

EM and Gradient Descent

共有 K 个 cluster 和 n 个样本点

$$k = 1 \dots K, i = 1 \dots n$$

 μ_k 和 σ_k^2 的似然函数为：

$$l(\{\mu_k, \sigma_k^2\}_{k=1}^K) = \sum_{i=1}^n \ln \left(\sum_{k=1}^K \pi_k \frac{1}{(2\pi)^{\frac{p}{2}} \cdot (\sigma_k^2)^{\frac{p}{2}}} \exp \left[-\frac{\|x_i - \mu_k\|^2}{2\sigma_k^2} \right] \right)$$

(P 为 x_i 的维度)

$$= \sum_{i=1}^n \ln \left(\sum_{k=1}^K \pi_k \frac{\exp \left(-\frac{1}{2\sigma_k^2} (x_i - \mu_k)^T (x_i - \mu_k) \right)}{(2\pi \sigma_k^2)^{p/2}} \right)$$

将 l 对 μ_k 求偏导：

$$\nabla_{\mu_k} l = \sum_{i=1}^n \frac{\pi_k \cdot N(x_i | \mu_k, \sigma_k^2 I)}{\sum_{j=1}^K \pi_j N(x_i | \mu_j, \sigma_j^2 I)} \cdot I \cdot \frac{(x_i - \mu_k)}{\sigma_k^2}$$

$$= \sum_{i=1}^n \frac{\pi_k \cdot N(x_i | \mu_k, \sigma_k^2 I)}{\sum_{j=1}^K \pi_j N(x_i | \mu_j, \sigma_j^2 I)} \cdot \frac{(x_i - \mu_k)}{\sigma_k^2}$$

↑ 这一部分正是下面 EM 算法中 E-step 的 \tilde{z}_{ik}

$$\tilde{z}_{ik} = \Pr(x_i \in \text{cluster}_i | \{\mu_j, \sigma_j^2\}_{j=1}^K, x_i)$$

$$= \frac{\pi_k \cdot N(x_i | \mu_k, \sigma_k^2 I)}{\sum_{j=1}^K \pi_j N(x_i | \mu_j, \sigma_j^2 I)}$$

$$= \sum_{i=1}^n \frac{\tilde{z}_{ik}}{\sigma_k^2} (x_i - \mu_k)$$

$$\Rightarrow \nabla_{\mu_k} l^{(t)} = \frac{1}{(\sigma_k^2)^{(t)}} \left[\sum_{i=1}^n \tilde{z}_{ik}^{(t+0.5)} x_i - \mu_k \sum_{i=1}^n \tilde{z}_{ik}^{(t+0.5)} \right]$$

$$\tilde{\pi}_k^{(t)} = \frac{(\sigma_k^2)^{(t)}}{\sum_{i=1}^n \tilde{z}_{ik}^{(t+0.5)}}$$

$$\mu_k^{(t+1)} = \mu_k^{(t)} + \tilde{\pi}_k^{(t)} \cdot \nabla_{\mu_k} l^{(t)} = \frac{\sum_{i=1}^n \tilde{z}_{ik}^{(t+0.5)} x_i}{\sum_{i=1}^n \tilde{z}_{ik}^{(t+0.5)}}$$

与 M-step 中 μ_k 相同

同理，可对 σ_k^2 求偏导

$$\nabla_{\sigma_k^2} \ell = \sum_{i=1}^n \underbrace{\left(\frac{\pi_k N(x_i | \mu_k, \sigma_k^2 I)}{\sum_{j=1}^k \pi_j N(x_i | \mu_j, \sigma_j^2 I)} \cdot \left[\frac{(x_i - \mu_k)^T I(x_i - \mu_k)}{2(\sigma_k^2)^2} - \frac{p}{2\sigma_k^2} \right] \right)}_{\uparrow \text{E-step中的 } \tilde{\pi}_{ik}}$$

$$= \sum_{i=1}^n \tilde{\pi}_{ik} \left[\frac{(x_i - \mu_k)^T I(x_i - \mu_k)}{2(\sigma_k^2)^2} - \frac{p}{2\sigma_k^2} \right]$$

$$\therefore S_k^{(t)} = \frac{2 \tilde{(\sigma_k^2)}^{(t)}}{p \cdot \sum_{i=1}^n \tilde{\pi}_{ik}^{(t+1)}}$$

$$\begin{aligned} (\sigma_k^2)^{(t+1)} &= (\sigma_k^2)^{(t)} + S_k^{(t)} \cdot \nabla_{\sigma_k^2} \ell^{(t)} \\ &= \frac{\sum_{i=1}^n \tilde{\pi}_{ik}^{(t+1)} (x_i - \mu_k)^{(t+1)T} I(x_i - \mu_k)^{(t+1)}}{p \cdot \sum_{i=1}^n \tilde{\pi}_{ik}^{(t+1)}} \end{aligned}$$

与 M-step 中 σ_k^2 相同

Mixture of multinomial Variables

1. Write down the likelihood function

$$X \sim \text{Multinomial}(\mu_1, \mu_2, \dots, \mu_N)$$

$$X = (x_1, x_2, \dots, x_N)$$

$$f(X | \mu_1, \dots, \mu_N) = \prod_{i=1}^N \mu_i^{x_i}$$

$$\text{记 } \Theta = (\mu_1, \dots, \mu_N), \mu_i = \Theta[i]$$

在混合模型中，有 K 种类别，记为 $\{1, 2, \dots, K\}$ ，
每种类别都各自有自己的参数 Θ_{class} , $\text{class} \in \{1, \dots, K\}$
引入隐变量 Y 表示 X 对应的类别， $Y \in \{1, 2, \dots, K\}$

考察样本容量为 M 的一个样本 $\bar{X} = (X_1, X_2, X_3, \dots, X_M)$ ，

对应的隐变量向量记为 $\bar{Y} = (Y_1, Y_2, Y_3, \dots, Y_M)$ ，

对应的样本参数集合记为 $\Theta_s = (\Theta_1, \Theta_2, \dots, \Theta_M)$

$$f(\bar{X} | \Theta_s) = f(X_1 | \Theta_1) \cdot f(X_2 | \Theta_2) \cdots f(X_M | \Theta_M)$$

$$= \prod_{i=1}^M f(X_{id} | \Theta_{id})$$

$$= \prod_{i=1}^M \sum_{\text{class}=1}^K \pi_{\text{class}} \prod_{\text{dim}=1}^N (\Theta_{\text{class}}^{[\text{dim}]})^{X_{id}^{[\text{dim}]}}$$

对数似然为：

$$\ell(\pi, \mu) = \ln f(\bar{X} | \pi, \mu) = \sum_{i=1}^M \ln \sum_{\text{class}=1}^K \pi_{\text{class}} \prod_{\text{dim}=1}^N (\Theta_{\text{class}}^{[\text{dim}]})^{X_{id}^{[\text{dim}]}}$$

2. Write down the Q-function

$$\ln L(\Theta_1, \Theta_2, \dots, \Theta_M | \bar{X}, \bar{Y}) = \ln P(\bar{X}, \bar{Y} | \Theta_1, \Theta_2, \dots, \Theta_M)$$

$$\text{其中: } P(\bar{X}, \bar{Y} | \Theta_s) = P_{\Theta_s}(\bar{X}, \bar{Y}) = P_{\Theta_s}(\bar{X} | \bar{Y}) P_{\Theta_s}(\bar{Y})$$

$$= \prod_{i=1}^M P_{\Theta_s} (X_{id} | Y_{id}) \cdot P_{\Theta_s} (Y_{id})$$

$$= \prod_{i=1}^M f(X_{id} | \Theta_{Y_{id}}) \cdot \pi_{Y_{id}}$$

$$= \prod_{i=1}^M \left\{ \left[\prod_{\text{dim}=1}^N (\Theta_{Y_{id}}^{[\text{dim}]})^{X_{id}^{[\text{dim}]}} \right] \cdot \pi_{Y_{id}} \right\}$$

$$\therefore \pi_s = (\pi_1, \pi_2, \dots, \pi_K)$$

$$P(Y_{id} | X_{id}, \Theta_s, \pi_s) = \frac{\pi_{y_{id}} f(X_{id} | \Theta_{y_{id}})}{\sum_{k=1}^K \pi_k f(X_{id} | \Theta_k)}$$

$$P(Y | \mathbf{X}, \Theta_s, \pi_s) = \prod_{id=1}^M \frac{\pi_{y_{id}} f(X_{id} | \Theta_{y_{id}})}{\sum_{k=1}^K \pi_k f(X_{id} | \Theta_k)}$$

$$\begin{aligned} & Q[(\Theta_s, \pi_s), (\Theta_s, \pi_s)^g] \\ &= \sum_{class=1}^K \sum_{id=1}^M \ln(\pi_{class}) P(class | X_{id}, \Theta_s^g, \pi_s^g) \\ &+ \sum_{class=1}^K \sum_{id=1}^M \ln f(X_{id} | \Theta_{class}) P(class | X_{id}, \Theta_s^g, \pi_s^g) \end{aligned}$$

3. 本小题设证, pass

4. Derive the updating rule in N -step

记 Q Function 的第一项为 A

$$A = \sum_{\text{class}=1}^K \sum_{id=1}^M \ln(\pi_{\text{class}}) P(\text{class} | X_{id}, \Theta_s^g, \pi_s^g)$$

使用拉格朗日极值法求其在 $\sum_{\text{class}=1}^K \pi_{\text{class}} = 1$ 时的条件极值

$$\frac{\partial}{\partial \pi_{\text{class}}} \{A + \lambda [\sum_{\text{class}=1}^K \pi_{\text{class}} - 1]\} = 0$$

$$\Rightarrow \sum_{id=1}^M \frac{1}{\pi_{\text{class}}} P(\text{class} | X_{id}, \Theta_s^g, \pi_s^g) + \lambda = 0$$

$$\Rightarrow \pi_{\text{class}} = \frac{1}{M} \sum_{id=1}^M P(\text{class} | X_{id}, \Theta_s^g, \pi_s^g)$$

$$= \frac{1}{M} \sum_{id=1}^M \frac{\pi_{\text{class}}^g \cdot f(X_{id} | \Theta_{\text{class}}^g)}{\sum_{k=1}^K \pi_k^g f(X_{id} | \Theta_k^g)}$$

$$= \frac{1}{M} \sum_{id=1}^M \frac{\pi_{\text{class}}^g \cdot \prod_{dim=1}^N (\Theta_{\text{class}}^g[\text{dim}])^{X_{id}[\text{dim}]}}{\sum_{k=1}^K \pi_k^g \cdot \prod_{dim=1}^N (\Theta_k^g[\text{dim}])^{X_{id}[\text{dim}]}}$$

记 Q Function 的第二项为 B

$$B = \sum_{\text{class}=1}^K \sum_{id=1}^M \ln f(X_{id} | \Theta_{\text{class}}) \cdot P(\text{class} | X_{id}, \Theta_s^g, \pi_s^g)$$

$$= \sum_{\text{class}=1}^K \sum_{id=1}^M \left(\ln \prod_{dim=1}^N (\Theta_{\text{class}}^g[\text{dim}])^{X_{id}[\text{dim}]} \right) \cdot \frac{\pi_{\text{class}}^g \cdot f(X_{id} | \Theta_{\text{class}}^g)}{\sum_{k=1}^K \pi_k^g f(X_{id} | \Theta_k^g)}$$

$$= \sum_{\text{class}=1}^K \sum_{id=1}^M \left[\sum_{dim=1}^N X_{id}[\text{dim}] \ln(\Theta_{\text{class}}^g[\text{dim}]) \right] \cdot \frac{\pi_{\text{class}}^g f(X_{id} | \Theta_{\text{class}}^g)}{\sum_{k=1}^K \pi_k^g f(X_{id} | \Theta_k^g)}$$

由多项分布性质 $\sum_{dim=1}^N X_{id}[\text{dim}] = 1$, $X_{id}[\text{dim}] \in \{0, 1\}$ 流量系数

$\therefore \exists! \dim \in \{1, \dots, N\}$, s.t. $X_{id}[\text{dim}] = 1$

因此, 让 $X_{id}[\text{dim}] = 1$ 的项对应的 $\Theta_{\text{class}}[\text{dim}] = 1$ 即可

$$\underline{\Theta_{\text{class}}[\text{dim}] = \prod (X_{id}[\text{dim}] = 1)}$$

EM Application

3.1 考察 $y^{(pr)} \sim N(\mu_p, \sigma_p^2)$ } 三者独立
 $z^{(pr)} \sim N(\nu_r, \tau_r^2)$
 $\xi^{(pr)} \sim N(0, \sigma^2)$

易知 $x^{(pr)} \sim \mu_p + \nu_r + \xi^{(pr)}$

随机向量 $(y^{(pr)}, z^{(pr)}, x^{(pr)})$ 的均值为:

$$(\mu_p, \nu_r, \mu_p + \nu_r)$$

协方差矩阵为:

$$\begin{bmatrix} \sigma_p^2 & 0 & \sigma_p^2 \\ 0 & \tau_r^2 & \tau_r^2 \\ \sigma_p^2 & \tau_r^2 & \sigma_p^2 + \tau_r^2 + \sigma^2 \end{bmatrix}$$

(2) $X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$

$$x_1/x_2 \sim N(\mu_1 + \Sigma_{12} \Sigma_{22}^{-1}(\mu_2 - \mu_1), \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21})$$

Q函数有如下形式:

$$Q_p(y^{(pr)}, z^{(pr)}) = P(y^{(pr)}, z^{(pr)} | x^{(pr)})$$

$$= N\left([\mu_p, \nu_r] + \frac{x^{(pr)} - (\mu_p + \nu_r)}{\sigma_p^2 + \tau_r^2 + \sigma^2} [\sigma_p^2, \tau_r^2], \frac{\sigma_p^2}{\sigma_p^2 + \tau_r^2 + \sigma^2} \right)$$

3.2 极大化 Q函数可推得:

$$(y_{(t+1)}^{(pr)}, z_{(t+1)}^{(pr)}) = (\mu_p^{(t)}, \nu_r^{(t)}) + \frac{[(\sigma_p^2)^{(t)}, (\tau_r^2)^{(t)}] (x^{(pr)} - \mu_p^{(t)} - \nu_r^{(t)})}{(\sigma_p^2)^{(t)} + (\tau_r^2)^{(t)} + \sigma^2}$$

$$\mu_p^{(t+1)} = \frac{1}{R} \sum_{r=1}^R y_{(t+1)}^{(pr)}$$

$$\nu_r^{(t+1)} = \frac{1}{P} \sum_{p=1}^P z_{(t+1)}^{(pr)}$$

$$(\sigma_p^2)^{(t+1)} = \frac{1}{R} \sum_{r=1}^R (y_{(t+1)}^{(pr)} - \mu_p^{(t+1)})^2$$

$$(\tau_r^2)^{(t+1)} = \frac{1}{P} \sum_{p=1}^P (z_{(t+1)}^{(pr)} - \nu_r^{(t+1)})^2$$