

$X \sim N(\mu, \Sigma)$  ← 3种形式.

$\phi(ct) = e^{it^T \mu - \frac{1}{2} t^T \Sigma t}$  ( $\varphi(ct) = e^{it\mu - \frac{1}{2} t^2 \sigma^2}$ )

$(X = AU + \mu)$   $AA^T = \Sigma$  ( $A = Q\Lambda = \sqrt{\Sigma}$ )

$U \stackrel{i.i.d.}{\sim} N(0, \sigma^2 I)$ .

marginal  $X_{r \times r} \sim N(\mu_r, \Sigma_{r \times r})$

$f(x) = \frac{1}{(\sqrt{2\pi})^p \sqrt{|\Sigma|}} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)}$  ( $U \rightarrow X$  证)

conditional  $X = \begin{pmatrix} X^1 \\ X^2 \end{pmatrix}_{p \times 1} \sim N(\mu, \Sigma)$  ( $\Sigma$  正定 (非退化) 或  $\Lambda, \Sigma$  非奇异)

(请见)  $(X^1 | X^2) \sim N_r(\mu_{1|2}, \Sigma_{1|2})$   $\rightarrow \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$  条件协方差阵  $\Sigma_{1|2}$

$\mu_{1|2} = \mu^1 + \Sigma_{12} \Sigma_{22}^{-1} (X^2 - \mu^2)$

$X^1$  对  $X^2$  回归 回归系数.

$E(X^1 | X^2)$  为对  $X^1$  最佳 (Variance) 预报.

$Z = \begin{pmatrix} X \\ Y \end{pmatrix}_{p+1} \sim N_{p+1} \left( \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix} \right)$

$Y \leftarrow X$  得  $\Sigma_{yx} \Sigma_{xx}^{-1}$  回归.

$R = \text{Corr}(Y, \Sigma_{yx} \Sigma_{xx}^{-1} X) = \frac{\Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{xy}}{\sigma_{yy}}$  全(复)相关系数

$\text{Vec}(\mu^T) = f \otimes \mu$

矩阵正态分布  $X \sim N_{n \times p}(\mu, I_n \otimes \Sigma)$ ,  $\mu = \mu^T$

$\begin{pmatrix} X_{n1} \\ \vdots \\ X_{np} \end{pmatrix}_{n \times p} Z = AXB^T + D, Z \sim N_{k \times q}(AMB^T, (AA^T) \otimes (B \Sigma B^T))$

estimation:  $\bar{x} = \frac{1}{n} X^T \mathbf{1}_n$   $X_{(i)}$  为第  $i$  个样品 ( $i=1, \dots, n$ ).

$S = \frac{1}{n-1} \sum_i (X_{(i)} - \bar{x})(X_{(i)} - \bar{x})^T = \frac{X^T X - n \bar{x} \bar{x}^T}{n-1} = X^T (I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T) X$

MLE  $\hat{\mu} = \bar{x}, \hat{\Sigma} = \frac{1}{n} A^{-1} A$  (求导/似然式)

(Q) 中心轴定理  $A \approx \sum_{i=1}^p Z_i Z_i^T, Z \stackrel{i.i.d.}{\sim} N(0, \Sigma)$   $\rightarrow \text{Cov}(Z_i, Z_j) = E(X^T \mathbf{e}_i \mathbf{e}_j^T X) = \delta_{ij} \Sigma$

$\bar{X} \sim N_p(\mu, \frac{1}{n} \Sigma), \bar{x} \text{ i.i.d.}$

$P(A > 0) = 1 \Leftrightarrow n > p. \leftarrow A = BB^T, B = (Z_1 \dots Z_{n-1})$

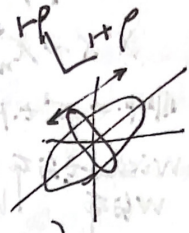
无/有秩, 相合, 充分...

$I(\mu) = \int \frac{\partial^2 f}{\partial \mu^2} dx = \int f dx \cdot (\Sigma^{-1} (x-\mu)^T)$

$(n \Sigma^{-1})^{-1} = \frac{\Sigma}{n} = \Sigma^{-1}$

(Q)  $I(\Sigma)?$

$\rightarrow E((x-\mu)(x-\mu)^T (x-\mu)(x-\mu)^T)$



$(A \Sigma B^T = 0)$  时  $AX$  与  $BX$  id.  $\Leftrightarrow BA=0$

$XAX$  与  $XBX$  id.  $\Leftrightarrow AB=BA=0.$

$\frac{\sigma_{ij} \cdot \sigma_{11} \dots \sigma_{11}}{\sqrt{\sigma_{11} \dots \sigma_{11} \dots \sigma_{11}}}$  偏相关系数

条件协方差阵  $\Sigma_{1|2}$

$(\Sigma_{12} = \Sigma_{21}^T)$

$\begin{pmatrix} I & -I \\ -\Sigma_{yx} \Sigma_{xx}^{-1} & 0 \end{pmatrix} \begin{pmatrix} \Sigma_{yx} \\ 0 \end{pmatrix} \begin{pmatrix} I \\ -\Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{xy} \end{pmatrix}$

$\mu_y - \Sigma_{yx} \Sigma_{xx}^{-1} \mu_x$

$\begin{pmatrix} \Sigma_{yx} \Sigma_{xx}^{-1} \\ I \end{pmatrix}$

$\begin{pmatrix} \Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{xy} \\ \Sigma_{yx} \Sigma_{yy} \end{pmatrix} \begin{pmatrix} \Sigma_{yy}^{-1} \Sigma_{xy} \\ I \end{pmatrix}$

$\Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{xy}$

$\Sigma_{yx} \Sigma_{xx}^{-1} \Sigma_{yy}$

$\Delta$  取迹 (变换顺序, 算E...) 的方法.

\* 各分布形状参数:  $\mu, \Sigma, \dots$

test: 1.  $X \sim N(\mu, I_n)$ ,  $\delta = \mu'\mu$ .

$X'X \sim \chi^2_{\delta}$

非中心  $\chi^2$  t.F 分布  $\rightarrow$  第2类 一般 错误

2. Wishart W 分布

$W = X'X$   $p=1$  时  $W \sim \sigma^2 \chi^2_n$   
 $W \sim W_p(n, \Sigma)$   
 $(X \sim N_p(\mu, \Sigma))$   
 $W = \sum_{i=1}^n X_i X_i'$  ( $W = \sum_{i=1}^n X_i^2$ )  
 $p \times p$

$X \sim N(0, \sigma^2 I)$   $A \text{ sym, } r(A)=r$

$X'AX \sim \sigma^2 \chi^2_r \Leftrightarrow A^2=A$  ( $\text{rank} \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 0 \end{pmatrix} = r$ )

$X \sim N(\mu, \Sigma)$ ,  $\Sigma > 0$ .

$X'\Sigma^{-1}X \sim \chi^2_{p, \delta}$ ,  $\delta = \mu'\Sigma^{-1}\mu$

$(X-\mu)'A(X-\mu) \sim \chi^2_r \Leftrightarrow A\Sigma A = A$

$(X-\mu)'A(X-\mu)$  与  $(X-\mu)'B(X-\mu)$  id.  $\Leftrightarrow A\Sigma B = 0$

$X \sim N_{np}$ ,  $X'AX$  与  $X'BX$  id. ( $A, B$  idempotent)  $\Leftrightarrow AB = 0$

$W_n(\sigma^2) = \sigma^2 \chi^2_n$

非中心 W:  $X \sim N_p(\mu, \Sigma)$ ,  $M = \mu\mu'$   $X_i \sim N_p(\mu_i, \Sigma)$ ,  $\delta = \mu'\mu$ ,  $M = \begin{pmatrix} \mu_1' \\ \vdots \\ \mu_n' \end{pmatrix}$   
 $W_p(n, \Sigma, \Delta)$ ,  $\Delta = M'M = n\mu\mu'$

$X \sim N_p(\mu, \Sigma)$ ,  $A \sim W_p(n-1, \Sigma)$   
 $(= \sum_{i=1}^{n-1} Z_i Z_i')$   $W_{n-1}(\Sigma)$

$X \sim N_{np}(\mu, I_n \otimes \Sigma)$ ,  $A \text{ sym, } r(A)=r$

$X'AX \sim W_p(\Sigma, \Delta)$ ,  $\Delta = M'M$  ( $\Leftrightarrow A^2=A$ )

$n$  可加,  $CWC' \sim W_n(C\Sigma C')$ ,  $E(W) = n\Sigma$

$(\sqrt{\Sigma} \otimes X = Y)$

对相乘边缘  $W_{ij} \sim \sigma_{ij}^2 \chi^2_n$

$aW \sim W_n(a\Sigma)$

$v'Wv \sim \chi^2_n(v'\Sigma v)$

特征 func:

$\phi_{\chi^2_n}(t) = (1-2it)^{-\frac{n}{2}}$

$\phi_{W_n}(t) = E(e^{i \text{tr}(Wt)}) = |I - 2it\Sigma|^{-\frac{n}{2}}$   
 $|W|^{-\frac{n-1}{2}} e^{-\text{tr}(\frac{\Sigma^{-1}W}{\lambda})}$

$f_{W_n}(w) = \frac{1}{2^{\frac{np}{2}} |\Sigma|^{\frac{n}{2}} \Gamma_p(\frac{n}{2})}$

3. Hotelling  $T^2 = nX'WX$  ( $X$  分  $\Sigma^{-1}X$  即  $T$ )

$T^2$  分布

与  $\Sigma$  无关 (对非退化变换不变)

$T^2 \sim T^2_{n,p}(\varphi)$  ( $X \sim N_p(\mu, \Sigma)$ ,  $W \sim W_n(\Sigma)$ ,  $\Sigma > 0$ ,  $n > p$ )

非中心  $\rightarrow T^2: X \sim N_p(\mu, \Sigma)$ ,  $T^2_{n,p}(\mu)$

$X_i \sim N_p(\mu, \Sigma)$

$T^2 = (n-1) \cdot n \cdot (\bar{X}-\mu)'A^{-1}(\bar{X}-\mu) \sim T^2_{n-1, p} = \frac{p}{n-p} (n-1) F_{p, n-p}$

$\frac{n-p+1}{np} T^2_{n,p} \sim F_{p, n-p+1}$

$n \rightarrow \infty$  时

$T^2_{n,p} \sim \chi^2_p$

$p=1, -\frac{1}{n} t^2 \sim F_{1, n}$

$T^2 = \frac{X'W^{-1}X}{p} = \frac{X'\Sigma^{-1}X}{p} \sim \chi^2_p(\delta=0) \checkmark$

$\frac{X'\Sigma^{-1}X}{X'W^{-1}X} \sim F_{p, n-p+1}$

$\frac{X'\Sigma^{-1}X}{X'W^{-1}X} \sim \chi^2_{n-p+1}$

$T^2 = (\bar{X}-\mu)'n\Sigma^{-1}(\bar{X}-\mu)$   
 $= Y'Y \sim \chi^2_p$

(F 分布. 也可:  $\chi^2_p$ )  
 $\frac{\chi^2_p}{n} \rightarrow 1$   
 仍然是  $\lambda \sim \chi^2$   
 似然比  $\lambda \sim \chi^2$

4. Wilks  $\Lambda$  分布

$f$  次方差  $|\Sigma|, |\mu_{n-1}|$

$A_1 \sim W_{n_1}(\Sigma), A_2 \sim W_{n_2}(\Sigma)$

$\Lambda = \frac{|A_1|}{|A_1+A_2|} \sim \Lambda_{n_1, n_2}(\varphi) = \frac{|W_{n_1}(\Sigma)|}{|W_{n_1+n_2}(\Sigma)|}$

$\Lambda_{n_1, n_2}(\varphi) = \beta(\frac{n_1}{2}, \frac{n_2}{2})$

$\Lambda_{n_1, p}(\varphi) = \frac{1}{1 + \frac{1}{n} T^2_{n,p}}$  ( $T^2_{n,p}(\varphi) = n \cdot \frac{1 - \Lambda_{n_1, p}(\varphi)}{\Lambda_{n_1, p}(\varphi)}$ )

$|W| = |W_1 + X_{n+1}' X_{n+1}| = |W_1 - X|$

$n_1 \rightarrow \infty$  时  $\Lambda \sim \chi^2_{pn_2}$   $= |W|(1 + X'_{n+1} W_1^{-1} X_{n+1})$

$\Lambda = \prod_{i=1}^p B_i$ ,  $B_i \sim \beta(\frac{n_1-p+i}{2}, \frac{n_2}{2})$

方差分解可对应  $\lambda$

仍然是  $\lambda \sim \chi^2$

$\alpha_2(\varphi) \Lambda_{n_1, n_2}(\varphi) = \Lambda_{p, n_1+n_2-p}$

1. Weistein - Aronszajn Idem.

$\det(I_m + AB) = \det(I_n + BA)$

推论:

$|I + c\bar{u}\bar{u}'| = |I + c\bar{u}'A^{-1}\bar{u}|$

$n_2 = 1/2$  时  $\Lambda$  可化为 F.  
 $p=1$  时  $\Lambda$  即  $\beta$  eta.

2.  $\lambda, A > 0$ .  $\lambda'AX \leq \lambda \Leftrightarrow XX' \leq \lambda A^{-1}$  then.

one-sample test:

均采用 LRT.

$\Sigma_0 \vee \sqrt{n}(\bar{x} - \mu) \sim N_p(0, \Sigma_0)$

$H_0$  时  $T_0^2 = n(\bar{x} - \mu_0)' \Sigma_0^{-1}(\bar{x} - \mu_0) \sim \chi_p^2$ .  $R = \{T_0^2 > \chi_p^2(\alpha)\}$  / P-值

$\Sigma \times A \sim W_{n-1}(\Sigma)$

( $\beta$ :  $T_0^2 \sim \chi_p^2(\delta)$ ,  $\delta = n(\mu_1 - \mu_0)' \Sigma_0^{-1}(\mu_1 - \mu_0)$ )

$H_0$  时  $T^2 = n(n-1)(\bar{x} - \mu_0)' A^{-1}(\bar{x} - \mu_0) \sim T_{n-1}^2(p)$

$\beta = P\{T_0^2 \leq \chi_p^2(\alpha)\}$

$F = \frac{n-p}{(n-1)p} T^2 \sim F_{p, n-p}$

LR E:  $H_0: \theta \in \Theta_0, H_1: \theta \notin \Theta_0, \Theta_0 \subset \Theta$

$\lambda = \frac{\max_{\theta \in \Theta_0} L(x; \theta)}{\max_{\theta \in \Theta} L(x; \theta)}$

$P(\lambda(x_1, \dots, x_n) < \lambda_0) = \alpha$

λ分布? 近似:  $n \rightarrow \infty$  时  $-2 \ln \lambda \sim \chi_p^2$  其中  $f = \dim \Theta - \dim \Theta_0$

N-P lemma.  $(\rightarrow$  UMVUE)

MLE:  $\max_{\mu, \Sigma > 0} L(\mu, \Sigma) = (2\pi)^{-\frac{np}{2}} e^{-\frac{np}{2}} | \frac{1}{n} A |^{-\frac{n}{2}} \lambda = \frac{|A_0|^{-\frac{n}{2}}}{|A|^{-\frac{n}{2}}} = \left( \frac{|A|}{|A_0|} \right)^{\frac{n}{2}} = \left( 1 + \frac{1}{n-1} T^2 \right)^{\frac{n}{2}}$

$R = \{T^2 > T^2(\alpha)\}$

confidence interval:

$\{F > F(\alpha)\}$

$A_0 = A + n(\bar{x} - \mu_0)(\bar{x} - \mu_0)'$   
 $|A_0| = |A| (1 + n(\bar{x} - \mu_0)' A^{-1}(\bar{x} - \mu_0))$

$T^2 = n(\bar{x} - \mu)' S^{-1}(\bar{x} - \mu) \leq \frac{(n-1)p}{n-p} F_{p, n-p}(\alpha) = \frac{n-p}{p} \frac{T^2}{n-1}$

μ 位于  $\bar{x}$  中的椭圆 (置信域) 内.

μ 的线性组合  $Z = a'X \sim N(a'\mu, a'Sa)$

$t = \frac{\sqrt{n}(a'\bar{x} - a'\mu)}{\sqrt{a'Sa}}$

$a'\mu \in a'\bar{x} \pm t \frac{\sqrt{a'Sa}}{\sqrt{n}}$  (单) 置信区间

推广到  $\text{ineq. } S > 0$ , Schafke:

$(a'b)^2 \leq (a'Sa)(b'S^{-1}b)$

$t^2 = n \frac{(a'\bar{x} - a'\mu)^2}{a'Sa} \leq t_{\frac{\alpha}{2}}^2$  换为  $\max t^2 = n(\bar{x} - \mu)' S^{-1}(\bar{x} - \mu) = T^2 \sim F$



(联合) 置信区间

$\forall a, a'\mu \in a'\bar{x} \pm \sqrt{\frac{(n-1)p}{n(n-p)} F_{p, n-p}(\alpha) a'Sa}$  比  $t_{\alpha} = C \cdot S^{-1}(\bar{x} - \mu)$

$\mu_i \in \bar{x}_i \pm \sqrt{\frac{(n-1)p}{n-p} F_{p, n-p}(\alpha) \frac{S_{ii}}{n}}$

multi-sample test:

(等  $\Sigma$ ) 双正态  $T^2 = \frac{nm}{n+m} (\bar{x} - \bar{y})' \left( \frac{A_x + A_y}{n+m-2} \right)^{-1} (\bar{x} - \bar{y})$

多总体均值检验:

(ANOVA) 多组 T = A + B

( $\Sigma$  一致下) 组内组间

$\Lambda = \frac{|A|}{|T|} \sim \Lambda(p)$   $\Sigma_i A_i$   $\tilde{W}_{n-k}(\varphi, \Sigma)$

2 组:

B id. A 且  $W_{p(k-1), \Sigma}$

$H_0 \sim T_{n+m-2}^2(p) = F_{p, n+m-p-1}$  (Wishart 可加性)

△ 回归直线的范围:

(单)  $T^2 = (\beta - \hat{\beta})' (X'X)^{-1} (\beta - \hat{\beta})$   $\beta_i$  需  $\pm$  改大 T.

$m(\alpha) \in \hat{\gamma}(x) \pm \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_x}}$   $(\max \frac{(x'(\hat{\beta} - \beta))^2}{\hat{\sigma}^2 \alpha' (X'X)^{-1} \alpha})$  T(α)

( $\downarrow$  LRE:  $\frac{\max \dots}{\max \dots}$ )

或  $R = \left( \frac{|A|}{|T|} \right)^{\frac{n}{2}}$  (αED.)

有  $\alpha'\beta \in \alpha'\hat{\beta} \pm T(\alpha) \cdot \hat{\sigma} \sqrt{\alpha' (X'X)^{-1} \alpha}$

(k=2 时与  $T^2$  检验一致)  $A = \sum A_i, |A|$

LR test  $\chi^2$  proof:  $L: H_0: \theta = \theta_0, H_1: \theta \neq \theta_0$

GLLR loglike  $\Lambda(\chi) = -2 \ln \lambda = 2(\ln(\hat{\theta}) - \ln(\theta_0))$

Taylor  $l(\theta_0) = l(\hat{\theta}) + (\hat{\theta} - \theta_0) l'(\hat{\theta}) + \frac{1}{2} (\hat{\theta} - \theta_0)^2 l''(\hat{\theta}) + \dots$

$\Lambda(\chi) = -(\hat{\theta} - \theta_0)^2 l''(\hat{\theta}) = +(\hat{\theta} - \theta_0)^2 I_{\theta\theta} \cdot \frac{-l'(\hat{\theta})}{I_{\theta\theta}}$

MLE is 弱相合:  $(\hat{\theta} - \theta_0) \sqrt{I_{\theta\theta}} \xrightarrow{P} N(0, 1)$

LLN (大数定律):  $\frac{-l'(\theta_0)}{I_{\theta\theta}} \xrightarrow{P} 1$

(Slutsky Th)  $\Lambda(\chi) \xrightarrow{P} \chi^2$

$\theta$  多元时有  $p$  个  $\chi^2$  相加.  $\leftarrow ? (\hat{\theta}_1 - \theta_{10}) (\hat{\theta}_2 - \theta_{20})$  独立?

Wilks' Th.

asymptotic dis. of the likelihood

ratio statistic:  $i=1, \dots, p$

$\Omega_0 \ni \theta_0$  (ii)  $A(\theta - \theta_0) = 0$  (iii)  $g_i(\theta) = 0$

$\theta = (\theta_1, \dots, \theta_k) \downarrow d.$   $p \times k$  mt.  $\downarrow d.$   $\chi_p^2$   $\chi_p^2$

Then  $2 \log \frac{L_n(\hat{\theta}_n)}{L_n(\theta_0)} \xrightarrow{d} \chi_k^2$   $p = \dim \Omega - \dim \Omega_0$

(if there are some  $\theta_1, \dots, \theta_p$  remains to be estimated  $\rightarrow$  the same.  $\Omega_0 \uparrow$  dim.)

$\chi^2$  (and  $\sqrt{\ln 2}$ ) 检验:

(Q 方法中)  $H_0: \pi_i, \dim(H_0) = 0$

$\hat{p}_i$  即 MLE.

$\Lambda = 2n \sum_i \hat{p}_i \ln \frac{\hat{p}_i}{\pi_i}$  Taylor  $\rightarrow 2n \cdot \frac{\sum_i (Y_i - n\pi_i)^2}{2n\pi_i} = \sum_i \frac{(Y_i - n\pi_i)^2}{n\pi_i}$

( $n \rightarrow \infty$  时  $\hat{p}_i \xrightarrow{P} \pi_i$ )

MLE:

与 Wilks Th. 一致.

( $\lambda \in [1]$ )

$H_0: \varphi; 1-P$  引理, 两类错误, 一致最优

依然地检验 (LRT) 与传统参数检验 (NP 理论) 的一致性?

$L(\mu, \Sigma) = \frac{1}{(2\pi)^{\frac{np}{2}}} \frac{1}{|\Sigma|^{\frac{n}{2}}} e^{-\frac{1}{2} \sum_i (X_i - \mu)' \Sigma^{-1} (X_i - \mu)}$

cov test:

1.  $H_0: \Sigma = I_p$  球形检验.  $\lambda = \dots$

2.  $H_0: \Sigma_0$   $Y = \sum_0 \frac{1}{\lambda} X$  变为 1,

3.  $H_0: \sigma^2 \Sigma_0$   $\Lambda_Y = \sum_0 \frac{1}{\sigma^2} \Lambda \Sigma_0 \frac{1}{\sigma^2}$

$\sigma^2$  待估:  $\hat{\sigma}^2 = \frac{1}{np} \text{tr}(\sum_0 A)$

$\ln L(\mu, \Sigma) = -\frac{np}{2} \ln 2\pi - \frac{n}{2} \ln |\Sigma| - \frac{1}{2} \text{tr}(\Sigma^{-1} \sum_i (X_i - \mu)(X_i - \mu)')$

$L(\hat{\mu}, \hat{\Sigma}) = L(\bar{X}, \frac{1}{n} A) = \left(\frac{n}{2\pi e}\right)^{\frac{np}{2}} |A|^{-\frac{n}{2}} \cdot \frac{1}{n} \sum_i (X_i - \bar{X})(X_i - \bar{X})'$

$\sim \chi^2 \left(\frac{p(p+1)}{2}\right)$

$\sim \chi^2 \left(\frac{p(p+1)}{2} - 1\right)$

多总体方差检验

$\max L(\mu^1, \dots, \mu^k, \Sigma^1, \dots, \Sigma^k)$

$\sim \chi^2 \frac{p(p+1)(k-1)}{2}$

independence test:

normality test:  $\chi^2$  test

(非参数检验)

K-S test  $D = \sup_x |F_n(x) - F_0(x)|$

偏峰. (JB test)

Wilks. D test

Q-Q/P-P  $\leftarrow \chi^2$  图

36 原则

( $A^2, W^2$  统计量)

edf:  $X_1 \leq \dots \leq X_n$

$F_n(x) = \frac{k}{n} (X_n \leq x \leq X_{k+1})$

$F_n(x) = 0 (x \leq X_1) / 1 (x \geq X_n)$

- 符号: Wilcoxon
- 符号: Cochran Q
- 游程

① 分布不正, 非正态 ② 等级/分类数据

对某性质(假设)检验.

分布特性

$P \rightarrow 1$  无

生成  $\chi^2$  图

Bayes  $\rightarrow$

参数检验: 基于对总体的假设, 对参数进行统计推断

① 正态分布

② 样本量化且独立

③ 均值与方差存在, 方差相等...

(目未知)

挑选: 分布; 样本大小; 等方差; 偏度; 待检量

△ 回归条件

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$x_1$  对  $x_2$  回归 (被  $x_2$  回归掉)

$R^2 \sim F?$

复相关系数  $(Y)$   $r(Y, \hat{Y}) = \frac{\sum yx \sum xx^{-1} \sum xy}{\sqrt{\sum y^2 \sum yx^2}}$

$R^2 = \frac{SSR}{SST}$  F 或开根 t.

偏相关系数 ( $x_2 \rightarrow x_1$  后剩余的方差)

偏回归显著性 (F) 检验:  $r_{ij} \dots$

逐步回归法  $SSR_{k-1} - R_{k-1} = \beta^T (X^T X)^{-1} \beta$

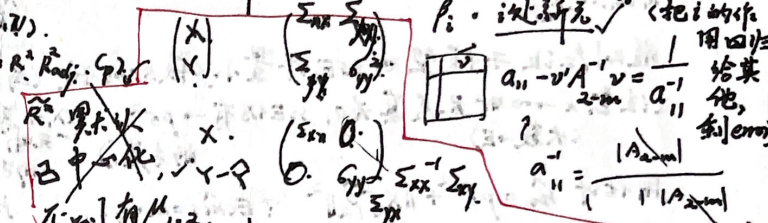
全子集法 ( $2^k - 1$ )

最优回归方程 (变量选择): (STEPWISE)

准则:

1.  $\sum d_i^2$  (SSE)  $\downarrow$   $R = \sqrt{\frac{SSR}{SST}}$   $\uparrow$   
 2.  $\hat{\sigma} = \sqrt{\frac{SSE}{n-k-1}}$   $\downarrow$

MIN/MAXR 增量法

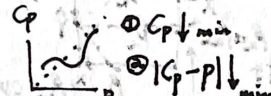


pre: 固定 k, SSE 对子集 ACK.

$S^2_{CK} = S^2_{CA} = \frac{SSE_{CK}}{n-k-1} \downarrow \min.$

② 选模型  $p = k+1$

全(回归)模型  $C_p = \frac{SSE_{CK}}{S^2} + 2p - n$



③  $\tilde{R}^2 = 1 - (1-R^2) \frac{n-1}{n-k-1}$

Overfitting.

$D_p = \hat{\sigma}^2 (n+k+1)$   
 $S_p = \frac{\hat{\sigma}^2}{n-k-2}$

选  $\lambda$  且  $n$  大 时  $EC_p$  评. Akaike Bayesian info criterion  $L = (2\pi)^{-\frac{n}{2}} \frac{1}{\sqrt{|SSE|}} e^{-\frac{n}{2}}$

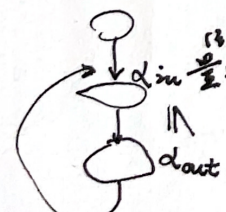
PRESS.

$AIC = 2k - 2 \ln L = 2k + n \ln \frac{SSE}{n}$

k 为参数个数 (每个  $\beta_j$  的)

SBC:  $2 \rightarrow \ln n$ .  $\ln n k + n \ln \frac{SSE}{n}$

BIC:  $2 \rightarrow \ln n$ .  $\ln n k + n \ln \frac{SSE}{n}$



只有其他是解释 (即  $\Delta R^2$ )  $\Delta R^2$   $\{ \max \lambda$

$R^2_{k+1} = \frac{SSR_{k+1}}{SST}$   $R^2_{k-1} = \frac{SSR_{k-1}}{SST}$

$R^2_k - R^2_{k-1} = \dots$

$\beta_1 = \begin{pmatrix} (X_1^T X_1)^{-1} X_1^T Y \\ 0 \end{pmatrix}$

$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} : \begin{pmatrix} \sum_{11} & \sum_{12} \\ \sum_{21} & \sum_{22} \end{pmatrix}$

$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} : \begin{pmatrix} \sum_{11} & 0 \\ 0 & \sum_{22} \end{pmatrix} \sum_{11}^{-1} \sum_{12}$

$\hat{y} = \sum_{j=1}^k \hat{\beta}_j X_j$   
 $\hat{y} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \end{pmatrix}$   
 $\hat{y} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \end{pmatrix}$   
 $\hat{y} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \end{pmatrix}$

k-S test:

$D_n = \sup_x |F_n(x) - F_0(x)|$

$D = \max (|F_n(x_i) - F_0(x_i)|, |F_n(x_i) - F_0(x_{i-1})|)$

$n \rightarrow \infty, \sqrt{n} D_n \rightarrow \sup_t |B(F(t))|$  Kolmogorov 分布.

Brownian bridge  $B(t) = W(t) - \frac{t}{T} W(T)$   $t \in [0, T]$

Wiener process  $W(t) \sim N(0, \sigma^2 t)$   $W(t) | W(T) = 0$

$f_{W(t)}(x) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}}$

证明: 消除  $\beta_1$  的干扰

$\beta_1 = \begin{pmatrix} \beta_{11} \\ \beta_{12} \end{pmatrix}$

$\beta_1 = \begin{pmatrix} \beta_{11} \\ \beta_{12} \end{pmatrix}$

△ Cp Criterion & Mallows's Cp =

子模型 (X<sub>1</sub>) 回归后剩

$$E(CHY - X\beta) = (H-I)X\beta = (H-I)(X_1\beta_1 + X_2\beta_2)$$

$$= -(I-H)X_2\beta_2$$

平方误差  $V(CHY - X\beta) = V(CHY) = \sigma^2 H \cdot \sigma^2$

总SSE =  $p\sigma^2 + \|X_2^\perp \beta_2\|^2 = m$

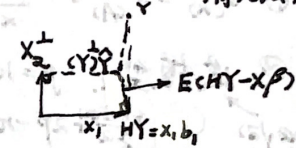
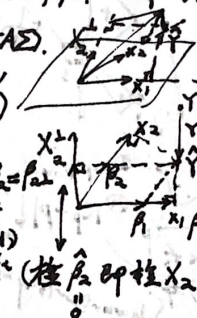
准则应让子模型的SSE尽量小。(较好的子) (与正交化 (值确实 (X<sub>1</sub>) 单独带有 1 即 β<sub>1</sub>, (注意 n → ∞ 时且 β<sub>2</sub> 真为 0, SSE 仍有 → pσ<sup>2</sup> (X<sub>1</sub> 为等同但 偏回归 (X<sub>2</sub>) 时无需带 1.) (大数 → E) 的方差) 无时) (H) 投影更 (hat mt: 用它 (X) 去估什么 (Y) 就来什么 (HY) 广的理解) 得到回归估计值)

用估计  $\hat{m} = p\sigma^2 + \|X_2^\perp \beta_2\|^2$  ? E(m̂) = m 吗?

σ<sup>2</sup> → σ<sup>2</sup> √. β<sub>2</sub> → β<sub>2</sub> √. E(CX) = μ 时通常 (f(x) ≠ f(y)) (注意 X = ((1) X<sub>1</sub> X<sub>2</sub>). 横着的 向量是 X<sub>1</sub> X<sub>2</sub>) 消无法为左乘.

考虑  $E(\|X_2^\perp \beta_2\|^2) = \beta_2' X_2^\perp X_2^\perp \beta_2 + \text{tr}(X_2^\perp X_2^\perp \sigma^2)$

$\beta \sim N(\beta, \sigma^2 (X'X)^{-1}) = \|X_2^\perp \beta_2\|^2 + \text{tr}(I_{m-k}) \sigma^2$



故无偏估计

$\hat{m} = \|X_2^\perp \beta_2\|^2 + 2p\sigma^2 - (m+1)\sigma^2$

子模型 SSE<sub>k</sub> - 全模型 SSE<sub>m</sub> =  $\|X_2^\perp \beta_2\|^2$

$\hat{m} = SSE_k + 2p\sigma^2 - n\sigma^2$

(标化)  $\hat{C}_p = \frac{\hat{m}}{\sigma^2} = \frac{SSE_k}{\sigma^2} + 2p - n$  → 子模型尽量 min 的预测误差.

Cp min 或 |Cp - p| min.

(BIC 基于 Bayes 框架)

△ AIC: K-L 距离度量预测误差:

真 y ~ g(y) 候选模型 f(y; θ).

$\hat{f}$  与 g 距离  $K(g, \hat{f}) = \int g \log(\frac{g}{\hat{f}}) \geq 0$

$K_{min} = \max(\int g \log f(y; \hat{\theta}) dy)$

$E(\frac{1}{n} \sum \log f(y_i; \hat{\theta})) = K(\hat{\theta})$

$E(\frac{1}{n} \sum \log f(y_i; \hat{\theta})) = E(K(\hat{\theta})) + \frac{k}{n} + o(1)$

用  $\bar{K} - \frac{k}{n} \rightarrow K(\hat{\theta})$

AIC =  $-2n \cdot (\bar{K} - \frac{k}{n}) = 2k - 2 \log L(\hat{\theta}) \rightarrow K(\hat{\theta})_{min}$  即 K-L min.

多元回归:  $Y = X\beta + E$

$n(y_1, \dots, y_p) = X(\beta_1, \dots, \beta_p) + (e_1, \dots, e_p)$

$\vec{Y} = (1' \otimes X)\vec{\beta} + \vec{E}$

$E_{(i)} = (E_{i1}, \dots, E_{ip}) \sim N(0, \Sigma)$

SSE =  $\sum_{ij} E_{ij}^2 = \vec{E}'\vec{E} = (\vec{Y} - X\hat{\beta})'(\vec{Y} - X\hat{\beta})$   $\min(\partial\hat{\beta}=0)$  (最小二乘法) estimation and the nature of the estimator.  
 残差平方和 投影(正规)方程(组)  $X'X\hat{\beta} = X'Y$

残差阵  $R = (Y - \hat{Y})'(Y - \hat{Y}) = Y'(I - H)Y$   $X'X(\beta_1, \dots, \beta_p) = X'(Y_1, \dots, Y_p)$

$\Sigma = \frac{R}{n-k-1}$   $(Y_1'(I-H)Y_1, \dots, Y_p'(I-H)Y_p)$  每行  $\sum Y_i - \sum Y_i X_i^{-1} \sum X_i Y_i$  同前所述.

(无k的 $\beta_k$ 的第i个分量)  $E(Y_i'(I-H)Y_i) = (n-m-1)\sigma^2$

若多对一列  $R = R_{ii}$ , (复)  $R = \sqrt{1 - R_{ii}}$  (SSE)  $(Y_i)_{ii}$

$Cov(\hat{\beta}_{ik}, \hat{\beta}_{jl}) = \sigma_{kl}^2 (X'X)^{-1}_{ij}$   $Y_i \sim N(X\beta_i, \sigma^2 I_n)$  (OLS估计, 定理, 取协)

则  $Cov(\hat{\beta}_i, \hat{\beta}_j) = \sigma_{ij}^2 (X'X)^{-1}$  技巧:  $e_i'(X'X)^{-1}X'Ee_k$

$Cov(\hat{\beta}_{(i)}, \hat{\beta}_{(j)}) = (X'X)^{-1} \sum (X'X)^{-1}_{ij} e_i e_j'$  用单位向量表示出元.

有  $\hat{\beta} \sim N_{mt}$ ,  $R \sim W_{n-k-1}(\Sigma)$ ,  $\hat{\beta}$  与  $R$  id. (独立)

$\hat{\beta}_i \sim N(\beta_i, \sigma_{ii}^2 (X'X)^{-1})$

$R = Y'(I-H)Y$   
 $\hat{\beta}'X'X\hat{\beta} = Y'HY$

(注:  $A = \alpha\alpha'$ ,  $\Lambda = \begin{pmatrix} \sigma^2 & & \\ & \dots & \\ & & \sigma^2 \end{pmatrix}$ )  
 $\Delta$  二次型独立 (A, B sym.):  $B\alpha = (0 \ \Delta) \dots$   
 $X'AX$  id.  $X'BX \iff AB=0$   $Y'Y$  与  $Y'QBQ'Y$  ...  
 (BA取')  
 hypo. test. of significance

$\beta_{(1)}, \beta_{(2)}, \dots, \beta_{(m_1)}, \beta_{(m_1+1)}, \dots, \beta_{(m_1+m_2)} = k$

$H_0: B_2 = 0$

细  $H_0: \beta_{(i)} = 0_p$   $\hat{\beta}_{(i)} / \hat{\sigma}_{ii} \sim N(0, \Sigma)$

$H_0$  对  $T^2 = (n-k-1) \hat{\beta}_{(i)}' R^{-1} \hat{\beta}_{(i)} / \hat{\sigma}_{ii} \sim T^2_{n-k-1}$

$R_1 - R = -Y'(H - H_1)Y = +Y(I - H_1)K(I - H_1)Y \sim W_{m_2}(\Sigma)$

(拆解H出  $H_1, H_2$ )  $K = X_2(X_2'(I - H_1)X_2)^{-1}X_2'$  的交互项  $V_i = \frac{\hat{\beta}_{(i)}' R^{-1} \hat{\beta}_{(i)}}{\hat{\sigma}_{ii}}$   $cp=1$  时  $V_i = \frac{\hat{\beta}_{(i)}^2}{\hat{\sigma}_{ii} \cdot SSE} = \frac{PSSR}{SSE}$  (SSR)

$H_1 = HH_1 = H_1H$  (理解)

$(I-H)(H-H_1) = 0$  则  $R_1 - R$  id. R. 欲求LRS:

$L = \omega \sqrt{\frac{p}{2}} |\Sigma|^{-\frac{n}{2}} e$   
 $\max_{\beta, \Sigma} L$  时  $\beta = \hat{\beta}$ ,  $\Sigma = \frac{1}{n}R$

$\lambda = \left(\frac{|R_1|}{|R|}\right)^{-\frac{n}{2}} = \left(\frac{|R|}{|R + (R_1 - R)|}\right)^{-\frac{n}{2}}$

$H_0$  对  $\Lambda \rightarrow 1$ .

单  $m_2=1$  时  $\Lambda = \frac{1}{1 + \frac{T^2}{n-k-1}}$   $Pvalue = P(\Lambda \leq \Lambda_{\alpha k}) \geq \alpha$

$\frac{n-k-p-1}{p} \frac{1-\Lambda}{\Lambda} = F_{p, n-k-p}$  (Wilks' Lambda)

多多下的 STEPREG:

变量  $u$  (外部) 对  $p$  个  $Y$  贡献  $V_u = u'(I-H)u \cdot \hat{\beta}_{(u)} \otimes \hat{\beta}_{(u)}$  原  $m$  个自变量,  $\alpha$  为残差  $R$  (阵) (未算  $\beta_0/Y$ ) 后  $(m+1)$  个.

$u = \begin{pmatrix} u_1 \\ \vdots \\ u_m \end{pmatrix}$

LR 有  $1 - V_u \rightarrow \Lambda$  ( $T^2 = u'(I-H)u \hat{\beta}_{(u)} \otimes \hat{\beta}_{(u)} = \frac{u'(I-H)u \hat{\beta}_{(u)} \otimes \hat{\beta}_{(u)}}{1 - u'(I-H)u \hat{\beta}_{(u)} \otimes \hat{\beta}_{(u)}}$ )  
 (1 =  $\frac{1}{1 + \frac{T^2}{n-m-2}}$ ) (Morrisson Formula)  $(n-m-2)$

(此处  $\beta_{(i)}$  上  $\beta_{(i)}$ )

$\beta_{(u)}$  的显著度/残差或的贡献量  $\frac{n-m-p-1}{p} \frac{V_i}{1-V_i} \rightarrow F_{(n-m-2)} \frac{V_i}{1-V_i} \rightarrow T^2$  (1) (2) 两种推导路径, (3) 为延伸

$(R_1 - R) = \hat{\beta}_{(u)}' u'(I-H)u \hat{\beta}_{(u)}$   $\Lambda$  去  $cp$   $\frac{|\alpha u|}{|\alpha u + W|} \geq \frac{|\alpha - \hat{\beta}_{(u)}' u'(I-H)u \hat{\beta}_{(u)}|}{|\alpha|} = 1 - V_i$

$p=1$  时  $\Delta SSR_i$

$p \geq 1$  时  $V_i (\frac{\Delta SSR_i}{SSE})$   
of  $K$  的

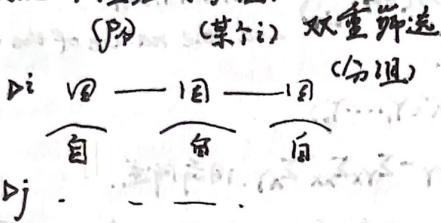
直接采取消元  $m$   $P$   
初相:  $L^{(0)} = \begin{pmatrix} XX & XY \\ YX & YY \end{pmatrix}^m$

(消去变换)

是  $\alpha_x$  (in=out),  $\alpha_y$ .

① 标准化/中心化, Cov 阵  $L$

最优方程组与方程:



DOUBLE STEPWISE 具体步骤?  $V_i / \min/\max V_i$ ; F 检验, 剔/引

$1 = \frac{|R|}{|Y|}$  (↓, 线性↑)

则  $\frac{1_i}{1} < 1 - \frac{1_i}{1}$ ,  $Y_i$  越显著

② 继续或转入自/因

③ 结果:  $Y \dots = X \dots \beta \dots + E$   
a.  $R \rightarrow \alpha$   $R = \sqrt{1 - \lambda}$   
b.  $t$  test.  $(X^2) = \sqrt{1 - \lambda}$   
c.  $(1 - \frac{1_i}{1}) \frac{1_i}{1} - 1$  做 F 检验

用绝对值公式把多出的一元扔出来,  $\frac{1_i}{1} - 1$  即  $V_i$  (Y 对 X 回归)

两模型等价. 若  $Y_i$  进入

$\Delta$  sweep. 消去变换/扫描算法:

STEPREG 重建:

- Wilks 定理
- $\frac{1_i}{1} \sim 1$  证明

Handwritten mathematical derivations and notes covering matrix algebra, regression theory, and statistical tests. Includes formulas for matrix inversion, determinant relationships, and statistical significance tests.



判别分析(归集):  $(dim) G_1, \dots, G_k, F_i(x) \checkmark, X \xrightarrow{new} F_i(G_i)$

overfitting 

1. 马氏距离  $d^2 = (X-\mu)^T \Sigma^{-1} (X-\mu)$

样本估计  $\mu_i, \Sigma_i$

(例) (5-集)

(66的判别) 各个G球性时为阿波罗尼斯球(判别)

$d_i^2(x) = \min d_i^2(x)$  则  $X \in G_i$

判别准则

0. 两总体同方差假设: 合并样本协方差阵  $S = \frac{1}{n_1+n_2-2} \sum_{i=1}^2 (X-\bar{X})(X-\bar{X})^T$

线性判别函数  $W(x) = d_2^2(x) - d_1^2(x) = 2(X - \frac{\bar{x}_1 + \bar{x}_2}{2})^T S^{-1} (\bar{x}_1 - \bar{x}_2)$

(划分)

2. Bayes 判别

先验  $G_i - \rho_i$  (历史: 样品  $\frac{n_i}{n}$ ; 同一)

LOOCV / k-fold CV

判别矩阵  $C_{ij}$

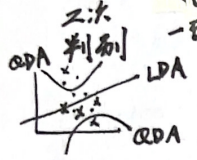
$P(1|2) = P(2|1)$

(7次平均) 判别 DISCRIM. esp. 综合效率最大

$P(j|i; D) = \int \rho_j(x) dx$

判别损失  $L(j|i)$

故  $\mu_1 \neq \mu_2$  显著时才有意义,  $d_{12}^2 = (\bar{x}_1 - \bar{x}_2)^T S^{-1} (\bar{x}_1 - \bar{x}_2)$



$\ln \rho_i - \frac{1}{2} \ln |S_i| - \frac{1}{2} d_i^2(x)$

平均  $LCD = \sum_i \rho_i \sum_j P(j|i) L(j|i)$

$e_i$  的判为  $j$  的损失

即  $D_i^* = d_i^2 + \ln |S_i| - 2 \ln \rho_i$  最小

Bayes Discrim. Solution:  $LCD^* = \min LCD$

$D_i^* = \{X | h_i(x) < h_j(x), j \neq i\}$  其中  $h_i(x) = \sum_j \rho_j f_j(x) L(j|i)$

3. Fisher 判别

(投影判别)  $W(X) = l^T X$

当  $L(j|i) = 1 - d_{ij}$  时,  $D_i^* = \{X | \rho_i f_i(x) > \rho_j f_j(x), j \neq i\}$

判别效率  $\frac{l^T B l}{l^T A l} = \Delta(l)$  判别效率 max.

$l = \lambda_i$ 's eigenvector,  $|A| = 1$   $\Delta$   $k=2$  时投影与距离等价于距离判别

准则 I:  $\lambda_1 (C^T A^{-1} B)$

$\lambda_i = (A^{-1} B)$ 's eigenvalue

$W(X) = \frac{1}{\sqrt{\lambda_1}} A^{-1} (\bar{x}_1 - \bar{x}_2)$  ( $A^{-1}$  与  $S^{-1}$  仅差倍数)  $(d^2 = \text{常数} = \sqrt{(\bar{x}_1 - \bar{x}_2)^T A^{-1} (\bar{x}_1 - \bar{x}_2)})$

再距离判别:  $u_j(x) = l_j^T X, \bar{u}_j(x) = l_j^T \bar{x}_j$

准则 II: 取  $l \propto r, P = \frac{r^T (x_1 - x_2)}{\|r\|} < 1$  ( $\xi = 0.7$ )

化为(无条件)距离判别 (1个不相关)

$\min_j \frac{|u_j(x) - \bar{u}_j|}{\sigma_j} = \min(\dots)$  则  $X \in G_j$

其中  $\sigma_j^2 = l_j^T S_j l_j$  ( $\frac{1}{n_j-1} l_j^T A_j l_j$ )

判别推论:

若有多个  $\lambda$ , 则序贯使用  $\lambda_1, \lambda_2$  再判

1. 判别效果 test:  $\mu_i = \mu_j, \dots$  若  $\sqrt{n}$  则无意义

( $\Sigma$  协方差矩阵)  $\Lambda = \frac{|\Lambda|}{|T|} \sim \Lambda^{(n-k)}$

逐步判别 STEPPWISE  $\Delta$  STEPDISC 重述

2. 判别能力 test: 变量  $H_0: \mu_{ih} = \mu_{jh}, \dots$  (仅  $2$  元时亦即  $(T^2) d^2 \sim F$ )

聚类分析: 系统聚类法, 动态聚类法, 有序聚类法

(均) 均值是否有显著差异

模糊 ~ 图论 ~ 聚类预报

R型聚类, Q型聚类

距离: Minkowski  $d_{ij}(p) = (\sum_k |x_{ik} - x_{jk}|^p)^{1/p}$

Lance  $d_{ij}(L) = \frac{1}{m} \sum_{t=1}^m |x_{it} - x_{jt}|$

Mahalanobis  $d_{ij}(M) = \sqrt{(x_i - x_j)^T S^{-1} (x_i - x_j)}$  ( $S$  使用全部样品计算效果  $X$ , 使用各类  $S_k X$ )

斜交空间距离  $d_{ij} = (\frac{1}{m^2} \sum_{k=1}^m \sum_{l=1}^m (x_{ik} - x_{jk})(x_{il} - x_{jl}) r_{kl})^{1/2}$ ,  $r_{kl}$  为  $\text{Corr}(X_k, X_l)$

相似系数:  $\cos d_{ij} = \frac{\sum_{k=1}^m x_{ik} x_{jk}}{\sqrt{\sum_{k=1}^m x_{ik}^2} \sqrt{\sum_{k=1}^m x_{jk}^2}}$

$\rho_{ij} = \frac{\sum (x_{i1} - \bar{x}_1)(x_{j1} - \bar{x}_1)}{\sqrt{\sum (x_{i1} - \bar{x}_1)^2} \sqrt{\sum (x_{j1} - \bar{x}_1)^2}}$

定性变量:  $d_{ij} = \frac{m_2}{m_1 m_2}$  或  $= \sum_{ij} (\delta_{ij} - d_{ij})^2 \dots$

系统聚类法:

$G_1, \dots, G_t$   
 $t=n$  开始  $\rightarrow$  计算类间距  $D_{ij}$   $\rightarrow$  合并最小两类  $\rightarrow G_1(t=1)$   $\rightarrow$  画谱系图, 各折点取类数

min; max; median; centroid; average; flexible average; MQR;  
 Ward  $\rightarrow$  类间平方和  $D_{pq}^2 = W_p + W_q - (W_p + W_q)^2 / (n_p + n_q)$  (欧氏  $d^2$  时  $\frac{n_p n_q}{n_p + n_q} (\bar{X}_p - \bar{X}_q)^2$ )  
 $d$  centroid

单调性: median  $X$ , centroid  $X$  (空间) 浓缩/扩张性  
 类的定义:  $\leq \text{Threshold}$   $\forall a, b$  划为两类,  $D(G_a, G_b) \leq T$   
 $\forall i, j, d_{ij} \leq T$

类的个数:

适当的  $d_0$ ; 散布图; 统计量:  $R_k^2 = 1 - \frac{P_k}{T} = \frac{B_k}{T}$   
 $DR_k^2 = R_{k+1}^2 - R_k^2$  (某步)  
 $\text{psudo } F = \frac{B}{P} \frac{n-k}{k-1} \times F$   
 $\text{psudo } t^2 = \frac{B_{kl}^2}{W_k + W_l}$  (某步, 合并  $k$  和  $l$ )  
 $\frac{B_{kl}^2}{N_k + N_l - 2}$  (某步)  
 $(B_{kl}^2 = W_{k+l} - W_k - W_l)$

动态聚类法:

初始分类  $\leftarrow$  凝聚点  
 挑选: (大致随  $k$ )  
 1. 人选 2. 重心 3. 密度 (形心) (画圈)  
 4. 均值图 5. 随机  $X$

分批修改:  
 a. min condensation point  $\rightarrow$  group  
 b. centroid as cond. point:  $\rightarrow$  mind  $d_i$   
 $\Rightarrow \sum W_i$  组内离差 min (Ward 的系统聚类一致) 每个修改 (k-means):  
 (证明: 此时随便更改一个都将增大  $W$ )  
 走  $k, \text{min, max}$  (first round) 前  $k$  个作 cond. p. (或其他方式)

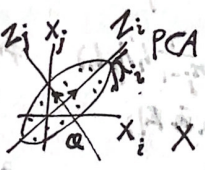
有序聚类法:

类直径 (类差和)  $D(i, j) = \sum (x_i - x_j)(x_i - x_j)$   
 最优分割法 (Fisher 算法)  
 $L(P, k) \leftarrow$  递推  $\min(L' + D)$   
 $D_{c(i, j)}$   $L(P, k)$  括  $k$  取用

exam.  $i, j \in O$   
 $d_{ij} \geq \text{Min.}$  否则合并取 means (centroid)  
 $\text{intro. } h \in O$   
 $d_{ih} \leq \text{Max.}$  归于最近点, 取 means (centroid)  
 否则  $> \text{Max}$  新成一点.  
 无 Min, Max 时: (分批) (取  $k$ )  $\rightarrow$  划入 min 中 重算  $k$  centroid

PCA 分类: (标化, 取  $R$ )

变量距离  $\|X_i - X_j\|^2 = \sum_{k=1}^m (x_{ik} - x_{jk})^2 \rightarrow \text{VARCLUS}$   
 因子载荷散布图 (此处  $l$  即  $P$ )  $(l_{i1}, \dots, l_{im})$  (样本 PCA 即  $\Sigma \rightarrow S = \frac{1}{n-1} X'X$  或标化后为  $R$ )  
 样品距离  $\|X_{ci} - X_{cj}\|^2 = \sum_{k=1}^m (x_{ck} - x_{jk})^2$  (也叫主成分得分)



PCA:  $Z = \alpha X$   
 $L = \alpha \Lambda (\alpha' \alpha)^{-1}$   
 $\lambda_1, \dots, \lambda_m$   $\text{tr } D (= \text{tr } \Sigma)$   
 $\Sigma = LL'$   
 $\Lambda = L'L$   
 $\text{Cov}(X, Z) = \alpha \Lambda$   
 $P(X, Z) = \frac{L}{\sqrt{D}} \cdot \frac{\text{Cov}(X, Z)}{\sqrt{\Lambda D}}$   
 $D = \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_m^2 \end{pmatrix}$   
 (行/列元素平方和  $\sum_i \sum_j l_{ij}^2$ )  
 (标化后  $\sigma_i^2 = 1$  即  $\text{tr } R = p$ )  
 $\Sigma = R, L = P \Lambda Z$   
 负荷  $L: l_{ij}$  为  $X_i$  分量 (的离差) 在主成分方向  $J$  上的长度 (投影)  
 $\Delta$  女子!

排序估计指数  $Z_i$

3. 排序估计指数  $Z_i$  (可加权  $X_i$ )  
 4. normality test.  $Z_i \sim Z_m$  无关, 作一元正态性.

$X_{n \times p} = Z_{n \times m} \alpha'_{m \times p} + E$  即 OLS 系数 (残差 min)  
 $(\text{复}) R^2 = \frac{\sum_{k=1}^m l_{ik}^2}{\sigma_i^2}$  (相对于上述定义的  $\alpha$  是重要)  
 $\text{SSR}_i = \alpha_i' (Z'Z)^{-1} \alpha_i$   
 $\Lambda_m$   
 解释难度 (逆变换回)

$Y \sim X \beta_X$   
 $\downarrow$   
 $Y \sim Z \alpha \beta_Z$   $\leftarrow$  有偏估计!

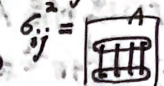
因子分析: 因子模型  $X_i = \sum_{k=1}^m a_{ik} F_k + \epsilon_i$

Q型使用样品相似下降, 寻找提炼样品的因子

简化结构 (变量/样品) 分类  
因子负荷 (m对上) (特殊因子)  
公共因子 (源)

正交因子模型  $X = \mu + AF + \epsilon$

A为loading mat.  $\Sigma = AA' + D$ .  $(F, \epsilon) \sim N(0, \begin{pmatrix} I & 0 \\ 0 & D \end{pmatrix})$



$\sigma_{ij}^2 = \sum_{k=1}^m a_{ik}^2 + \epsilon_i^2$

$F, \forall i=1, \dots, m$   
 $a_{ij} = \text{Cov}(X_i, F_j)$

因子得分: 估计  $F_{(i)}$ .  $X = AF + \epsilon$

Bartlett — 加权最小二乘 (WLS)  
min  $\epsilon'D\epsilon$ .  $\hat{F} = (A'D^{-1}A)^{-1}A'D^{-1}X$   
( $D = V(\epsilon)$ )



(或  $L_{max}$ .  $L = -\frac{1}{2} \epsilon'D^{-1}\epsilon - \frac{1}{2} \ln |2\pi D|$ )

$\hat{F}$ 与主成分得分差一倍数 =  $\frac{\sum_{ij} x_{ij}^2}{\sum_{ij} a_{ij}^2}$

Thompson — 回归 (主成分) 解常不加权

$F = BX$   
 $n \times n$   $n \times p$   $p \times n$  (因子得分函数)

由载荷阵估计B:  $A = E(XF')$

$B = A\Sigma^{-1} = \Sigma B'$

$\hat{F} = A'\Sigma^{-1}X$  ← Bayes思想

(常三代S或R)

右验分布的均值 (先验:  $(X, F) \sim N(0, \begin{pmatrix} \Sigma & A \\ A' & I \end{pmatrix})$ )  
 $E(F - A'\Sigma^{-1}X) = 0$

△比较:  $F_B = (A'D^{-1}A)^{-1}A'D^{-1}X$   
 $F_T = A'(AA'+D)^{-1}X$

①  $F_B = (I + A'D^{-1}A)^{-1}F_T$  常近似相等.  
②  $E(F_B) = F$ .  $E(F_T) = A'\Sigma^{-1}AF$  有偏.

(需要一点矩阵等式)

Q型: 矩阵大 × 标准难 (低秩) (给定  $F, X \sim N(AF, D)$ )

$E((F_B - F)(F_B - F)') = (A'D^{-1}A)^{-1}$

$E((F_T - F)(F_T - F)') = (I + A'D^{-1}A)^{-1}$ , 误差更小.

相似系数 (cos) 阵求特征向量 (右旋转)

可以从代表性 (cos) 系数看出样本聚类等 (或  $F_i$  聚类) (各因子)

对应分析: 列联表的一类加权主成分分析.

(R-Q 因子分析) 克服变量和样品间量级的差异.

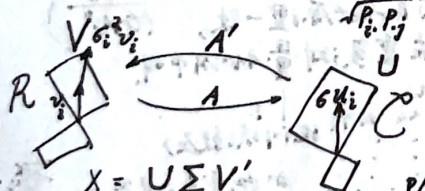
$X \rightarrow Z$   $z_{ij} = \frac{p_{ij} - p_i \cdot p_j}{\sqrt{p_i \cdot p_j} \sqrt{x_{ij}}}$  ( $p_{ij}$  对应阵)

data transformation:

中心化, 标准化, 极差标准化/规格化

卡方 (对应, 列联) 变换

函数变换, Box-Cox 变换  $\lambda$  用 MLE 等.  $y' = \begin{cases} \frac{y^\lambda - 1}{\lambda} & (\lambda \neq 0) \\ \ln y & (\lambda = 0) \end{cases}$   $y' = X\beta + \epsilon$



$X = U\Sigma V'$

$S_R = X'X$

$S_Q = XX'$

$S = LL'$

$A = \Sigma^2 = L'L$

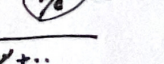
加权平方距离 (卡方距离)  $\frac{1}{p_i} (\frac{p_{ij} - p_i \cdot p_j}{p_i})^2$

总惯量  $Q = \sum_{ij} p_{ij} \frac{1}{p_i} (\frac{p_{ij} - p_i \cdot p_j}{p_i})^2$

(行点/列点) 至重心 (的) 加权距离平方和

行轮廓 (形影)  $G_r = G_Q = D_r^{-\frac{1}{2}} U \Sigma$

列轮廓 (坐标)  $G_c = G_R = D_c^{-\frac{1}{2}} V \Sigma$



$Z: u_1 \sqrt{\lambda} v + \dots$

$R (v \sqrt{\lambda}) \quad v \lambda v' + \dots$  ( $Z$  及其  $\Sigma = \epsilon_{ij}^2$ )  
 $Q (u \sqrt{\lambda}) \quad u \lambda u' + \dots$  (拆解)

$\text{sum}(\text{sum}(z)) = \lambda$

$(X^2 \text{ 乘以 } \sqrt{\lambda} \cdot \frac{y_0 - f_0}{f_0})^2$

$\sim df = (m-1)(p-1)$

△? coordinates and graphical representation

see in Wiki.

$\chi^2 = T \cdot \text{tr} S_R = T \cdot \text{tr} S_Q$   
( $T = ZZ'$ ) =  $T \sum_{ij} \lambda_i$   
卡方分解 ( $Q = \sum_{ij} \lambda_i$ ) (变量)  
一个  $\lambda$  → 解释了一部分 inertia  
→ 一个因子

PCA, LDA, FDA 关系重述:

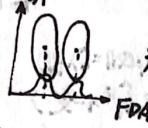
$G_{max} \frac{x^T A x}{x^T B x} = \max x^T (B^{-\frac{1}{2}} A B^{-\frac{1}{2}}) x$  也称. 称为瑞利商  $R_q$ .

取  $p$  (最大特征值), 方向为  $(x^T) B^{-\frac{1}{2}} A B^{-\frac{1}{2}}$  特征方向;  
或用求导 (Lagrange  $\lambda$ ) 得到.

LDA: 假设各类样本  $Cov$  相同 (且满秩),  $S^{-1}$  (马氏距离).

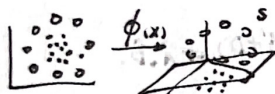
FDA: 逐方向 (拉大类间距离) 判别 esp.  $m=1$  维时与差不同.  $(W(X)) = d_1^2 - d_2^2 \geq 0$  也是线性判别的. 可开方  $d_1 - d_2 \geq 0$

$u(x) = l^T X$  PCA —  $A+B$  特征方向  
注意 FDA —  $A^{-1}B$  特征方向



QDA:  $Cov$  不同, 只能写  $d^2$ . Bayes: 如  $p_i, p_j, S_i, S_j$

KFDA: kernel '核方法' ~



$k(x_i, x_j) = \phi(x_i) \cdot \phi(x_j)$  核函数

$X = (x_1, \dots, x_n)$   $n$  样本  
 $\phi(X) = (\phi(x_1), \dots, \phi(x_n))$   $m$  变量

非线性 线性可分, 再 FDA.

KPCA 同理.

$S = \frac{1}{n-1} \phi(X) \phi(X)^T$   $S_p = \lambda p$   
不重要.

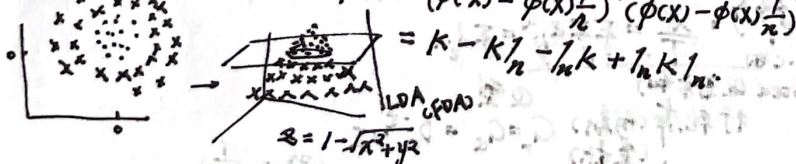
kernel trick:  $\phi(X) \phi(X)^T p = \lambda p$  (SVD 角度:  $(\phi(X))$  的奇异向量)

$p = \frac{1}{\lambda} \sum \phi(x_i) [\phi(x_i)^T p]$  令  $\alpha = \phi(x_i)^T p$   
 $p = \phi(X) \alpha$   
 $\alpha = \phi(X)^T p$

$K = \phi(X) \phi(X)^T$ ,  $k_{ij} = \phi(x_i) \cdot \phi(x_j)$   
 $(p^T p = 1 \rightarrow \alpha^T K \alpha = 1)$  (半) 正定核.

polynomial —  $(x^T y + c)^d$   
Gaussian / RBF —  $\exp(-\frac{\|x-y\|^2}{2\sigma^2})$  (Manchly, sph. test  $W = \lambda \frac{p^T W}{p^T W}$ )  
sigmoid —  $\tanh(ax^T y + r)$  与 Bartlet 原理一致, 常在重复测量 ANOVA 中叫.

centralize:  $\tilde{\phi}(x_i) = \phi(x_i) - \frac{1}{n} \sum \phi(x_j)$   
 $u(x) = p^T \phi(x)$



球形性) 检验 ( $H_0: \sigma^2 I$ )

sphericity test:  
Pearson  $\chi^2$  分布  
Bartlet 球形检验  $H_0: I$  (对相关阵)

$KMO = \frac{\sum_{i,j} r_{ij}^2}{\sum_{i,j} r_{ij}^2 + \sum_{i,j} d_{ij}^2}$  简单相关系数  
偏  $r_{ij} (i, j \dots)$

相关性 检验 (因子分析前: 变量是否独立的 提供信息?)  $KMO \uparrow$  越有相关性 适/否做.  $KMO \geq 0.5$  (0.7)

Bartlet:  $p$  前  $Cov$  test.

$\lambda = \frac{|\Sigma_0^{-1} A|^{p/2}}{(\frac{tr(\Sigma_0^{-1} A)}{p})^{p/2}}$   $\frac{\partial \ln L(x, \sigma^2)}{\partial \sigma^2} = 0$

变量为相关阵.  $\Sigma_0 = I$ .

$\chi^2 \left( \frac{p(p-1)}{2} \rightarrow 0 \right) \sim -2 \ln \lambda = -n \ln |A|$   
(详细版公式带  $p \dots$ ) 即相关阵.

(关于求  $KMO$  方法 — Matlab 代码).

$AIS = \frac{1}{D_A^{-1}} \cdot R^{-1} \cdot \frac{1}{D_A}$  ?

$AIR = \frac{1}{\sqrt{D_{AIS}}} \cdot AIS \cdot \frac{1}{\sqrt{D_{AIS}}}$   $(= \frac{1}{\sqrt{D_A}} \cdot R^{-1} \cdot \frac{1}{\sqrt{D_A}})$   
证明:  $R = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$  简单 ~ 与  $\lambda$  有关.

$\sqrt{a_{11} - v_1 A^{-1} v_1} \quad \sqrt{a_{22} - v_2 A^{-1} v_2}$   $\frac{|A|}{|S|}$   
(可与先前的  $\frac{f_i^2}{6}$  作一对比)  $\frac{|A|}{|S|} \cdot \frac{|A|}{|S|} = \frac{|A|^2}{|S|^2}$

与 Bartlet 原理一致, 常在重复测量 ANOVA 中叫. (如  $A^B$ )  
two-factor: (mixed anova) 组内效 (交互)

\* 把重复测量视 作另一变量 (组内效) 的关键是球形检验.

$Y = \bar{Y} + A_i + B_j + AB_{ij} + e$  (16 个样本, 看 4 个变量 相关性) 应无关 海次以抽 8 个样本)  
然后再检验 B 间, A 间效应. AB 交互. (2 阶效应)

如 A:  $df = 1$   
 $df = 14$

CCA, RDA, PLS:

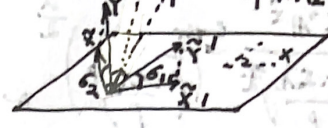
△? RDA 问: 是提取  $\hat{Y}$  还是  $\hat{X}$  的主轴还是  $\alpha, \beta$  轴?

典型相关分析, 典型冗余分析, 偏最小二乘法

(样本维: 可以做列  $\hat{X}, \hat{Y}$  的  $\Sigma$ )

$\hat{X} = \alpha' X$  (设计型)  
 $\hat{Y} = \beta' Y$  ( $X = X\alpha, Y = Y\beta$ )

$\max \frac{\alpha' \Sigma_{12} \beta}{\sqrt{\alpha' \Sigma_{11} \alpha} \sqrt{\beta' \Sigma_{22} \beta}} = \max \frac{\alpha' T \beta}{\sqrt{\alpha' \alpha} \sqrt{\beta' \beta}}$



$\alpha = \Sigma_{11}^{-1/2} U, \beta = \Sigma_{22}^{-1/2} V$

$T = \Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1/2} = U \Sigma V'$   
 $\Sigma \hat{Y} = \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \beta' \Sigma_{22} \beta = \Sigma^2$  (长  $\hat{Y}$ )  
 (有些地况况对  $\hat{Y} = HY$  作主轴 ( $\beta$ ) 也对)

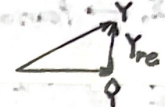
△解决  $X(Y)$  病态 (collinearity), 剥离共线性 (挑出前  $k$  对)

△相子于因子和 PCA. ( $Y = \hat{Y} + Y_{re}$ )

predictor mt.  $X = F_X L_{X\hat{X}} + E_X$  (loading mt.)

response mt.  $Y = F_Y L_{Y\hat{Y}} + E_Y$  (error mt.)

但作了旋转  $U$  (转后不能写  $L'L = I$ );



(共同的是, 载荷要正规与  $L' \Sigma_{11}^{-1} L = I$ )

特别是  $\omega(0,0)$ , 且  $U$  考虑了  $Y$  的信息.

$k$  principle components.

$\alpha' \Sigma_{11} \alpha = I, \beta' \Sigma_{22} \beta = I.$

$Cov(X, \hat{Y}) = Cov(X, \hat{X}) \Sigma$

$Cov(Y, \hat{X}) = Cov(Y, \hat{Y}) \Sigma.$

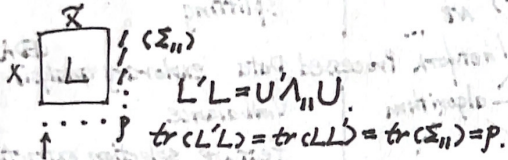
$\Sigma$  即为  $\hat{X}, \hat{Y}$  回归系数.

( $L_{XX} \Sigma_{11}^{-1} L_{XX}' = I$ )

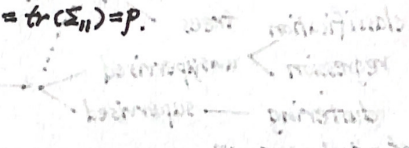
仍有  $L_{XX} \Sigma_{11}^{-1} L_{XX}' = \Sigma_{11}$  (中间夹  $I$ )

$L_{XY} \Sigma_{11}^{-1} L_{XY}' = \Sigma_{12}$ . 依此类推.

$\Sigma_{11}^{-1/2} U \Sigma \Sigma_{11}^{-1/2} = \Sigma_{11}^{-1/2} U = L_{XX}$   
 $\Sigma_{22}^{-1/2} V \Sigma \Sigma_{22}^{-1/2} = \Sigma_{22}^{-1/2} V = L_{YY}$



$\hat{X}$  解释占比 ( $\frac{\hat{X}}{X}$ )



△ Bartlett  $\Sigma_0 \leftrightarrow$  id. test? 有区别.

$H_0: \sigma^2 \Sigma_0, L(\bar{x}, \sigma^2 \Sigma_0) + \hat{\sigma}^2$

$$\Lambda = \frac{|\Sigma_0^{-1} A|}{\left(\frac{\text{tr}(\Sigma_0^{-1} A)}{p}\right)^p} = \frac{|A|}{\left(\frac{\text{tr}(A)}{p}\right)^p} \times \Lambda = \left(\frac{|A|}{\prod |A_{ii}|}\right)^{\frac{n}{2}}$$

Bartlett 又估一个  $\sigma^2$ .

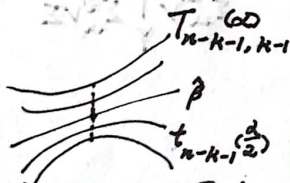
假设好了各元的方差比例关系:

idn. test 估每个元各自的方差. 知  $\Lambda_{Bart} < \Lambda_{id}$ .

△ Bartlett  $\Sigma_0 \leftrightarrow$  Pearson  $t = r \sqrt{\frac{n-2}{1-r^2}}$ ?

$-n \ln |R| \sim \chi^2 \left(\frac{p(p-1)}{2}\right) (n-2)$   
 $r \sqrt{\frac{n-2}{1-r^2}} \sim t_{(n-2)}$

$(\chi^2 \sim \text{cat}(\frac{1}{2}, \frac{1}{2})) \xrightarrow{\text{cut.}} \bar{\chi}_n^2 \sim N(1, \frac{2}{n})$   
 $(n \rightarrow \infty)$



△ 一般回归直线的联合置信区间?: 见置信椭圆球处(大T区间)

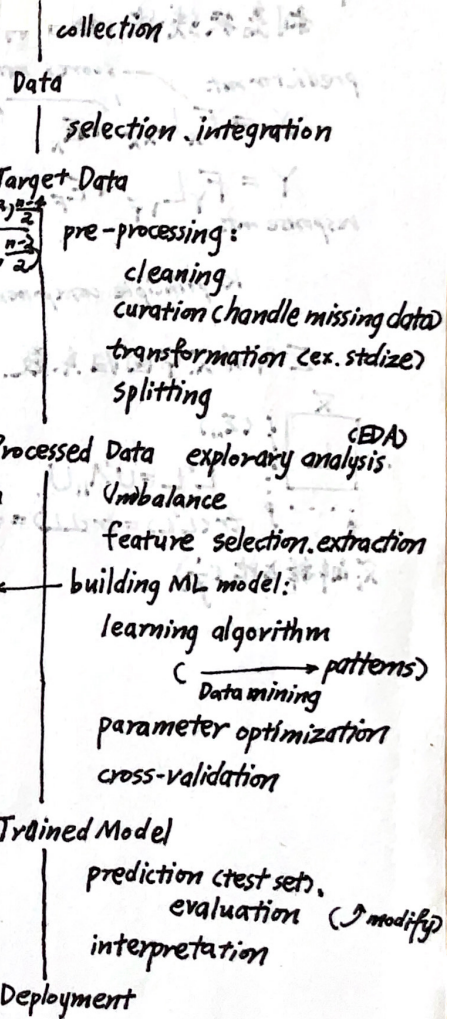
id. test  $H_0: \Sigma_{ij} = 0, \forall i \neq j$

$$\prod_i L_i(\bar{x}_i, \Sigma_{ii}) = \frac{|A|}{\prod |A_{ii}|}$$

△ skills for data analysis:

- 1. programming
- 2. mathematics
- 3. software engineering
- 4. statistics
- 5. machine learning
- 6. data visualization
- 7. soft skills

△ common process of data ana.:



Fisher 变换:

$$z = \text{arctanh } r = \frac{1}{2} \ln \frac{1+r}{1-r}$$

$$z \approx N\left(\frac{1}{2} \ln \frac{1+\rho}{1-\rho}, \frac{1}{n-3}\right) \text{ NB}$$

逆  $r = \frac{e^{2z} - 1}{e^{2z} + 1}$

- classification
- regression
- dustering
- neutral network
- svm
- trees
- unsupervised
- supervised

△ over-fitting:

1. more data
2. punish complexity (regularization)
3. less parameter (simpler model)
4. dedimension
  - feature selection
  - feature extraction

filter  $r, \chi^2, I(x,y), \text{Var.}$   
 wrapper (screen)  
 embedded eval func  $\rightarrow$  sub-set ML scores.