The Application of Expetation-Maximize Algorithm: 3 Coins Problem and Gaussian Mixture Model

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1. （a）推导三硬币模型的 EM 算法中隐变量后验分布的计算公式以及参数更新公式；
（b）假设硬币 A、B、C 正面向上的概率分别是 0.7、0.3、0.6，按照三硬币模型的数据生成过程独立地重复 100 次试验并记录观测结果的序列；
（c）利用 EM 算法根据上述观测序列估计各硬币正面向上的概率。
2. 参考《The Matrix Cookbook》推导高斯混合模型的 EM 算法中 M 步的参数更新公式。
3. 按下列参数生成高斯混合模型的数据，共有三个高斯混合成分，每个成分生成 300 个数据点。

$$
\begin{aligned}
\boldsymbol{\mu}_1 &= (3,1) & \Sigma_1 &= ((1,-0.5);(-0.5,1)) \\
\boldsymbol{\mu}_2 &= (8,10) & \Sigma_2 &= ((2,0.8);(0.8,2)) \\
\boldsymbol{\mu}_3 &= (12,2) & \Sigma_3 &= ((1,0);(0,1))
\end{aligned}
$$

使用 scikit-learn 库中的高斯混合模型实现上述数据的学习过程，计算在不同个数的高斯混合成分下模型的 AIC 和 BIC 值，并将学习得到的模型参数与真实模型参数进行对比。

1.（a）

解：

$$
J(\theta, Q(z)) = \sum_i \sum_{z_i} Q(z_i) \cdot \log(\frac{P(x_i, z_i|\theta)}{Q(z_i)}), \quad \theta = (\pi, p, q)
$$

E step:

$$
Q^{t+1}(z) = \arg\max_{Q(z)} \ J(\theta^t, Q(z))
$$

$$
Q(z_i) = P(z_i|x_i, \theta^t) \Leftarrow \begin{cases} \dfrac{P(x_i, z_i|\theta^t)}{Q(z_i)} = c, \\ \sum\limits_{z_i} Q(z_i) = 1 \end{cases}
$$

$$
\begin{cases}
P(z|x,\theta) &= \dfrac{P(x,z|\theta)}{P(x|\theta)} \\
P(x,z|\theta) &= \pi^z p^x (1-p)^{1-x} + (1-\pi)^{1-z} q^x (1-q)^{1-x} \\
P(x|\theta) &= P(x, z=1|\theta) + P(x, z=0|\theta)
\end{cases}
$$

$$
\begin{aligned}
Q^{t+1}(z_i) &= P(z_i|x_i, \theta^t) \\
&= \frac{(\pi^t)^{z_i} (p^t)^{x_i} (1-p^t)^{1-x_i} + (1-\pi^t)^{1-z_i} (q^t)^{x_i} (1-q^t)^{1-x_i}}{(\pi^t)(p^t)^{x_i}(1-p^t)^{1-x_i} + (1-\pi^t)(q^t)^{x_i}(1-q^t)^{1-x_i}}
\end{aligned}
$$

$$
Q^{t+1}(z_i = 1) = \frac{(\pi^t)(p^t)^{x_i}(1-p^t)^{1-x_i}}{(\pi^t)(p^t)^{x_i}(1-p^t)^{1-x_i} + (1-\pi^t)(q^t)^{x_i}(1-q^t)^{1-x_i}}
$$

M step:

$$\theta^{t+1} = \arg\max_{\theta} \ J(\theta, Q^{t+1}(z))$$
$$= \arg\max_{\theta} \ \sum_i \sum_{z_i} Q(z_i) \cdot \log(P(x_i, z_i|\theta))$$

$$① \ \frac{\partial J(\theta, Q^{t+1}(z))}{\pi} = \sum_i \sum_{z_i} \frac{Q^{t+1}(z_i)}{P(x_i, z_i|\theta)} \cdot \frac{\partial P(x_i, z_i|\theta)}{\partial \pi}$$
$$= \sum_i [\frac{Q^{t+1}(z_i=1)}{\pi p^{x_i}(1-p)^{1-x_i}} \cdot p^{x_i}(1-p)^{1-x_i} - \frac{Q^{t+1}(z_i=0)}{(1-\pi)q^{x_i}(1-q)^{1-x_i}} \cdot q^{x_i}(1-q)^{1-x_i}]$$
$$= \frac{1}{\pi}\sum_i Q^{t+1}(z_i=1) - \frac{1}{1-\pi}\sum_i Q^{t+1}(z_i=0)$$

$$\frac{\partial J(\theta, Q^{t+1}(z))}{\pi}|_{\pi=\pi^{t+1}} = 0$$
$$\pi^{t+1} = \frac{\sum\limits_i Q^{t+1}(z_i=1)}{\sum\limits_i [Q^{t+1}(z_i=0) + Q^{t+1}(z_i=1)]}$$
$$= \frac{1}{n}\sum_i Q^{t+1}(z_i=1)$$

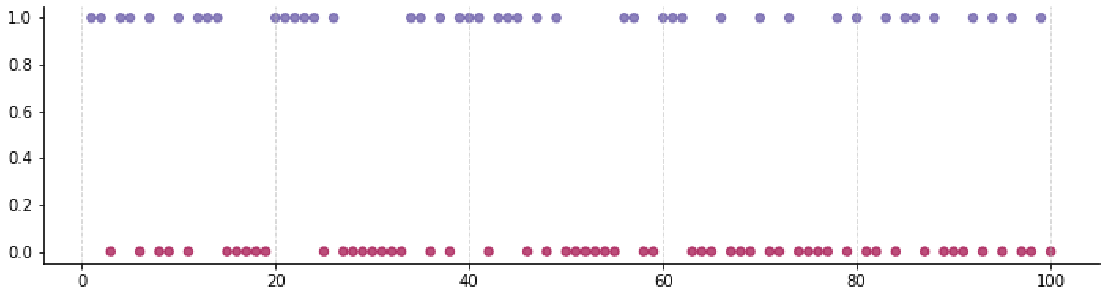
$$② \ \frac{\partial J(\theta, Q^{t+1}(z))}{p} = \sum_i \sum_{z_i} \frac{Q^{t+1}(z_i)}{P(x_i, z_i|\theta)} \cdot \frac{\partial P(x_i, z_i|\theta)}{\partial p}$$
$$= \sum_i \frac{Q^{t+1}(z_i=1)}{\pi p^{x_i}(1-p)^{1-x_i}} \cdot [\pi x_i p^{x_i-1}(1-p)^{1-x_i} - \pi p^{x_i}(1-x_i)(1-p)^{-x_i}]$$
$$= \sum_i Q^{t+1}(z_i=1)(\frac{x_i}{p} - \frac{1-x_i}{1-p})$$

$$\frac{\partial J(\theta, Q^{t+1}(z))}{p}|_{p=p^{t+1}} = 0$$
$$p^{t+1} = \frac{\sum\limits_i Q^{t+1}(z_i=1)x_i}{\sum\limits_i Q^{t+1}(z_i=1)}$$

$$③ \ \frac{\partial J(\theta, Q^{t+1}(z))}{q} = \sum_i \sum_{z_i} \frac{Q^{t+1}(z_i)}{P(x_i, z_i|\theta)} \cdot \frac{\partial P(x_i, z_i|\theta)}{\partial q}$$
$$= \sum_i Q^{t+1}(z_i=0)(\frac{x_i}{q} - \frac{1-x_i}{1-q})$$
$$q^{t+1} = \frac{\sum\limits_i Q^{t+1}(z_i=0)x_i}{\sum\limits_i Q^{t+1}(z_i=0)}$$
$$= \frac{\sum\limits_i (1-Q^{t+1}(z_i=1))x_i}{\sum\limits_i (1-Q^{t+1}(z_i=1))}$$

由推导过程可知，θ 中三个参数的更新都需要计算 $Q^{t+1}(z=1)$ ，提前计算有利于提高算法效率。

（b）生成的观测序列如图：



（c）预测结果如下：

	π	p	q	LL
真实参数	0.700	0.300	0.600	-0.4943
预测 1	0.248	0.776	0.329	-0.5798
预测 2	0.598	0.440	0.440	-0.5798
预测 3	0.047	0.760	0.424	-0.5798
$\cdots$		$\cdots$		$\cdots$

尽管有无穷多解，但它们的似然几乎相等。

2.

解：

$$J(\theta, Q(z)) = \sum_i \sum_{z_i} Q(z_i) \cdot \log(\frac{P(\mathbf{x}_i, z_i|\theta)}{Q(z_i)}), \quad \theta = \{\alpha_k, \boldsymbol{\mu}_k, \Sigma_k\}_{k=1}^K$$

E step:

$$Q^{t+1}(z) = \arg\max_{Q(z)} \; J(\theta^t, Q(z))$$

$$\begin{aligned} Q^{t+1}(z_i) &= P(z_i|\mathbf{x}_i, \theta^t) \\ &= \frac{P(\mathbf{x}_i|z_i, \theta^t)P(z_i|\theta^t)}{\sum\limits_{z_i} P(\mathbf{x}_i|z_i, \theta^t)P(z_i|\theta^t)} \end{aligned}$$

$$Q^{t+1}(z_i = k) = \frac{\alpha_k P(\mathbf{x}_i|\boldsymbol{\mu}_k^t, \Sigma_k^t)}{\sum\limits_{k=1}^K \alpha_k P(\mathbf{x}_i|\boldsymbol{\mu}_k^t, \Sigma_k^t)}$$

M step:

$$
\begin{aligned}
\theta^{t+1} &= \arg\max_{\theta}\ J(\theta, Q^{t+1}(z)) \\
&= \arg\max_{\theta}\ \sum_i \sum_{z_i} Q(z_i)\cdot \log(P(\mathbf{x}_i, z_i|\theta))
\end{aligned}
$$

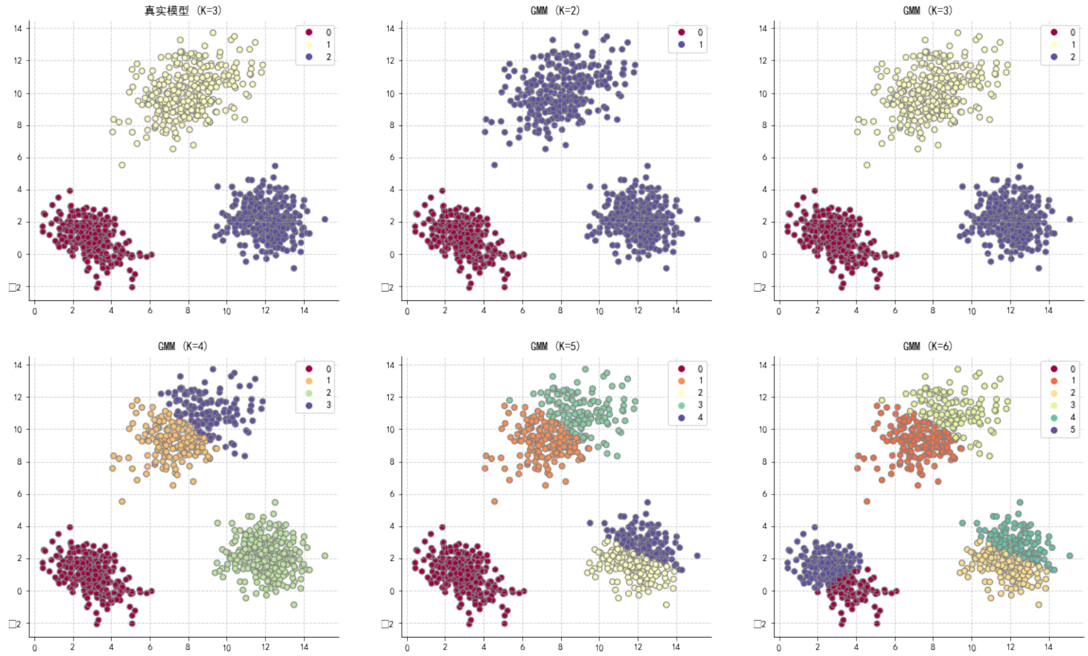
$$
\begin{aligned}
① \ L(\boldsymbol{\alpha}, \nu) &= \sum_i \sum_{z_i} Q^{t+1}(z_i)\log P(\mathbf{x}_i, z_i|\theta) + \nu(\sum_{k=1}^{K}\alpha_k - 1) \\
\frac{\partial L}{\partial \alpha_k} &= \sum_i \frac{Q^{t+1}(z_i = k)}{\alpha_k P(\mathbf{x}_i|\boldsymbol{\mu}_k, \Sigma_k)} + \nu \\
&= \sum_i \frac{Q^{t+1}(z_i = k)}{\alpha_k} + \nu \\
\frac{\partial L}{\partial \alpha_k}&|_{\alpha_k = \alpha_k^{t+1}} = 0 \\
\sum_i \frac{Q^{t+1}(z_i = k)}{\alpha_k^{t+1}} &+ \nu = 0 \\
\sum_k \alpha_k^{t+1} &= \frac{\sum_i \sum_k Q^{t+1}(z_i = k)}{-\nu} \\
&= \frac{m}{-\nu} = 1 \\
\alpha_k^{t+1} &= \frac{1}{m}\sum_i Q^{t+1}(z_i = k)
\end{aligned}
$$

$$
\begin{aligned}
② \ \log P(\mathbf{x}_i, z_i = k|\theta) &= \log \alpha_k \cdot P(\mathbf{x}_i|\boldsymbol{\mu}_k, \Sigma_k) \\
&= \log \alpha_k - \frac{n}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_k| - \\
&\qquad \frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \Sigma_k^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k) \\
\frac{\partial J(\theta, Q^{t+1}(z))}{\partial \boldsymbol{\mu}_k} &= -\sum_i Q^{t+1}(z_i = k)\Sigma_k^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k) \\
\frac{\partial J(\theta, Q^{t+1}(z))}{\partial \boldsymbol{\mu}_k}&|_{\boldsymbol{\mu}_k = \boldsymbol{\mu}_k^{t+1}} = 0 \\
\boldsymbol{\mu}_k^{t+1} &= \frac{\sum_i Q^{t+1}(z_i = k)\mathbf{x}_i}{\sum_i Q^{t+1}(z_i = k)}
\end{aligned}
$$

$$
\begin{aligned}
③ \ \frac{\partial J(\theta, Q^{t+1}(z))}{\partial \Sigma_k}|_{\Sigma_k = \Sigma_k^{t+1}} &= \frac{1}{2}\sum_i Q^{t+1}(z_i = k)\cdot[-(\Sigma_k^{t+1})^{-1} + \\
&\qquad (\Sigma_k^{t+1})^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T(\Sigma_k^{t+1})^{-1}] = 0 \\
&\sum_i Q^{t+1}(z_i = k)\cdot[\Sigma_k^{t+1} + (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T] = 0 \\
\Sigma_k^{t+1} &= \frac{\sum_i Q^{t+1}(z_i = k)\cdot(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T}{\sum_i Q^{t+1}(z_i = k)}
\end{aligned}
$$

3.

生成样本与高斯混合模型预测的分类结果如下：



AIC 和 BIC 值情况如下：