indicating which mixture x_i belongs to. The core problem then simply boils down to a single Gaussian fitting.

2 Preliminaries

2.1 Convex function



$$f\left((1-t)x_1 + tx_2\right) \leq (1-t)f(x_1) + tf(x_2) \qquad t \in (0 \ldots 1) \tag{4}$$

2.2 Jensen's inequality

Using notation ϕ instead of f:

$$\phi\left((1-t)x_1 + tx_2\right) \leq (1-t)\phi(x_1) + t\phi(x_2) \qquad t \in (0 \ldots 1) \tag{5}$$

Can be generalized further for any convex combination, i.e., let $\sum_{i=1}^{n} p_i = 1$:

$$\begin{aligned}
\phi\left(p_1x_1 + p_2x_2 + \ldots p_nx_n\right) \leq p_1\phi(x_1) + p_2\phi(x_2) \ldots p_n\phi(x_n) \qquad \sum_{i=1}^{n} p_i = 1 \\
\implies \phi\Big(\sum_{i=1}^{n} p_i x_i\Big) \leq \sum_{i=1}^{n} p_i \phi(x_i) \\
\implies \phi\Big(\sum_{i=1}^{n} p_i f(x_i)\Big) \leq \sum_{i=1}^{n} p_i \phi(f(x_i)) \qquad \text{by replacing } x_i \text{ with } f(x_i)
\end{aligned} \tag{6}$$

generalize to the continuous case:

$$\phi\left(\int_x f(x)p(x)\right) \leq \int_x \phi(f(x))p(x) \implies \phi\big(\mathbb{E}[f(x)]\big) \leq \mathbb{E}[\phi(f(x))] \tag{7}$$

2.2.1 Jensen's inequality example: $-\log(x)$

$\phi(x) = -\log(x)$ is a convex function:

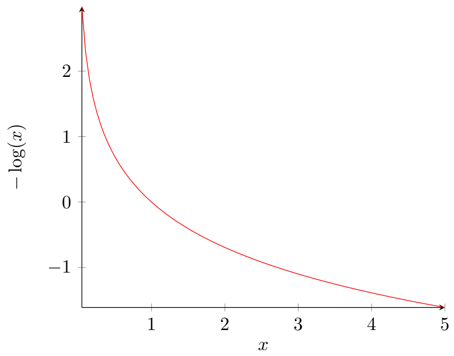


Figure 2: example of convex function $-\log(x)$

1. when $\phi(.)$ is convex:

$$\begin{aligned} &\phi(\mathbb{E}[f(\mathbf{x})]) \leq \mathbb{E}[\phi(f(\mathbf{x}))] \\ \text{e.g.} \quad &-\log(\mathbb{E}[f(\mathbf{x})]) \leq \mathbb{E}[-\log(f(\mathbf{x}))] \end{aligned} \tag{8}$$

2. when $\phi(.)$ is concave:

$$\begin{aligned} &\phi(\mathbb{E}[f(\mathbf{x})]) \geq \mathbb{E}[\phi(f(\mathbf{x}))] \\ \text{e.g.} \quad &\log(\mathbb{E}[f(\mathbf{x})]) \geq \mathbb{E}[\log(f(\mathbf{x}))] \end{aligned} \tag{9}$$

3 Expectation-Maximization Algorithm

Instead of perform:

$$\begin{aligned} \Theta^{\text{MLE}} &= \arg\max_{\Theta} \mathcal{L}(\Theta|X) \\ &= \arg\max_{\Theta} (\log[p(X|\Theta)]) \end{aligned} \tag{10}$$

The trick is to assume some "latent" variable Z to the model
For each iteration of the E-M algorithm, we perform:

$$\Theta^{(g+1)} = \arg\max_{\Theta} \left(\int_z \log\left(p(X, Z|\Theta)\right) p(Z|X, \Theta^{(g)}) \right) \mathrm{d}Z \tag{11}$$

However, before we apply it, we must ensure convergence, i.e.,

$$\begin{aligned} \log(p(X|\Theta^{(g+1)})) &= \mathcal{L}(\Theta^{(g+1)}|X) \\ &\geq \mathcal{L}(\Theta^{(g)}|X) \\ &= \log(p(X|\Theta^{(g)})) \quad \forall g \end{aligned} \tag{12}$$

Note the difference between variable Θ and the constant $\Theta^{(g)}$. Also note that gradient ascend is **not** suitable for many E-M problems, as they can be **non-concave**.

4 Proof of convergence: Maximization-Maximization

We have seen it from variational inference literature, for the ELBO-KL decomposition:

$$
\begin{aligned}
\mathcal{L}(\Theta|X) &= \log\left(p(X|\Theta)\right) \\
&= \log\left(\frac{p(X,Z|\Theta)}{p(Z|X,\Theta)}\right) \\
&= \log\left(\frac{p(X,Z|\Theta)}{q(Z)} \times \frac{q(Z)}{p(Z|X,\Theta)}\right) \\
&= \log\left(\frac{p(X,Z|\Theta)}{q(Z)}\right) + \log\left(\frac{q(Z)}{p(Z|X,\Theta)}\right) \\
&= \int_Z \log\left(\frac{p(X,Z|\Theta)}{q(Z)}\right) q(Z) + \int_Z \log\left(\frac{q(Z)}{p(Z|X,\Theta)}\right) q(Z) \\
&= \text{ELBO}(\Theta, q) + \text{KL}\big(q(Z)\|p(Z|X,\Theta)\big)
\end{aligned}
\tag{13}
$$

or to use Jensen's inequality:

$$
\begin{aligned}
\mathcal{L}(\Theta|X) &= \log p(X|\Theta) = \log \int_Z p(X,Z|\Theta) \\
&= \log\Big(\int_Z \frac{p(X,Z|\Theta)}{q(Z)} q(Z)\Big) \\
&\geq \int_Z \log\Big(\frac{p(X,Z|\Theta)}{q(Z)}\Big) q(Z) \\
&= \text{ELBO}(\Theta, q)
\end{aligned}
\tag{14}
$$

4.1 Maximization of ELBO

When applying E-M as a Maximization-Maximization algorithm, we only need to optimize ELBO, let's revisit the ELBO-KL decomposition again:

$$
\begin{aligned}
\mathcal{L}(\Theta|X) &= \int_Z \log\left(\frac{p(X,Z|\Theta)}{q(Z)}\right) q(Z) + \int_Z \log\left(\frac{q(Z)}{p(Z|X,\Theta)}\right) q(Z) \\
&= \text{ELBO}(\Theta, q) + \text{KL}(q(Z)\|p(Z|X,\Theta))
\end{aligned}
\tag{15}
$$

STEP 1: fix $\Theta = \Theta^{(g)}$, maximize $q(Z)$ for ELBO

$$
\begin{aligned}
q^*(Z) &= \arg\max_q \{\text{ELBO}(\Theta^{(g)}, q)\} \\
&= \arg\max_q \Big\{ \int_Z \log\left(\frac{p(X,Z|\Theta^{(g)})}{q(Z)}\right) q(Z) \Big\} \\
&= p(Z|X,\Theta^{(g)}) \\
\implies \ \text{ELBO}(\Theta^{(g)}, q^*) &= \mathcal{L}(\Theta^{(g)}|X)
\end{aligned}
\tag{16}
$$

This can be done with the realization that when fixing $\Theta = \Theta^{(g)}$, ELBO is upperbounded by $\mathcal{L}(\Theta^{(g)}|X)$, and maximum occurs, i.e., when $\text{KL}(q^*\|p(Z|X,\Theta^{(g)})) = 0$

STEP 1 is invisible to the algorithm, but needs to be considered for interpretation convergence.

STEP 2 Fix $q(Z) = p(Z|X,\Theta^{(g)})$, maximize Θ

substitute $q^* = p(Z|X, \Theta^{(g)})$ back into the ELBO:

$$\begin{aligned}
\Theta^{(g+1)} &= \arg\max_{\Theta} \left\{ \text{ELBO}(\Theta, q^* = p(Z|X, \Theta^{(g)})) \right\} \\
&= \arg\max_{q(Z)} \left\{ \int_Z \log\left(\frac{p(X, Z|\Theta^{(g)})}{p(Z|X, \Theta^{(g)})}\right) p(Z|X, \Theta^{(g)}) \right\} \\
&= \arg\max_{\Theta} \left(\int_Z \log\left(p(X, Z|\Theta)\right) p(Z|X, \Theta^{(g)}) \mathrm{d}Z \right) \qquad \text{remove constant terms}
\end{aligned} \tag{17}$$

after obtaining $\Theta^{(g+1)}$, it will introduce a new likelihood function $\mathcal{L}(\Theta^{(g+1)}|X)$ for which the upper bound of the ELBO($\Theta^{(g+1)}, q$) is increased for **STEP 1**

4.2 Proof of convergence without ELBO

let's decompose $\mathcal{L}(\Theta|X)$ into:

$$\begin{aligned}
\mathcal{L}(\Theta|X) &= \log(p(X|\Theta)) \\
&= \log(p(Z, X, \Theta)) - \log(p(Z|X, \Theta))
\end{aligned} \tag{18}$$

take expectation with respect to both sides with respect to $p(Z|X, \Theta^{(g)})$:

$$\mathcal{L}(\Theta|X) = \underbrace{\int_Z \log(p(Z, X, \Theta)) p(Z|X, \Theta^{(g)}) \mathrm{d}Z}_{Q(\Theta|\Theta^{(g)})} \underbrace{- \int_Z \log(p(Z|X, \Theta)) p(Z|X, \Theta^{(g)}) \mathrm{d}Z}_{H(\Theta|\Theta^{(g)})} \tag{19}$$

where $H(\Theta|\Theta^{(g)}) = \text{Cross-Entropy}\big(p(Z|X, \Theta^{(g)}) \| p(Z|X, \Theta)\big)$.

Eq.(19) can be considered as a simpler version of the ELBO-KL decomposition of $\mathcal{L}(\Theta|X)$ we have seen previously:

$$\mathcal{L}(\Theta|X) = \int_Z \log\left(\frac{p(Z, X|\Theta)}{p(Z|X, \Theta^{(g)})}\right) p(Z|X, \Theta^{(g)}) \mathrm{d}Z \; - \int_Z \log\left(\frac{p(Z|X, \Theta)}{p(Z|X, \Theta^{(g)})}\right) p(Z|X, \Theta^{(g)}) \mathrm{d}Z \tag{20}$$

i.e., the added term $\log\big(p(Z|X, \Theta^{(g)})\big) p(Z|X, \Theta^{(g)})$ of the two terms cancel out and equivalent to Eq.(19).

4.2.1 why only $Q(\Theta|\Theta^{(g)})$ needs to be maximized

In E-M, we only maximize non Θ part of ELBO:

$$\begin{aligned}
\Theta^{(g+1)} &= \arg\max_{\Theta} Q(\Theta|\Theta^{(g)}) \\
&= \arg\max_{\Theta} \left(\int_Z \log\left(p(X, Z|\Theta)\right) p(Z|X, \Theta^{(g)}) \mathrm{d}Z \right)
\end{aligned} \tag{21}$$

instead of maximizing the entire Eq.(19), i.e., $Q(\Theta|\Theta^{(g)}) + H(\Theta|\Theta^{(g)})$

the **trick** is, if we can prove:

$$H(\Theta|\Theta^{(g)}) \geq H(\Theta^{(g)}|\Theta^{(g)}) \qquad \forall \Theta \tag{22}$$

then we can show:

$$
\begin{aligned}
\mathcal{L}(\Theta^{(g+1)}) &= Q(\Theta^{(g+1)}|\Theta^{(g)}) + H(\Theta^{(g+1)}|\Theta^{(g)}) \\
&\geq \underbrace{Q(\Theta^{(g)}|\Theta^{(g)})}_{\text{Eq.(21)}} + \underbrace{H(\Theta^{(g)}|\Theta^{(g)})}_{\text{Eq.(22)}} \\
&= \mathcal{L}(\Theta^{(g)})
\end{aligned} \tag{23}
$$

it is obvious that:

$$
\begin{aligned}
\bar{\Theta} &= \arg\max_{\Theta} \left\{Q(\Theta|\Theta^{(g)}) + H(\Theta|\Theta^{(g)})\right\} \\
\implies \mathcal{L}(\Theta^{(g+1)}) &\neq \mathcal{L}(\bar{\Theta})
\end{aligned} \tag{24}
$$

4.2.2 $H(\Theta|\Theta^{(g)}) \geq H(\Theta^{(g)}|\Theta^{(g)}) \qquad \forall\Theta$

1. cross entropy

$$
\begin{aligned}
H(\Theta|\Theta^{(g)}) &= -\int_Z \log(p(Z|X,\Theta))p(Z|X,\Theta^{(g)})\mathrm{d}Z \\
&= \text{Cross-Entropy}\big(p(Z|X,\Theta^{(g)})\|p(Z|X,\Theta)\big) \\
\implies \arg\min_{\Theta}\{H(\Theta|\Theta^{(g)})\} &= \Theta^{(g)} \\
\implies \min_{\Theta}\{H(\Theta|\Theta^{(g)})\} &= \text{Entropy}(p(Z|X,\Theta^{(g)}))
\end{aligned} \tag{25}
$$

2. directly

$$
\begin{aligned}
&H(\Theta|\Theta^{(g)}) - H(\Theta^{(g)}|\Theta^{(g)}) \\
&= \int_Z -\log(p(Z|X,\Theta))p(Z|X,\Theta^{(g)})\mathrm{d}z - \int_Z -\log\big(p(Z|X,\Theta^{(g)})\big)p(Z|X,\Theta^{(g)})\mathrm{d}Z \\
&= \int_Z \log\left(\frac{p(Z|X,\Theta^{(g)})}{p(Z|X,\Theta)}\right)p(Z|X,\Theta^{(g)})\mathrm{d}Z \\
&= \int_Z -\log\left(\frac{p(Z|X,\Theta)}{p(Z|X,\Theta^{(g)})}\right)p(Z|X,\Theta^{(g)})\mathrm{d}Z \\
&\geq -\log\left(\int_Z \frac{p(Z|X,\Theta)}{p(Z|X,\Theta^{(g)})}p(Z|X,\Theta^{(g)})\mathrm{d}Z\right) \\
&= 0 \quad \because \phi = -\log \text{ a convex unction}
\end{aligned} \tag{26}
$$

5 E-M Example: Gaussian Mixture Model

Gaussian Mixture Model (k-mixture) (GMM):

$$
\begin{gathered}
p(X|\Theta) = \sum_{l=1}^{k} \alpha_l \mathcal{N}(X|\mu_l, \Sigma_l) \qquad \sum_{l=1}^{k} \alpha_l = 1 \\
\text{and } \Theta = \{\alpha_1, \dots \alpha_k, \mu_1, \dots \mu_k, \Sigma_1, \dots \Sigma_k\}
\end{gathered}
\tag{27}
$$

For data $X = \{x_1, \dots x_n\}$ we introduce "latent" variable $Z = \{z_1, \dots z_n\}$, each z_i indicates which mixture component x_i belong to.

Looking at the E-M algorithm:

$$
\Theta^{(g+1)} = \arg\max_{\Theta} \left[q(\Theta, \Theta^{(g)}) \right] = \arg\max_{\Theta} \left(\int_z \log\left(p(X, Z|\Theta)\right) p(Z|X, \Theta^{(g)}) \mathrm{d}z \right) \tag{28}
$$

All we need to do is to define both $p(X, Z|\Theta)$ and $p(Z|X, \Theta)$

5.1 Gaussian Mixture Model in action

$$
p(X|\Theta) = \sum_{l=1}^{k} \alpha_l \mathcal{N}(X|\mu_l, \Sigma_l) = \prod_{i=1}^{n} \sum_{l=1}^{k} \alpha_l \mathcal{N}(X|\mu_l, \Sigma_l) \tag{29}
$$

How to define $p(X, Z|\Theta)$

$$
p(X, Z|\Theta) = \prod_{i=1}^{n} p(x_i, z_i|\Theta) = \prod_{i=1}^{n} \underbrace{p(x_i|z_i, \Theta)}_{\mathcal{N}(\mu_{z_i}, \Sigma_{z_i})} \underbrace{p(z_i|\Theta)}_{\alpha_{z_i}} = \prod_{i=1}^{n} \alpha_{z_i} \mathcal{N}(\mu_{z_i}, \Sigma_{z_i}) \tag{30}
$$

Notice that $p(X, Z|\Theta)$ is actually simple than $p(X|\Theta)$.

How to define $p(Z|X, \Theta)$

$$
p(Z|X, \Theta) = \prod_{i=1}^{n} p(z_i|x_i, \Theta) = \prod_{i=1}^{n} \frac{\alpha_{z_i} \mathcal{N}(\mu_{z_i}, \Sigma_{z_i})}{\sum_{l=1}^{k} \alpha_l \mathcal{N}(\mu_l, \Sigma_l)} \tag{31}
$$

5.2 The E-Step:

$$
\begin{aligned}
q(\Theta, \Theta^{(g)}) &= \int_z \log\left(p(X, Z|\Theta)\right) p(Z|X, \Theta^{(g)}) \mathrm{d}z \\
&= \int_{z_1} \cdots \int_{z_n} \left(\sum_{i=1}^{n} \log p(z_i, x_i|\Theta) \prod_{i=1}^{n} p(z_i|x_i, \Theta^{(g)}) \right) \mathrm{d}z_1, \dots \mathrm{d}z_n
\end{aligned}
\tag{32}
$$

5.3 Some derivation to help

let $p(Y)$ be the joint pdf: $P(y_1, \dots y_n)$, also let $F(Y)$ be a linear function, where each term involves only one variable y_i, i.e.,

$$
F(Y) = f_1(x_1) + \dots f_n(x_n) = \sum_{i=1}^{n} f_i(y_i) \tag{33}
$$

then,

$$\int_{y_1} \cdots \int_{y_n} \Big(\sum_{i=1}^{n} f_i(y_i) \Big) P(Y) \mathrm{d}Y = \sum_{i}^{N} \Big(\int_{y_i} f_i(y_i) P_i(y_i) \mathrm{d}y_i \Big) \tag{34}$$

5.3.1 Proof

$$\int_{Y} F(Y)p(Y)\mathrm{d}Y = \int_{y_1} \int_{y_2} \cdots \int_{y_N} \Big(\sum_{i=1}^{N} f_i(y_i) \Big) p(Y) \mathrm{d}y_1, \ldots \mathrm{d}y_n \tag{35}$$

Expand it out, this equation has N sum terms. The first term is:

$$\begin{aligned}
&= \int\limits_{y_1} \int\limits_{y_2} \cdots \int\limits_{y_N} f_1(y_1) p(y_1, \ldots, y_N) \prod_{i=1}^{N} (\mathrm{d}y_i) + \cdots + \int\limits_{y_1} \int\limits_{y_2} \cdots \int\limits_{y_N} f_N(y_N) p(y_1, \ldots, y_N) \prod_{i=1}^{N} (\mathrm{d}y_i) \\
&= \int\limits_{y_1} f_1(y_1)\mathrm{d}y_1 \Big(\int\limits_{y_2} \cdots \int\limits_{y_N} p(y_1, \ldots, y_N) \prod_{i=2}^{N} (\mathrm{d}y_i) \Big) + \cdots + \int\limits_{y_N} f_N(y_N)\mathrm{d}y_N \int\limits_{y_1} \cdots \int\limits_{y_{N-1}} p(y_1, \ldots, y_N) \prod_{i=1}^{N-1} (\mathrm{d}y_i)
\end{aligned} \tag{36}$$

inside the first big bracket becomes the marginal probability density of $p(y_1)$, therefore, the first term becomes:

$$\int_{y_1} f_1(y_1) p(y_1) \mathrm{d}y_1 \tag{37}$$

Apply this to each of the N terms, therefore:

$$\int_{Y} (F(Y)) P(Y) \mathrm{d}Y = \int_{y_1} f_1(y_1) P_1(y_1) \mathrm{d}y_1 + \cdots + \int_{y_n} f_n(y_n) P_n(y_n) \mathrm{d}y_n \tag{38}$$

now apply Eq.(34), we have:

$$\begin{aligned}
q(\Theta, \Theta^{(g)}) &= \int_{z_1} \cdots \int_{z_n} \left(\sum_{i=1}^{n} \log p(z_i, x_i|\Theta) \prod_{i=1}^{n} p(z_i|x_i, \Theta^{(g)}) \right) \mathrm{d}z_1, \ldots \mathrm{d}z_n \\
&= \sum_{i=1}^{n} \Big(\int_{z_i} \log p(z_i, x_i|\Theta) p(z_i|x_i, \Theta^{(g)}) \mathrm{d}z_i \Big) \qquad z_i \in \{1, \ldots, k\} \\
&= \sum_{z_i=1}^{k} \sum_{i=1}^{n} \log p(z_i, x_i|\Theta) p(z_i|x_i, \Theta^{(g)}) \qquad \text{swap the summation terms} \\
&= \sum_{l=1}^{k} \sum_{i=1}^{n} \log[\alpha_l \mathcal{N}(x_i|\mu_l, \Sigma_l)] p(l|x_i, \Theta^{(g)}) \qquad \text{substitute Gaussan and replace } z_i \rightarrow l
\end{aligned} \tag{39}$$

5.4 The M-Step objective function

$$\begin{aligned}
q(\Theta, \Theta^{(g)}) &= \sum_{l=1}^{k} \sum_{i=1}^{n} \log[\alpha_l \mathcal{N}(x_i|\mu_l, \Sigma_l)] p(l|x_i, \Theta^{(g)}) \\
&= \sum_{l=1}^{k} \sum_{i=1}^{n} \log(\alpha_l) p(l|x_i, \Theta^{(g)}) + \sum_{l=1}^{k} \sum_{i=1}^{n} \log[\mathcal{N}(x_i|\mu_l, \Sigma_l)] p(l|x_i, \Theta^{(g)})
\end{aligned} \tag{40}$$

5.4.1 computing responsibilities

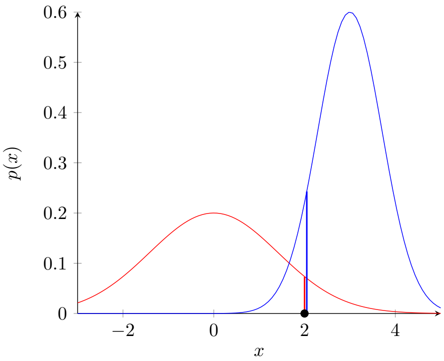


Figure 3: compute responsibility probabilities, red and blue each indicate its own un-normalized responsibilities

$$p(l|x_i, \Theta^{(g)}) = \frac{\alpha_l \mathcal{N}(\mathbf{x}_i; \mu_l, \Sigma_l)}{\sum_{s=1}^{k} \alpha_s \mathcal{N}(\mathbf{x}_i|\mu_s, \Sigma_s)} \tag{41}$$

Eq.(40) shows that the first term contains only α and the second term contains only μ, Σ. So we can maximize both terms independently.

5.5 The M-Step: maximizing α

Maximizing α means that:

$$\frac{\partial \sum_{l=1}^{k} \sum_{i=1}^{n} \log(\alpha_l) p(l|x_i, \Theta^{(g)})}{\partial \alpha_1, \ldots, \partial \alpha_k} = [0 \ldots 0] \qquad \text{subject to} \sum_{l=1}^{k} \alpha_l = 1 \tag{42}$$

This is to be solved using Lagrange Multiplier

$$\mathbb{LM}(\alpha_1, \ldots \alpha_k, \lambda) = \sum_{l=1}^{k} \log(\alpha_l) \underbrace{\left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \right)}_{\text{contains no } \alpha} + \lambda \left(\sum_{l=1}^{k} \alpha_l - 1 \right) \tag{43}$$

taking derivative with respect to just one α_l:

$$\begin{aligned}
\frac{\partial \mathbb{LM}}{\partial \alpha_l} &= \frac{1}{\alpha_l} \left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \right) + \lambda = 0 \\
\implies -\lambda &= \frac{1}{\alpha_l} \left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \right) \\
\implies -\lambda \alpha_l &= \left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \right) \\
\implies -\lambda \sum_{l=1}^{k} \alpha_l &= \sum_{l=1}^{k} \left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \right) \\
\implies \lambda &= -n
\end{aligned} \tag{44}$$

substitute $\lambda = -n$ into Eq.(44):

$$\begin{aligned} \frac{1}{\alpha_l}\left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)})\right) + \lambda = 0 \\ \implies \frac{1}{\alpha_l}\left(\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)})\right) - n = 0 \\ \implies \alpha_l = \frac{1}{n}\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)}) \end{aligned} \tag{45}$$

5.6 Optional The M-Step: maximizing μ, Σ

Here I jot down the MLE steps for the parameters of a single multidimensional Gaussian distribution. The MLE of a single 1D Gaussian distribution can be easily found in your previous work.

So, maximizing μ, Σ means that:

$$\frac{\partial \sum_{l=1}^{k} \sum_{i=1}^{n} \log(\alpha_l) p(l|x_i, \Theta^{(g)})}{\partial \mu_1, \ldots, \partial \mu_k, \partial \Sigma_1, \ldots, \partial \Sigma_k} = [0 \ldots 0] \tag{46}$$

- You will need some linear algebra identities to solve this. It's quite involved. For details, please refer:
- J. Bilmes. "A Gentle Tutorial on the EM Algorithm and its Application to Parameter Estimation for Gaussian Mixture and Hidden Markov Models"

5.6.1 Some formulas to remember

- derivatives of log of determinant (**with** determinant)

$$\frac{\partial \log |\mathbf{X}|}{\partial \mathbf{X}} = (\mathbf{X}^{-1})^{\top} \tag{47}$$

- Derivatives of Traces

$$\frac{\partial \text{Tr}(F(\mathbf{X}))}{\partial \mathbf{X}} = (f(\mathbf{X}))^{\top} \tag{48}$$

where $f(\cdot)$ is the scalar derivative of $F(\cdot)$

- Derivatives of Traces of inverse, fact 1

$$\frac{\partial \text{Tr}(\mathbf{AXB})}{\partial \mathbf{X}} = \mathbf{A}^{\top}\mathbf{B}^{\top} \tag{49}$$

- Derivatives of Traces of inverse, fact 2

$$\frac{\partial \text{Tr}((\mathbf{X}+\mathbf{A})^{-1})}{\partial \mathbf{X}} = -\left((\mathbf{X}+\mathbf{A})^{-1}(\mathbf{X}+\mathbf{A})^{-1}\right)^{\top} \tag{50}$$

- Derivatives of Traces of inverse, fact 3

$$\frac{\partial \text{Tr}(\mathbf{AX}^{-1}\mathbf{B})}{\partial \mathbf{X}} = -(\mathbf{X}^{-1}\mathbf{BAX}^{-1})^{\top} \tag{51}$$

5.6.2 Maximization μ_l

$$\begin{aligned}\text{second part of } q(\Theta,\Theta^{(g)}) &= \sum_{l=1}^{k}\sum_{i=1}^{n}\log[\mathcal{N}(x_i|\mu_l,\mathbf{\Sigma}_l)]p(l|x_i,\Theta^{(g)}) \\ &= \sum_{i=1}^{n}\sum_{l=1}^{k}\log\left(\frac{1}{\sqrt{(2\pi)^d|\mathbf{\Sigma}_l|}}\exp\left(-\frac{1}{2}(x_i-\boldsymbol{\mu})^\top\mathbf{\Sigma}^{-1}(x_i-\boldsymbol{\mu})\right)\right)p(l|x_i,\Theta^{(g)})\end{aligned} \tag{52}$$

Let $\mathbf{Y}$ be zero-meaned data matrix, where each column of $\mathbf{Y}$ is $\mathbf{x}_i-\boldsymbol{\mu}_l$:

$$\mathcal{L}\equiv\mathcal{L}(p(\mathbf{Y}|\mathcal{K})) = -\frac{DN}{2}\log(2\pi)-\frac{D}{2}\log|\mathcal{K}|-\frac{1}{2}\mathrm{Tr}\big(\mathcal{K}^{-1}\mathbf{Y}\mathbf{Y}^\top\big) \tag{53}$$

$$\begin{aligned}\text{second part of } q(\Theta,\Theta^{(g)}) &= \sum_{l=1}^{k}\sum_{i=1}^{n}\log[\mathcal{N}(x_i|\mu_l,\mathbf{\Sigma}_l)]p(l|x_i,\Theta^{(g)}) \\ &= \sum_{i=1}^{n}\sum_{l=1}^{k}\log\left(\frac{1}{\sqrt{(2\pi)^d|\mathbf{\Sigma}_l|}}\exp\left(-\frac{1}{2}(x_i-\boldsymbol{\mu})^\top\mathbf{\Sigma}^{-1}(x_i-\boldsymbol{\mu})\right)\right)p(l|x_i,\Theta^{(g)}) \\ \Longrightarrow \mathcal{S}(\mu_l,\mathbf{\Sigma}_l) &= \sum_{i=1}^{n}-\frac{1}{2}\log(|\mathbf{\Sigma}_l|)p(l|x_i,\Theta^{(g)})-\sum_{i=1}^{n}\frac{1}{2}(x_i-\boldsymbol{\mu}_l)^T\mathbf{\Sigma}^{-1}(x-\boldsymbol{\mu}_l)p(l|x_i,\Theta^{(g)})\end{aligned} \tag{54}$$

$$\begin{aligned}\Longrightarrow \mathcal{S}(\mu_l,\Sigma_l^{-1}) &= -\mathrm{Tr}\left(\frac{\Sigma_l^{-1}}{2}\sum_{i=1}^{n}(x_i-\mu_l)(x-\mu_l)^Tp(l|x_i,\Theta^{(g)})\right)+\text{ Constant} \\ \Longrightarrow \frac{\partial\mathcal{S}(\mu_l,\Sigma_l^{-1})}{\partial\mu_l} &= \frac{\Sigma^{-1}}{2}\sum_{i=1}^{n}2(x_i-\mu_l)p(l|x_i,\Theta^{(g)})=0 \\ \Longrightarrow \sum_{i=1}^{n}x_ip(l|x_i,\Theta^{(g)}) &= \mu_l\sum_{i=1}^{n}p(l|x_i,\Theta^{(g)}) \\ \Longrightarrow \mu_l &= \frac{\sum_{i=1}^{n}x_ip(l|x_i,\Theta^{(g)})}{\sum_{i=1}^{n}p(l|x_i,\Theta^{(g)})}\end{aligned} \tag{55}$$

5.6.3 Maximization of covariance

$$\begin{aligned}\text{second part of } q(\Theta,\Theta^{(g)}) &= \sum_{l=1}^{k}\sum_{i=1}^{n}\log[\mathcal{N}(x_i|\mu_l,\mathbf{\Sigma}_l)]p(l|x_i,\Theta^{(g)}) \\ &= \sum_{i=1}^{n}\sum_{l=1}^{k}\log\left(\frac{1}{\sqrt{(2\pi)^d|\mathbf{\Sigma}_l|}}\exp\left(-\frac{1}{2}(x_i-\boldsymbol{\mu}_l)^\top\mathbf{\Sigma}^{-1}(x_i-\boldsymbol{\mu}_l)\right)\right)p(l|x_i,\Theta^{(g)})\end{aligned} \tag{56}$$

- let $\mathbf{Y}$ be zero-meaned data matrix, where each column of $\mathbf{Y}$ is $x_i-\boldsymbol{\mu}_l$
- let $\mathbf{P}$ be diagonal matrix in which $\mathbf{P}_{ii}$ correspond to $p(l|x_i,\Theta^{(g)})$

$$\mathcal{L}\equiv\mathcal{L}(p(\mathbf{Y}|\boldsymbol{\mu}_l,\mathbf{\Sigma}_l)) = -\frac{d\times\mathrm{Tr}(\mathbf{P})}{2}\log(2\pi)-\frac{\mathrm{Tr}(\mathbf{P})}{2}\log|\mathbf{\Sigma}_l|-\frac{1}{2}\mathrm{Tr}\big(\mathbf{\Sigma}_l^{-1}\mathbf{Y}\mathbf{P}\mathbf{Y}^\top\big) \tag{57}$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \mathbf{\Sigma}_l} &= \mathbf{\Sigma}_l{}^{-1}\mathbf{Y}\mathbf{P}\mathbf{Y}^\top\mathbf{\Sigma}_l^{-1} - \text{Tr}(\mathbf{P})\mathbf{\Sigma}_l^{-1} = \mathbf{0} \\
\implies \mathbf{\Sigma}_l{}^{-1}\mathbf{Y}\mathbf{P}\mathbf{Y}^\top\mathbf{\Sigma}_l^{-1} &= \text{Tr}(\mathbf{P})\mathbf{\Sigma}_l^{-1} \\
\implies \mathbf{Y}\mathbf{P}\mathbf{Y}^\top\mathbf{\Sigma}_l^{-1} &= \text{Tr}(\mathbf{P}) \implies \mathbf{\Sigma}_l^{-1} = \text{Tr}(\mathbf{P})(\mathbf{Y}\mathbf{P}\mathbf{Y}^\top)^{-1} \\
\implies \mathbf{\Sigma}_l &= \text{Tr}(\mathbf{P})^{-1}(\mathbf{Y}\mathbf{P}\mathbf{Y}^\top) = \frac{(\mathbf{Y}\mathbf{P}\mathbf{Y}^\top)}{\text{Tr}(\mathbf{P})} \\
&= \frac{\sum_{i=1}^{n}(x_i - \mu_l)(x - \mu_l)^T p(l|x_i, \Theta^{(g)})}{\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)})}
\end{aligned} \tag{58}
$$

$$
\mathcal{S}(\mu_l, \Sigma_l^{-1}) = \sum_{i=1}^{n}\left(-\frac{1}{2}\log(|\Sigma_l|) - \frac{1}{2}(x_i - \mu_l)^T\Sigma^{-1}(x - \mu_l)\right)p(l|x_i, \Theta^{(g)}) \tag{59}
$$

Change Σ to Σ^{-1}, this is so that after taking derivative of $\log(X)$, the result is in terms of X^{-1}

$$
= \left(\sum_{i=1}^{n}\log(|\Sigma_l^{-1}|)p(l|x_i, \Theta^{(g)}) - \frac{1}{2}\text{tr}\left(\Sigma^{-1}\underbrace{\sum_{i=1}^{n}(x_i - \mu_l)(x - \mu_l)^T p(l|x_i, \Theta^{(g)})}_{M_l}\right)\right)
$$

$$
\begin{aligned}
\implies \frac{\partial \mathcal{S}(\mu_l, \Sigma_l^{-1})}{\partial \Sigma_l^{-1}} &= \frac{2\sum_{i=1}^{n}\Sigma_l p(l|x_i, \Theta^{(g)}) - \sum_{i=1}^{n}\text{diag}(\Sigma)p(l|x_i, \Theta^{(g)})}{2} - \frac{2M_l - \text{diag}(M_l)}{2} = 0 \\
&\implies 2(\sum_{i=1}^{n}\Sigma p(l|x_i, \Theta^{(g)}) - M_l) - \sum_{i=1}^{n}\text{diag}(\Sigma p(l|x_i, \Theta^{(g)}) - M_l) = 0 \\
&\implies \sum_{i=1}^{n}\Sigma p(l|x_i, \Theta^{(g)}) - M_l = 0 \\
&\implies \Sigma = \frac{\sum_{i=1}^{n} M_l}{\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)})} = \frac{\sum_{i=1}^{n}(x_i - \mu_l)(x - \mu_l)^T p(l|x_i, \Theta^{(g)})}{\sum_{i=1}^{n} p(l|x_i, \Theta^{(g)})}
\end{aligned} \tag{60}
$$

5.7 Summary of Gaussian Mixture Model

Maximizing μ, Σ means that to update $\Theta^{(g)} \to \Theta^{(g+1)}$:

$$
\alpha_l^{(g+1)} = \frac{1}{N}\sum_{i=1}^{N} p(l|x_i, \Theta^{(g)}) \tag{61}
$$

$$
\mu_l^{(g+1)} = \frac{\sum_{i=1}^{N} x_i p(l|x_i, \Theta^{(g)})}{\sum_{i=1}^{N} p(l|x_i, \Theta^{(g)})} \tag{62}
$$

$$
\Sigma_l^{(g+1)} = \frac{\sum_{i=1}^{N}[x_i - \mu_l^{(i+1)}][x_i - \mu_l^{(i+1)}]^\top p(l|x_i, \Theta^{(g)})}{\sum_{i=1}^{N} p(l|x_i, \Theta^{(g)})} \tag{63}
$$

One can verify that when the number of component $K = 1 \implies p(l = 1|x_i, \Theta^{(g)}) = 1$, then:

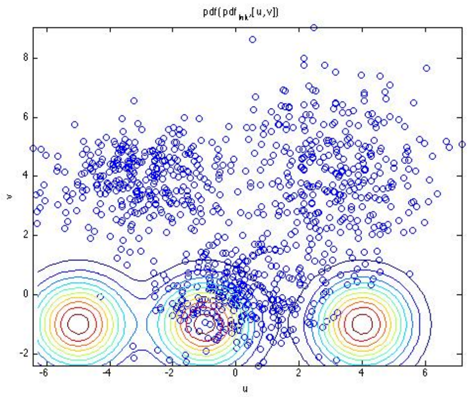
$$\alpha_l^{(g+1)} = 1 \tag{64}$$

$$\mu_l^{(g+1)} = \frac{1}{N}\sum_{i=1}^{N} x_i \tag{65}$$

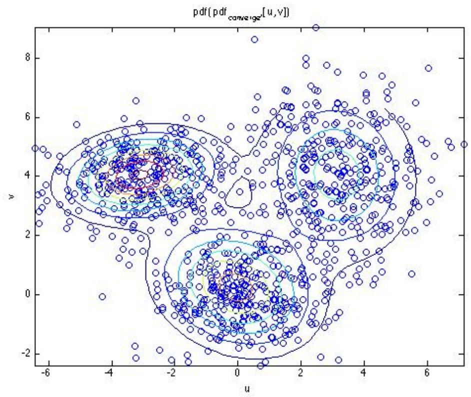
$$\Sigma_l^{(g+1)} = \frac{1}{N}\sum_{i=1}^{N}[x_i - \mu_l^{(i+1)}][x_i - \mu_l^{(i+1)}]^\top \tag{66}$$

which becomes the parameter update of a single Gaussian

5.8 To show the diagram again



(a) GMM at initialization: $\Theta^{(1)}$



(b) GMM at convergence: $\Theta^{(f)}$