

EM算法

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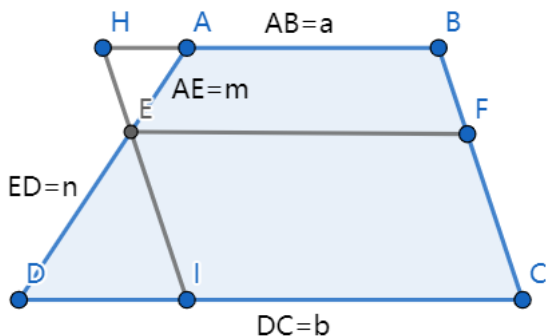
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1. 背景知识

1.1. 相似三角形

- 1. 定理：两角分别对应相等的两个三角形相似。
- 2. 定理：相似三角形任意对应线段的比等于相似比。

1.2. 梯形中位线推论



已知：在梯形ABCD中， $AB \parallel DC$ ， $AB = a$ ， $DC = b$ ，E为边AB上的任意一点， $EF \parallel DC$ ，且EF与BC相交与点F。

结论：
$$EF = \frac{n \cdot a + m \cdot b}{m + n}$$

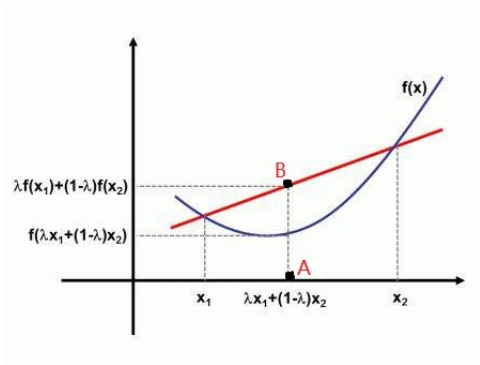
证明：过E做直线HI平行于BC，由相似三角形定理可知， $\triangle AEH \sim \triangle EDI$ 。

所以，
$$\frac{AE}{ED} = \frac{HA}{DI} = \frac{EF - a}{b - EF} = \frac{m}{n}$$

化简可得：
$$EF = \frac{n \cdot a + m \cdot b}{m + n}$$

特别地，当 $m + n = 1$ 时， $EF = n \cdot a + (1 - n) \cdot b$

1.3. Jensen(琴生)不等式



若 f 是凸函数，则：

$$f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda)f(x_2) \quad \text{其中 } \lambda \in [0, 1]。 \text{如果 } f \text{ 是凹函数，则 } (33) \leq \text{ 换为 } \geq \text{ 即可。}$$

证明1: 令 $x = \lambda x_1 + (1 - \lambda)x_2$, 直线与曲线相交的两点分别为 $(x_1, f(x_1))$, $(x_2, f(x_2))$ 。

$$\text{根据直线两点式, 可得直线方程为 } \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{f(x) - f(x_1)}{x - x_1}$$

$$\text{当 } x = \lambda x_1 + (1 - \lambda)x_2 \text{ 时, } y = \lambda f(x_1) + (1 - \lambda)f(x_2)$$

证明2: 令 $x = \lambda x_1 + (1 - \lambda)x_2$

因为 $\lambda \in [0, 1]$, 所以 $x \in [x_1, x_2]$ 。

$$\text{因为 } \frac{x - x_1}{x_2 - x_1} = \frac{\lambda x_1 + (1 - \lambda)x_2 - x_1}{x_2 - \lambda x_1 - (1 - \lambda)x_2} = \frac{(1 - \lambda)(x_2 - x_1)}{\lambda(x_2 - x_1)} = \frac{1 - \lambda}{\lambda}$$

根据梯形推导公式可得:

$$y = AB = \lambda f(x_1) + (1 - \lambda)f(x_2)$$

将上式中的 λ 推广到 n 个同样成立, 即:

$$f(\lambda_1 x_1 + \lambda_2 x_2 + \dots + \lambda_n x_n) \leq \lambda_1 f(x_1) + \lambda_2 f(x_2) + \dots + \lambda_n f(x_n) \quad \text{其中, } \lambda_1, \lambda_2, \dots, \lambda_n \in [0, 1], \sum_{i=1}^n \lambda_i = 1$$

如果将 i 看做概率分布, 则在概率论中:

$$f(E[X]) \leq E[f(x)] \quad (33)$$

其中, f 是凸函数, X 是随机变量, $E[X]$ 为 X 的期望

1.4. 期望

对随机变量 x_i , 对应的概率为 p_i , 则随机变量 x 的期望为:

$$E(x) = \sum_{i=1}^n x_i p_i \quad (34)$$

2. 三硬币模型引入

问题: 假设有3枚硬币, 分别记作A, B, C。这些硬币正面出现的概率分别是 π, p 和 q 。进行如下掷硬币试验: 先掷硬币A, 根据其结果选出硬币B或硬币C, 正面选硬币B, 反面选硬币C; 然后掷选出的硬币, 掷硬币的结果, 出现正面记作1, 出现反面记作0; 独立地重复 n 次试验 (这里, $n=10$) , 观测结果如下:

1, 1, 0, 1, 0, 0, 1, 0, 1, 1

假设只能观测到掷硬币的结果, 不能观测掷硬币的过程。问如何估计三硬币正面出现的概率, 即三硬币模型的参数。

解: 对每一次试验可如下建模

$$\begin{aligned} P(y | \theta) &= \sum_z P(y, z | \theta) \\ &= \sum_z P(z | \theta) P(y | z, \theta) \\ &= P(z = 1 | \theta) P(y | z = 1, \theta) + P(z = 0 | \theta) P(y | z = 0, \theta) \\ &= \begin{cases} \pi p + (1 - \pi)q, & \text{if } y = 1; \\ \pi(1 - p) + (1 - \pi)(1 - q), & \text{if } y = 0; \end{cases} \\ &= \pi p^y (1 - p)^{1-y} + (1 - \pi) q^y (1 - q)^{1-y} \end{aligned} \quad (35)$$

其中, 随机变量 y 是观测变量, 表示一

则观测数据的似然函数为:

$$\begin{aligned} P(Y | \theta) &= \sum_Z P(Y, Z | \theta) \\ &= \sum_Z P(Z | \theta) P(Y | Z, \theta) \\ &= \prod_{j=1}^n P(y_j | \theta) \end{aligned} \quad (36)$$

$$= \prod_{j=1}^n [\pi p^{y_j} (1-p)^{1-y_j} + (1-\pi) q^{y_j} (1-q)^{1-y_j}]$$

考虑求模型参数 $\theta = (\pi, p, q)$ 的极大似然估计，即使用对数似然函数来进行参数估计，可得：

$$\begin{aligned}\hat{\theta} &= \arg \max_{\theta} \ln P(Y | \theta) \\ &= \arg \max_{\theta} \ln \prod_{j=1}^n [\pi p^{y_j} (1-p)^{1-y_j} + (1-\pi) q^{y_j} (1-q)^{1-y_j}] \\ &= \arg \max_{\theta} \sum_{j=1}^n \ln [\pi p^{y_j} (1-p)^{1-y_j} + (1-\pi) q^{y_j} (1-q)^{1-y_j}]\end{aligned}\quad (37)$$

上式没有解析解，也就是没有办法直接通过求导方式解出 (π, p, q) 的值，只能使用迭代法进行求解。

3. EM算法

3.1. 为什么需要EM算法

概率模型有时候既含有观测变量又含有隐变量。如果概率模型的变量都是观测变量，那么给定数据，可以直接使用极大似然法估计或贝叶斯估计进行求解。但是，当模型含有隐变量时，就不能简单地使用这些估计方法。

EM算法就是解决含有隐变量的概率模型参数的极大似然估计。

3.2. EM算法推导

当面对含有隐变量的模型时，目标是极大化观测数据 Y 关于参数 θ 的对数似然函数，即极大化：

$$L(\theta) = \ln P(Y | \theta) = \ln \sum_Z P(Y, Z | \theta) = \ln \left(\sum_Z P(Y | Z, \theta) P(Z | \theta) \right) \quad (38)$$

注意到这一极大化的主要困难是上式中有未观测数据 Z 并有包含和（ Z 为离散型时）或者积分（ Z 为连续型时）的对数。EM算法采用的是通过迭代逐步近似极大化 $L(\theta)$ 。

假设在第 i 次迭代后 θ 的估计值是 $\theta^{(i)}$ ，我们希望新的估计值 θ 能使 $L(\theta)$ 增加，即 $L(\theta) > L(\theta^{(i)})$ 并逐步达到极大值。为此，我们考虑两者的差：

$$\begin{aligned}L(\theta) - L(\theta^{(i)}) &= \ln \left(\sum_Z P(Y | Z, \theta) P(Z | \theta) \right) - \ln P(Y | \theta^{(i)}) \\ &= \ln \left(\sum_Z P(Z | Y, \theta^{(i)}) \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)})} \right) - \ln P(Y | \theta^{(i)}) \\ &\geq \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)})} - \ln P(Y | \theta^{(i)}) \\ &= \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)})} - 1 \cdot \ln P(Y | \theta^{(i)}) \\ &= \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)})} - \sum_Z P(Z | Y, \theta^{(i)}) \cdot \ln P(Y | \theta^{(i)}) \\ &= \sum_Z P(Z | Y, \theta^{(i)}) \left(\ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)})} - \ln P(Y | \theta^{(i)}) \right) \\ &= \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)}) P(Y | \theta^{(i)})}\end{aligned}\quad (39)$$

将 $L(\theta^{(i)})$ 移项，令：

$$B(\theta, \theta^{(i)}) = L(\theta^{(i)}) + \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta) P(Z | \theta)}{P(Z | Y, \theta^{(i)}) P(Y | \theta^{(i)})} \quad (40)$$

则：

$$L(\theta) \geq B(\theta, \theta^{(i)}) \quad (41)$$

即函数 $B(\theta, \theta^{(i)})$ 是 $L(\theta)$ 的一个下界函数。

此时，若设 θ^{i+1} 使得 $B(\theta, \theta^{(i)})$ 达到极大，也就意味着：

$$B(\theta^{(i+1)}, \theta^{(i)}) \geq B(\theta^{(i)}, \theta^{(i)}) \quad (42)$$

由于：

$$\begin{aligned}B(\theta^{(i)}, \theta^{(i)}) &= L(\theta^{(i)}) + \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y | Z, \theta^{(i)}) P(Z | \theta^{(i)})}{P(Z | Y, \theta^{(i)}) P(Y | \theta^{(i)})} \\ &= L(\theta^{(i)}) + \sum_Z P(Z | Y, \theta^{(i)}) \ln \frac{P(Y, Z | \theta^{(i)})}{P(Z, Y | \theta^{(i)})} \\ &= L(\theta^{(i)})\end{aligned}\quad (43)$$

进一步可推得：

$$L(\theta^{(i+1)}) \geq B(\theta^{(i+1)}, \theta^{(i)}) \geq B(\theta^{(i)}, \theta^{(i)}) = L(\theta^{(i)}) \quad (44)$$

即：

$$L\left(\theta^{(i+1)}\right) \geq L\left(\theta^{(i)}\right) \quad (45)$$

因此，任何能使得 $B\left(\theta, \theta^{(i)}\right)$ 增大的 θ ，也可以使 $L(\theta)$ 增大。于是，问题就转化为求解能使得 $B\left(\theta, \theta^{(i)}\right)$ 到达极大的 θ^{i+1} ，即：

$$\begin{aligned} \theta^{(i+1)} &= \arg \max_{\theta} B\left(\theta, \theta^{(i)}\right) \\ &= \arg \max_{\theta} \left(L\left(\theta^{(i)}\right) + \sum_Z P\left(Z \mid Y, \theta^{(i)}\right) \ln \frac{P(Y \mid Z, \theta) P(Z \mid \theta)}{P\left(Z \mid Y, \theta^{(i)}\right) P\left(Y \mid \theta^{(i)}\right)} \right) \\ &= \arg \max_{\theta} \left(\sum_Z P\left(Z \mid Y, \theta^{(i)}\right) \ln \left(P(Y \mid Z, \theta) P(Z \mid \theta) \right) \right) \\ &= \arg \max_{\theta} \left(\sum_Z P\left(Z \mid Y, \theta^{(i)}\right) \ln P(Y, Z \mid \theta) \right) \\ &= \arg \max_{\theta} Q\left(\theta, \theta^{(i)}\right) \end{aligned} \quad (46)$$

至此，完成了EM算法的一次迭代，求出的 $\theta^{(i+1)}$ 作为下一次迭代的初始 $\theta^{(i)}$ 。

综上所述，可以总结出EM算法的“E步”和“M步”分别为：

1. E步：导出Q函数

计算完全数据的对数似然函数 $\ln P(Y, Z \mid \theta)$ 关于给定观测数据Y和当前参数 θ 下对未观测数据Z的条件概率分布 $P(Z \mid Y, \theta^{(i)})$ 的期望，也即Q函数：

$$Q\left(\theta, \theta^{(i)}\right) = E_Z \left[\ln P(Y, Z \mid \theta) \mid Y, \theta^{(i)} \right] = \sum_Z P\left(Z \mid Y, \theta^{(i)}\right) \ln P(Y, Z \mid \theta) \quad (47)$$

2. M步：Q函数极大

求使得Q函数达到极大的 $\theta^{(i+1)}$ 。

4. 使用EM求解三硬币模型

求解思路：

1. E步：导出Q函数

2. M步：求使得Q函数达到极大的 $\theta^{(i+1)} = (\pi^{(i+1)}, p^{(i+1)}, q^{(i+1)})$

4.1. E步：导出Q函数

$$\begin{aligned} Q\left(\theta \mid \theta^{(i)}\right) &= \sum_Z P\left(Z \mid Y, \theta^{(i)}\right) \ln P(Y, Z \mid \theta) \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \ln \left[\prod_{j=1}^N P\left(y_j, z_j \mid \theta\right) \right] \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \left[\sum_{j=1}^N \ln P\left(y_j, z_j \mid \theta\right) \right] \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \left[\ln P\left(y_1, z_1 \mid \theta\right) + \sum_{j=2}^N \ln P\left(y_j, z_j \mid \theta\right) \right] \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) + \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \left[\sum_{j=2}^N \ln P\left(y_j, z_j \mid \theta\right) \right] \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) \right\} + \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \left[\sum_{j=2}^N \ln P\left(y_j, z_j \mid \theta\right) \right] \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) \right\} + \\ &\quad \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_2, z_2 \mid \theta\right) \right\} + \\ &\quad \dots + \\ &\quad \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_N, z_N \mid \theta\right) \right\} \end{aligned} \quad (48)$$

单独考察 $\sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) \right\}$

$$\begin{aligned} &\sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) \right\} \\ &= \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=2}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot P\left(z_1 \mid y_1, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 \mid \theta\right) \right\} \\ &= \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P\left(z_j \mid y_j, \theta^{(i)}\right) \cdot P\left(z_1 = 1 \mid y_1, \theta^{(i)}\right) \cdot \ln P\left(y_1, z_1 = 1 \mid \theta\right) \right\} \end{aligned}$$

$$\begin{aligned}
& + \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P(z_j | y_j, \theta^{(i)}) \cdot P(z_1 = 0 | y_1, \theta^{(i)}) \cdot \ln P(y_1, z_1 = 0 | \theta) \right\} \\
& = P(z_1 = 1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 = 1 | \theta) \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P(z_j | y_j, \theta^{(i)}) \right\} \\
& \quad + P(z_1 = 0 | y_1, \theta^{(i)}) \ln P(y_1, z_1 = 0 | \theta) \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P(z_j | y_j, \theta^{(i)}) \right\} \\
& = \left[P(z_1 = 1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 = 1 | \theta) + P(z_1 = 0 | y_1, \theta^{(i)}) \ln P(y_1, z_1 = 0 | \theta) \right] \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P(z_j | y_j, \theta^{(i)}) \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \sum_{z_2, \dots, z_N} \left\{ \prod_{j=2}^N P(z_j | y_j, \theta^{(i)}) \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \left\{ \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \cdot P(z_2 = 1 | y_2, \theta^{(i)}) \right] + \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \cdot P(z_2 = 0 | y_2, \theta^{(i)}) \right] \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \left\{ P(z_2 = 1 | y_2, \theta^{(i)}) \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \right] + P(z_2 = 0 | y_2, \theta^{(i)}) \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \right] \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \left\{ \left[P(z_2 = 1 | y_2, \theta^{(i)}) + P(z_2 = 0 | y_2, \theta^{(i)}) \right] \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \right] \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \left\{ \sum_{z_2} P(z_2 | y_2, \theta^{(i)}) \sum_{z_3, \dots, z_N} \left[\prod_{j=3}^N P(z_j | y_j, \theta^{(i)}) \right] \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \left\{ \sum_{z_2} P(z_2 | y_2, \theta^{(i)}) \times \sum_{z_3} P(z_3 | y_3, \theta^{(i)}) \times \dots \times \sum_{z_N} P(z_N | y_N, \theta^{(i)}) \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \times \{1 \times 1 \times \dots \times 1\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta)
\end{aligned}$$

所以,

$$\sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P(z_j | y_j, \theta^{(i)}) \cdot \ln P(y_1, z_1 | \theta) \right\} = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) \quad (50)$$

将其带回Q函数可得:

$$\begin{aligned}
Q(\theta | \theta^{(i)}) & = \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P(z_j | y_j, \theta^{(i)}) \cdot \ln P(y_1, z_1 | \theta) \right\} + \\
& \quad \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P(z_j | y_j, \theta^{(i)}) \cdot \ln P(y_2, z_2 | \theta) \right\} + \\
& \quad \dots + \\
& \quad \sum_{z_1, z_2, \dots, z_N} \left\{ \prod_{j=1}^N P(z_j | y_j, \theta^{(i)}) \cdot \ln P(y_N, z_N | \theta) \right\} \\
& = \sum_{z_1} P(z_1 | y_1, \theta^{(i)}) \ln P(y_1, z_1 | \theta) + \dots + \sum_{z_N} P(z_N | y_N, \theta^{(i)}) \ln P(y_N, z_N | \theta) \\
& = \sum_{j=1}^N \left[\sum_{z_j} P(z_j | y_j, \theta^{(i)}) \ln P(y_j, z_j | \theta) \right] \\
& = \sum_{j=1}^N \left[P(z_j = 1 | y_j, \theta^{(i)}) \ln P(y_j, z_j = 1 | \theta) + P(z_j = 0 | y_j, \theta^{(i)}) \ln P(y_j, z_j = 0 | \theta) \right]
\end{aligned} \quad (51)$$

由于:

$$\begin{cases} P(y_j, z_j = 1 | \theta) = \pi p^{y_j} (1-p)^{1-y_j} \\ P(y_j, z_j = 0 | \theta) = (1-\pi) q^{y_j} (1-q)^{1-y_j} \\ P(z_j = 1 | y_j, \theta^{(i)}) = \frac{P(z_j=1, y_j | \theta^{(i)})}{P(y_j | \theta^{(i)})} = \frac{\pi^{(i)} [p^{(i)}]^{y_j} (1-p^{(i)})^{1-y_j}}{\pi^{(i)} [p^{(i)}]^{y_j} (1-p^{(i)})^{1-y_j} + (1-\pi^{(i)}) [q^{(i)}]^{y_j} (1-q^{(i)})^{1-y_j}} = \mu_j^{(i+1)} \\ P(z_j = 0 | y_j, \theta^{(i)}) = 1 - P(z_j = 1 | y_j, \theta^{(i)}) = (1 - \mu_j^{(i+1)}) \end{cases} \quad (52)$$

所以, Q函数的最终形式为:

$$Q(\theta | \theta^{(i)}) = \sum_{j=1}^N \left\{ \mu_j^{(i+1)} \ln [\pi p^{y_j} (1-p)^{1-y_j}] + (1 - \mu_j^{(i+1)}) \ln [(1-\pi) q^{y_j} (1-q)^{1-y_j}] \right\} \quad (53)$$

4.2. 求Q函数达到极大的参数

该步骤求使得Q函数达到极大的 $\theta^{(i+1)} = (\pi^{(i+1)}, p^{(i+1)}, q^{(i+1)})$ 。

4.2.1. 对 π 求偏导

对Q函数关于 π 求一阶偏导数，并令一阶偏导数为0：

$$\begin{aligned}
 \frac{\partial Q(\theta | \theta^{(i)})}{\partial \pi} &= \sum_{j=1}^N \frac{\partial}{\partial \pi} \left\{ \mu_j^{(i+1)} \ln [\pi p^{y_j} (1-p)^{1-y_j}] + (1 - \mu_j^{(i+1)}) \ln [(1-\pi) q^{y_j} (1-q)^{1-y_j}] \right\} \\
 &= \sum_{j=1}^N \left\{ \mu_j^{(i+1)} \frac{p^{y_j} (1-p)^{1-y_j}}{\pi p^{y_j} (1-p)^{1-y_j}} + (1 - \mu_j^{(i+1)}) \frac{-q^{y_j} (1-q)^{1-y_j}}{(1-\pi) q^{y_j} (1-q)^{1-y_j}} \right\} \\
 &= \sum_{j=1}^N \left\{ \frac{\mu_j^{(i+1)} (1-\pi) p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}}{\pi (1-\pi) p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}} + \frac{(\mu_j^{(i+1)} - 1) \pi p_j (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}}{\pi (1-\pi) p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}} \right\} \\
 &= \sum_{j=1}^N \left\{ \frac{\mu_j^{(i+1)} p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j} - \pi p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}}{\pi (1-\pi) p^{y_j} (1-p)^{1-y_j} q^{y_j} (1-q)^{1-y_j}} \right\} \\
 &= \sum_{j=1}^N \left[\frac{\mu_j^{(i+1)} - \pi}{\pi (1-\pi)} \right] \\
 &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} - \sum_{j=1}^N \pi}{\pi (1-\pi)} \\
 &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} - N\pi}{\pi (1-\pi)}
 \end{aligned} \tag{54}$$

令上式为0，可得：

$$\begin{aligned}
 \frac{\partial Q(\theta | \theta^{(i)})}{\partial \pi} &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} - N\pi}{\pi (1-\pi)} = 0 \\
 \sum_{j=1}^N \mu_j^{(i+1)} - N\pi &= 0 \\
 N\pi &= \sum_{j=1}^N \mu_j^{(i+1)} \\
 \pi &= \frac{1}{N} \sum_{j=1}^N \mu_j^{(i+1)} \Rightarrow \pi^{(i+1)} = \frac{1}{N} \sum_{j=1}^N \mu_j^{(i+1)}
 \end{aligned} \tag{55}$$

4.2.2. 对 p 求偏导

对Q函数关于 p 求一阶偏导数，并令一阶偏导数为0：

$$\begin{aligned}
 \frac{\partial Q(\theta | \theta^{(i)})}{\partial p} &= \sum_{j=1}^N \frac{\partial}{\partial p} \left\{ \mu_j^{(i+1)} \ln [\pi p^{y_j} (1-p)^{1-y_j}] + (1 - \mu_j^{(i+1)}) \ln [(1-\pi) q^{y_j} (1-q)^{1-y_j}] \right\} \\
 &= \sum_{j=1}^N \frac{\partial}{\partial p} \left\{ \mu_j^{(i+1)} \ln [\pi p^{y_j} (1-p)^{1-y_j}] \right\} \\
 &= \sum_{j=1}^N \frac{\partial}{\partial p} \left\{ \mu_j^{(i+1)} [\ln \pi + y_j \ln p + (1-y_j) \ln (1-p)] \right\} \\
 &= \sum_{j=1}^N \frac{\partial}{\partial p} \left\{ \mu_j^{(i+1)} \ln \pi + \mu_j^{(i+1)} y_j \ln p + \mu_j^{(i+1)} (1-y_j) \ln (1-p) \right\} \\
 &= \sum_{j=1}^N \frac{\partial}{\partial p} \left\{ \mu_j^{(i+1)} y_j \ln p + \mu_j^{(i+1)} (1-y_j) \ln (1-p) \right\} \\
 &= \sum_{j=1}^N \left\{ \frac{\mu_j^{(i+1)} y_j}{p} + \frac{(-1) \cdot \mu_j^{(i+1)} (1-y_j)}{(1-p)} \right\} \\
 &= \sum_{j=1}^N \frac{\mu_j^{(i+1)} y_j}{p} - \sum_{j=1}^N \frac{\mu_j^{(i+1)} (1-y_j)}{(1-p)} \\
 &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{p} - \frac{\sum_{j=1}^N \mu_j^{(i+1)} (1-y_j)}{(1-p)}
 \end{aligned} \tag{56}$$

令上式等于0可得：

$$\begin{aligned}
 \frac{\partial Q(\theta | \theta^{(i)})}{\partial p} &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{p} - \frac{\sum_{j=1}^N \mu_j^{(i+1)} (1-y_j)}{(1-p)} = 0 \\
 \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{p} &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} (1-y_j)}{(1-p)} \\
 (1-p) \sum_{j=1}^N \mu_j^{(i+1)} y_j &= p \sum_{j=1}^N \mu_j^{(i+1)} (1-y_j) \\
 \sum_{j=1}^N \mu_j^{(i+1)} y_j - p \sum_{j=1}^N \mu_j^{(i+1)} y_j &= p \sum_{j=1}^N \mu_j^{(i+1)} - p \sum_{j=1}^N \mu_j^{(i+1)} y_j \\
 \sum_{j=1}^N \mu_j^{(i+1)} y_j &= p \sum_{j=1}^N \mu_j^{(i+1)} \\
 n &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{p} \Rightarrow n^{(i+1)} = \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{p}
 \end{aligned} \tag{57}$$

$$\sum_{j=1}^N \mu_j^{(i+1)} = \sum_{j=1}^N \mu_j^{(i+1)}$$

4.2.3. 对q求偏导

对Q函数关于q求一阶偏导数，并令一阶偏导数为0：

$$\begin{aligned} \frac{\partial Q(\theta | \theta^{(i)})}{\partial q} &= \sum_{j=1}^N \frac{\partial}{\partial q} \left\{ \mu_j^{(i+1)} \ln [\pi p^{y_j} (1-p)^{1-y_j}] + (1-\mu_j^{(i+1)}) \ln [(1-\pi) q^{y_j} (1-q)^{1-y_j}] \right\} \\ &= \sum_{j=1}^N \frac{\partial}{\partial q} \left\{ (1-\mu_j^{(i+1)}) \ln [(1-\pi) q^{y_j} (1-q)^{1-y_j}] \right\} \\ &= \sum_{j=1}^N \frac{\partial}{\partial q} \left\{ (1-\mu_j^{(i+1)}) [\ln(1-\pi) + y_j \ln q + (1-y_j) \ln(1-q)] \right\} \\ &= \sum_{j=1}^N \frac{\partial}{\partial q} \left\{ (1-\mu_j^{(i+1)}) \ln(1-\pi) + (1-\mu_j^{(i+1)}) y_j \ln q + (1-\mu_j^{(i+1)}) (1-y_j) \ln(1-q) \right\} \\ &= \sum_{j=1}^N \frac{\partial}{\partial q} \left\{ (1-\mu_j^{(i+1)}) y_j \ln q + (1-\mu_j^{(i+1)}) (1-y_j) \ln(1-q) \right\} \\ &= \sum_{j=1}^N \left\{ \frac{(1-\mu_j^{(i+1)}) y_j}{q} + \frac{(-1) \cdot (1-\mu_j^{(i+1)}) (1-y_j)}{(1-q)} \right\} \\ &= \sum_{j=1}^N \frac{(1-\mu_j^{(i+1)}) y_j}{q} - \sum_{j=1}^N \frac{(1-\mu_j^{(i+1)}) (1-y_j)}{(1-q)} \\ &= \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{q} - \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j)}{(1-q)} \end{aligned} \quad (58)$$

令上式等于0可得：

$$\begin{aligned} \frac{\partial Q(\theta | \theta^{(i)})}{\partial q} &= \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{q} - \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j)}{(1-q)} = 0 \\ \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{q} &= \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j)}{(1-q)} \\ (1-q) \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j &= q \sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j) \\ \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j - q \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j &= q \sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j) - q \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j \\ \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j &= q \sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j) + q \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j \\ q &= \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{\sum_{j=1}^N (1-\mu_j^{(i+1)}) (1-y_j) + \sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j} = \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{\sum_{j=1}^N (1-\mu_j^{(i+1)})} \end{aligned} \quad (59)$$

4.2.4. 总结

综上所述，为了求Q函数的极大值，可使用如下公式进行参数迭代：

$$\begin{aligned} \pi^{(i+1)} &= \frac{1}{N} \sum_{j=1}^N \mu_j^{(i+1)} \\ p^{(i+1)} &= \frac{\sum_{j=1}^N \mu_j^{(i+1)} y_j}{\sum_{j=1}^N \mu_j^{(i+1)}} \\ q^{(i+1)} &= \frac{\sum_{j=1}^N (1-\mu_j^{(i+1)}) y_j}{\sum_{j=1}^N (1-\mu_j^{(i+1)})} \end{aligned} \quad (60)$$

5. 参考文档

1. [从最大似然到EM算法：一致的理解方式 - 科学空间|Scientific Spaces](#)
2. [\(47条消息\) EM算法之三硬币模型求解zsdust的博客-CSDN博客三硬币模型](#)
3. [人人都懂EM算法 - 知乎\(zhuhu.com\)](#)
4. [EM算法详解 - 知乎\(zhuhu.com\)](#)
5. [【机器学习】EM——期望最大（非常详细） - 知乎\(zhuhu.com\)](#)