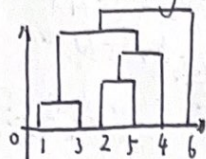


清华大学

L12 聚类分析 1. Hierarchical

Agglomerative 自下而上.

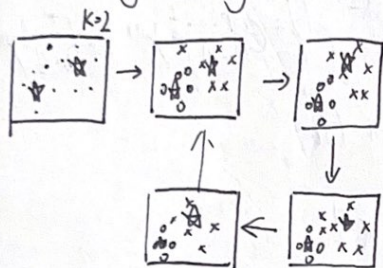
距离 { 欧式
single (min): 对形状敏感
complete (max): 不易受异常值影响
Group Average
Ward's linkage (SSE)



X方向上坐标无要求
Y方向上高低一定严格不同.

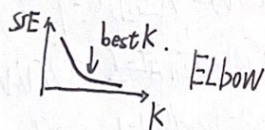
不足: 计算复杂度太高, 不能纠错.

2. Partitioning Clustering (K-Means)



Picking K:

$$① SSE = \sum_{i=1}^K \sum_{x \in C_i} \text{dist}^2(x, \mu_i)$$



② Empirical $K \approx \sqrt{n}$

③ Cross validation.

L11 LDA 判别分析.

Fisher Approach: Assumption $\bar{Z}_1 = \bar{Z}_2$

$$\max_{\vec{\alpha}} \frac{(\vec{\alpha}^T (\bar{x}_1 - \bar{x}_2))^2}{\vec{\alpha}^T S_{\text{pooled}} \vec{\alpha}} \quad \hat{\alpha} = S_{\text{pooled}}^{-1} \vec{d} \quad \vec{d} = \bar{x}_1 - \bar{x}_2$$

$$S_{\text{pooled}} = \frac{(n_1 - 1)S_1 + (n_2 - 1)S_2}{n_1 + n_2 - 2} \quad y = \hat{\alpha}^T \vec{x}$$

$$\text{maximum } D^2 = (\bar{x}_1 - \bar{x}_2)^T S_{\text{pooled}}^{-1} (\bar{x}_1 - \bar{x}_2)$$

ECM方法: p_1, p_2 为 π_1, π_2 先验概率, 需知 f_1, f_2 先验分布, 以及代价.

$$\begin{aligned} ECM &\triangleq C(2|1) P(x \in R_1, x \in R_2) + C(1|2) P(x \in R_2, x \in R_1) \\ &= C(2|1) p_1 + \int_{R_1} [C(1|2) p_2 f_2(x) - C(2|1) p_1 f_1(x)] dx \text{ 求 min} \\ \Rightarrow R_1 &= \{x: \frac{C(1|2) p_2}{C(2|1) p_1} < \frac{f_1(x)}{f_2(x)}\} \quad R_2 = R_1^c \end{aligned}$$

正态分布下的结论

$$\bar{z}_1 = \bar{z}_2 \quad f_i(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_i)^T \Sigma^{-1} (x - \mu_i) \right\}$$

$$R_1: (\mu_1 - \mu_2)^T \Sigma^{-1} x - \frac{1}{2} (\mu_1 - \mu_2)^T \Sigma^{-1} (\mu_1 + \mu_2) \geq \ln \left[\frac{C(1|2) p_2}{C(2|1) p_1} \right]$$

$$\text{sample} \Rightarrow (\mu_1, \mu_2)^T S_{\text{pooled}}^{-1} x - \frac{1}{2} (\bar{x}_1 - \bar{x}_2)^T S_{\text{pooled}}^{-1} (\bar{x}_1 + \bar{x}_2) \geq \ln \left[\frac{C(1|2) p_2}{C(2|1) p_1} \right]$$

$$\text{if } \frac{C(1|2) p_2}{C(2|1) p_1} = 1 \Rightarrow \hat{y} \geq \frac{1}{2} (\hat{y}_1 + \hat{y}_2) \Rightarrow \text{LDA}$$

$\bar{z}_1 \neq \bar{z}_2$ QDA.

$$R_1: -\frac{1}{2} x^T (\bar{z}_1^{-1} - \bar{z}_2^{-1}) x + (\bar{z}_1^T \bar{z}_1^{-1} - \bar{z}_2^T \bar{z}_2^{-1}) x - k \geq \ln \left[\frac{C(1|2) p_2}{C(2|1) p_1} \right]$$

APER: Confusion matrix

	predicted membership		
Actual membership	π_1	π_2	
	n_{1c}	n_{1m}	n_1
	π_2	π_1	
	n_{2m}	n_{2c}	n_2

$$\text{APER} = \frac{n_{1m} + n_{2m}}{n_1 + n_2}$$

Cross validation: 样本均分为m份, 每份中用其他样本作为训练集, 以验证.

L8-9 因子分析.

$$\psi = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_p \end{bmatrix}$$

$$X - \mu = L F + \Sigma \quad E(F) = 0 \quad E(\Sigma F) = 0 \quad \text{Cov } F = I_{m \times m} \quad \text{Cov } (\Sigma) = \psi_{p \times p}$$

PCA法

$$\text{Cov}(\Sigma, F) = 0_{p \times m}$$

$$S = \underbrace{L L^T}_{p \times m} + \underbrace{\hat{\psi}}_{p \times p} \quad \hat{L} = [\hat{\lambda}_1 e_1, \dots, \hat{\lambda}_m e_m]$$

special variance: $S - \hat{L} \hat{L}^T$

$$\hat{\lambda}_1^2 + \dots + \hat{\lambda}_p^2 = \hat{\lambda}_i$$

$$\text{proportion} \quad \frac{\hat{\lambda}_1^2 + \dots + \hat{\lambda}_m^2}{\text{tr}(S)}$$

MLE法:

$$L(u, \Sigma) = (2\pi)^{-\frac{(n-1)p}{2}} |\Sigma|^{-\frac{(n-1)}{2}} \exp \left\{ -\frac{1}{2} \text{tr} \left[\Sigma^{-1} \left(\sum_{j=1}^n (\bar{x}_j - \bar{x})(\bar{x}_j - \bar{x})^T \right) \right] \right\}$$

$$+ \frac{1}{2} \sum_{j=1}^n (\bar{x}_j - \bar{x})^T \Sigma^{-1} (\bar{x}_j - \bar{x})$$

假设: common factors 和 specific factors 都是正态的

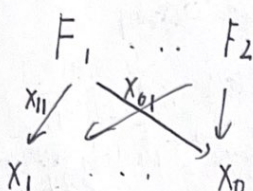
$$F \sim N(0, I) \quad \varepsilon \sim N_p(0, \Psi) \quad F \perp \varepsilon$$

common factors

$$\hat{h}_i^2 = \hat{L}_{i1}^2 + \dots + \hat{L}_{ip}^2 \quad \text{for } i=1, 2, \dots, p \quad \text{公共方差}$$

$$\psi_i = G_{ii} - \hat{h}_i^2 \quad \text{特殊方差}$$

$$\bar{Z} = \begin{bmatrix} \hat{L}_{11} \\ \vdots \\ \hat{L}_{ip} \end{bmatrix} = \begin{bmatrix} \hat{L}_{11}^T \\ \vdots \\ \hat{L}_{ip}^T \end{bmatrix} \begin{bmatrix} \hat{L}_{11} \\ \vdots \\ \hat{L}_{ip} \end{bmatrix} + \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_p \end{bmatrix}$$



(Proportion of total sample variance due to j-th factor) = $\frac{\hat{L}_{1j}^2 + \hat{L}_{2j}^2 + \dots + \hat{L}_{pj}^2}{S_{11} + \dots + S_{pp}}$ 因子比例

$$\hat{h}_i^2 = \hat{L}_{i1}^2 + \hat{L}_{i2}^2 + \dots + \hat{L}_{ip}^2$$

$$\Sigma = E[(X - W)(X - W)^T] = E[(LF + \varepsilon)(LF + \varepsilon)^T]$$

$$= E[LF F^T L^T + L F \varepsilon^T + \varepsilon \varepsilon^T L^T + \varepsilon \varepsilon^T]$$

$$= L E(F F^T) L^T + E(\varepsilon \varepsilon^T) = L I L^T + \Psi = L L^T + \Psi$$

$$\hat{L}^* = V^{\frac{1}{2}} \hat{L}_Z \quad \hat{\Psi}^* = V^{\frac{1}{2}} \hat{\Psi}_Z V^{\frac{1}{2}} \quad V = \text{diag}(\hat{\Sigma}) = \text{diag}(G_{ii})$$

V 即正则化项

两种做法优劣: PC: 随 m 增大计算方便

MLE: 相关数与协方差之间联系可直接转化

选择更合适的: 看可解释性

因子个数限制 $m < p$

Fisher Approach

目标: $\frac{\bar{y}_1 - \bar{y}_2}{S_y} \quad S_y^2 = \frac{\sum (y_i - \bar{y})^2}{n + n_2 - 2}$

优化: $\max_a \frac{(\bar{y}_1 - \bar{y}_2)^2}{S_y^2}$

$$\hat{y} = \hat{a}^T X = (\bar{x}_1 - \bar{x}_2)^T \text{Spooled } X \quad \text{s.t.} \quad \max_a \frac{(a^T (\bar{x}_1 - \bar{x}_2))^2}{a^T \text{Spooled } a}$$

典型相关分析:

$$X^{(1)} = \begin{bmatrix} X_1^{(1)} \\ \vdots \\ X_p^{(1)} \end{bmatrix} \quad X^{(2)} = \begin{bmatrix} X_1^{(2)} \\ \vdots \\ X_q^{(2)} \end{bmatrix} \quad \bar{Z} = \begin{bmatrix} \bar{Z}_{11} & \bar{Z}_{12} \\ \bar{Z}_{21} & \bar{Z}_{22} \end{bmatrix}$$

目标: 找到最佳 a, b s.t. $\text{corr}(U, V)$ 最大 $U = a^T X^{(1)}$

$$\Rightarrow \max_{a, b \neq 0} \frac{a^T \bar{Z}_{12} b}{\sqrt{a^T \bar{Z}_{11} a} \sqrt{b^T \bar{Z}_{22} b}} = \max \frac{a^T \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}} \bar{Z}_{22}^{\frac{1}{2}} b}{\sqrt{a^T \bar{Z}_{11} a} \sqrt{b^T b}} = \max \frac{a^T \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}} \bar{Z}_{22}^{\frac{1}{2}} b}{|a| |b|}$$

对 $\bar{Z}_{11}^{-\frac{1}{2}} \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}}$ 作奇异值分解 \Rightarrow 求 $\bar{Z}_{11}^{-\frac{1}{2}} \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}}$ 的特征值

第 i 个特征值为 ρ_i^2 $U = e_i^T \bar{Z}_{11}^{-\frac{1}{2}} X^{(1)}$ $V = \bar{Z}_{22}^{-\frac{1}{2}} X^{(2)}$

$$f_i = \frac{1}{\rho_i^2} \bar{Z}_{22}^{-\frac{1}{2}} \bar{Z}_{21} \bar{Z}_{11}^{-\frac{1}{2}} e_i$$

$$U = A X^{(1)} \quad V = B X^{(2)}$$

$$\text{Cov}(U, V) = A \bar{Z}_{12} B^T = \begin{bmatrix} \rho_1^2 & & \\ & \ddots & \\ & & \rho_p^2 \end{bmatrix}$$

$$\text{Cov}(U, U) = A \bar{Z}_{11} A^T = I \quad \text{Cov}(U, V) = B \bar{Z}_{22} B^T = I$$

$$\text{Var}(U_k) = \text{Var}(V_k) = 1 \quad \text{Cov}(U_k, V_l) = \text{corr}(U_k, V_l) = 0 \quad k \neq l$$

$$\text{Cov}(U_k, V_k) = \text{corr}(U_k, V_k) = 0 \quad k \neq 0$$

$$\text{corr}(U, X^{(1)}) = A \bar{Z}_{11}^{-\frac{1}{2}}$$

$$\text{corr}(U, X^{(2)}) = A \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}}$$

$$\text{corr}(V, X^{(1)}) = B \bar{Z}_{21} \bar{Z}_{11}^{-\frac{1}{2}}$$

$$\text{corr}(V, X^{(2)}) = B \bar{Z}_{22}^{-\frac{1}{2}}$$

$$\text{Cov}(U, X^{(1)}) = \text{Cov}(A X^{(1)}, X^{(1)}) = A \bar{Z}_{11}$$

$$\text{Cov}(U, X^{(2)}) = \text{Cov}(U, V \bar{Z}_{22}^{\frac{1}{2}} X^{(2)}) = A \bar{Z}_{12} \bar{Z}_{22}^{-\frac{1}{2}}$$

$$V_{11} = \text{diag}(\bar{Z}_{11})$$

标准化不会影响结果

从几何上看, 标准化后 $X^{(1)}, X^{(2)}$ 张成空间不变, $\therefore U, V$ 也不变