A Brief Summary of Statistics Course

统计学课程知识总结

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目录

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Chapter. I 概率论部分

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Section 1.1 Some Important Distributions

X	$p_X(k)//f_X(x)$	E	σ^2	PGF	MGF
$B(p)$		p	pq		$q+pe^s$
$B(n,p)$	$C_n^k p^k(1-p)^{n-k}$	np	npq	$(q+ps)^n$	$(q+pe^s)^n$
$G(p)$	$(1-p)^{k-1}p$	$\frac{1}{p}$	$\frac{q}{p^2}$	$\frac{ps}{1-qs}$	$\frac{pe^s}{1-qe^s}$
$H(n,M,N)$	$\frac{C_M^k C_{N-M}^{n-k}}{C_N^n}$	$n\frac{M}{N}$	$\frac{nM(N-n)(N-M)}{N^2(n-1)}$		
$P(\lambda)$	$\frac{\lambda^k}{k!}e^{-\lambda}$	λ	λ	$e^{\lambda(s-1)}$	$e^{\lambda(e^s-1)}$
$U(a,b)$	$\frac{1}{b-a}$	$\frac{a+b}{2}$	$\frac{(b-a)^2}{12}$		$\frac{e^{sb}-e^{sa}}{(b-a)s}$
$N(\mu,\sigma^2)$	$\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$	μ	σ^2		$e^{\frac{\sigma^2 s^2}{2}+\mu s}$
$\epsilon(\lambda)$	$\lambda e^{-\lambda x}$	$\frac{1}{\lambda}$	$\frac{1}{\lambda^2}$		$\frac{\lambda}{\lambda-s}$
$\Gamma(\alpha,\lambda)$	$\frac{\lambda^\alpha}{\Gamma(\alpha)}x^{\alpha-1}e^{-\lambda x}$	$\frac{\alpha}{\lambda}$	$\frac{\alpha}{\lambda^2}$		
$B(\alpha,\beta)$	$\frac{1}{B(\alpha,\beta)}x^{\alpha-1}(1-x)^{\beta-1}$	$\frac{\alpha}{\alpha+\beta}$	$\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$		
χ_n^2	$\frac{1}{2^{\frac{n}{2}}\Gamma(\frac{n}{2})}x^{\frac{n}{2}-1}e^{-\frac{x}{2}}$	n	$2n$		
t_ν	$\frac{\Gamma(\frac{\nu+1}{2})}{\sqrt{\nu\pi}\Gamma(\frac{\nu}{2})}(1+\frac{x^2}{\nu})^{-\frac{\nu+1}{2}}$	0	$\frac{\nu}{\nu-2}$		
$F_{m,n}$	$\frac{\Gamma(\frac{m+n}{2})}{\Gamma(\frac{m}{2})\Gamma(\frac{n}{2})}\frac{m^{\frac{m}{2}}n^{\frac{n}{2}}x^{\frac{m}{2}-1}}{(mx+n)^{\frac{m+n}{2}}}$	$\frac{n}{n-2}$	$\frac{2n^2(m+n-2)}{m(n-2)^2(n-4)}$		

Definition of PGF, MGF, CF see section. 1.5.

More Properties of χ^2, t, F see section. 1.8.2.

Relation between distributions and more properties see http://www.math.wm.edu/~leemis/chart/UDR/UDR.html

Section 1.2 Probability and Probability Model

What is **Probability**?

A 'belief' in the chance of an event occurring?

1.2.1 Sample and σ-Field

Def. sample space Ω: The set of all possible outcomes of one particular experiment.

Def. $\mathscr{F}$ a σ-field(or a σ-algebra) as a collection of some subsets of Ω **if**

- $\Omega \in \mathscr{F}$

- if $A \in \mathscr{F}$,then $A^{\complement} \in \mathscr{F}$
- if $A_n \in \mathscr{F}$, then $\bigcup_{n=1}^{\infty} A_n \in \mathscr{F}$

And $(\Omega, \mathscr{F})$ is a measurable space.

1.2.2 Axioms of Probability

$\mathbb{P}(\cdot)$ is probability measure (or probability function) defined on $(\Omega, \mathscr{F})$ describing the possibility that some event $A \in \Omega$ happens. Definition of probability $\mathbb{P}(A)$ in useful models:

$$\mathbb{P}(A) := \begin{cases} \dfrac{\#A}{\#\Omega} & \text{Classical Model} \\ \dfrac{m(A)}{m(\Omega)} & \text{Geometric Model} \end{cases}$$

□ **Basic Axioms of Probability Mearure** $\mathbb{P}(\cdot)$

- Nonnegativity

$$\mathbb{P}(A) \geq 0 \qquad \forall A \in \Omega \tag{1.1}$$

- Normalization

$$\mathbb{P}(\Omega) = 1 \tag{1.2}$$

- Countable Additivity

$$\mathbb{P}(A_1 \cup A_2 \cup \cdots) = \mathbb{P}(A_1) + \mathbb{P}(A_2) + \cdots \quad, (A_i \perp\!\!\!\perp A_j \quad \forall i \neq j) \tag{1.3}$$

Then $(\Omega, \mathscr{F}, \mathbb{P})$ is probability space.

□ **Properties of Probability:**

- Monotonicity

$$\mathbb{P}(A) \leq \mathbb{P}(B) \quad \text{for } A \subset B \tag{1.4}$$

- Finite Subadditivity (Boole Inequality)

$$\mathbb{P}(\bigcup_{i=1}^{n} A_i) \leq \sum_{i=1}^{n} \mathbb{P}(A_i) \tag{1.5}$$

- Inclusion-Exclusion Formula(Jordan Formula)

$$\mathbb{P}(\Cup_{i=1}^{n} A_i) = \sum_{1 \leq i \leq n} \mathbb{P}(A_i) - \sum_{1 \leq i < j \leq n} \mathbb{P}(A_i \cap A_j) \tag{1.6}$$

$$+ \sum_{1 \leq i < j < k \leq n} \mathbb{P}(A_i \cap A_j \cap A_k) - \cdots \tag{1.7}$$

$$+ (-1)^{n-1} \mathbb{P}(A_1 \cap A_2 \cap \cdots \cap A_n) \tag{1.8}$$

- Borel-Cantelli Lemma

$$\sum_{n=1}^{\infty} \mathbb{P}(A_n) < \infty \Rightarrow \mathbb{P}(\lim_{n \to \infty} \sup A_n) = 0 \tag{1.9}$$

$$\sum_{n=1}^{\infty} \mathbb{P}(A_n) = \infty \Rightarrow \mathbb{P}(\lim_{n \to \infty} \sup A_n) = 1 \quad \text{if } A_i \text{ independent} \tag{1.10}$$

1.2.3 Conditional Probability

Def. **Conditional Probability** of B given A:

$$\mathbb{P}(B|A) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(A)} \tag{1.11}$$

(Actually a change of σ-field: $\Omega \to B$)

☐ **Application of conditional probability:**

- Multiplication Formula

$$\mathbb{P}(\Cap_{i=1}^{n} A_i) = \mathbb{P}(A_1) \prod_{i=2}^{n} \mathbb{P}(A_i | A_1 \cap A_2 \cap \cdots \cap A_{i-1}) \tag{1.12}$$

- Total Probability Thm.

$$\mathbb{P}(B) = \sum_{i=1}^{n} \mathbb{P}(A_i)\mathbb{P}(B|A_i) \tag{1.13}$$

  where $\{A_i\}$ is a partition of Ω.

- Bayes's Rule

$$\mathbb{P}(A_i|B) = \frac{\mathbb{P}(A_i)\mathbb{P}(B|A_i)}{\sum_{j=1}^{\mathbb{P}}(A_j)\mathbb{P}(B|A_j)}, \quad 1 \le i \le n \tag{1.14}$$

  where $\{A_i\}$ is a partition of Ω.

- Statistically Independence

$$\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B), \text{ for } A \perp\!\!\!\perp B \tag{1.15}$$

Section 1.3 Properties of Random Variable and Vector

1.3.1 Random Variable

Def. Random Variable: a **function** X defined on sample space Ω, mapping from Ω to some $\mathscr{X} \in \mathbb{R}$.

Then def. Cumulative Distribution Function (CDF).

$$F_X(x) = \mathbb{P}(X \le x) \tag{1.16}$$

For Discrete case, consider CDF as **right-continuity**.

- PMF:

$$p_X(x) = F_X(x^+) - F_X(x^-) \tag{1.17}$$

  PDF:

$$f_X(x) = \frac{\mathrm{d}F_X(x)}{\mathrm{d}x} \tag{1.18}$$

- Indicator function:

$$I_{x \in A}(x) = \begin{cases} 1 & x \in A \\ 0 & x \notin A \end{cases} \tag{1.19}$$

- Convolution

  - $W = X + Y$

$$f_W(w) = \int_{-\infty}^{\infty} f_X(x) f_Y(w - x) \mathrm{d}x \tag{1.20}$$

- $V = X - Y$

$$f_V(v) = \int_{-\infty}^{\infty} f_X(x) f_Y(x-v) \mathrm{d}x \tag{1.21}$$

- $Z = XY$

$$f_Z(z) = \int_{-\infty}^{\infty} \frac{1}{|x|} f_X(x) f_Y(\frac{z}{x}) \mathrm{d}x \tag{1.22}$$

- Order Statistics

  Def $X_{(1)}, X_{(2)}, \cdots, X_{(n)}$ as order statistics of $\vec{X}$

$$g_{X_{(i)}} = n! \prod_i f(x_i) \qquad \text{for}\, x_1 < x_2 \cdots < x_n \tag{1.23}$$

  PDF of $X_{(k)}$

$$g_k(x_k) = nC_{n-1}^{k-1} [F(x_k)]^{k-1} [1 - F(x_k)]^{n-k} f(x_k) \tag{1.24}$$

- p-fractile

$$\xi_p = F^{-1}(p) = \inf\{x | F(x) \geq p\} \tag{1.25}$$

1.3.2 Random Vector

A general case of random variable.

n-dimension Random Vector $\vec{X} = (X_1, X_2, \ldots, X_n)$ defined on $(\Omega, \mathscr{F}, \mathbb{P})$.

CDF $F(x_1, \ldots, x_n)$ defined on $\mathbb{R}^n$:

$$F(x_1, \ldots, x_n) = \mathbb{P}(X_1 \leq x_1, \ldots, X_n \leq x_n) \tag{1.26}$$

Joint PDF of random vector:

$$f(x_1, \ldots, x_n) = \frac{\partial^n F(x_1, \ldots, x_n)}{\partial x_1 \ldots \partial x_n} \tag{1.27}$$

k-dimensional Marginal Distribution: For $1 \leq k < n$ and index set $S_k = \{i_1 \ldots, i_k\}$, distribution of $\vec{X} = (X_{i_1}, X_{i_2}, \ldots, X_{i_k})$

$$F_{S_k}(x_{i_1}, X_{i_2} \leq x_{i_2} \ldots, x_{i_k}) = \mathbb{P}(X_{i_1} \leq x_{i_1}, \ldots, X_{i_k} \leq x_{i_k}; X_{i_{k+1}}, \ldots, X_{i_n} \leq \infty) \tag{1.28}$$

Marginal distribution:

$$g_{S_k}(x_{i_1}, \ldots, x_{i_k}) = \int_{\mathbb{R}^{n-k}} f(x_1, \ldots, x_n) \mathrm{d}x_{i_{k+1}} \ldots \mathrm{d}x_{j_n} = \frac{\partial^{n-k} F(x_1, \ldots, x_n)}{\partial x_{i_{k+1}} \ldots \partial x_{i_n}} \tag{1.29}$$

Δ **Function of r.v.**

For $\vec{X} = (X_1, X_2, \cdots, X_n)$ with PDF $f(\vec{X})$ and define

$$\vec{Y} = (Y_1, Y_2, \cdots, Y_n) = \left(y_1(\vec{X}), y_2(\vec{X}), \cdots, y_n(\vec{X})\right) \tag{1.30}$$

with inverse mapping

$$\vec{X} = (X_1, X_2, \cdots, X_n) = \left(x_1(\vec{Y}), x_2(\vec{Y}), \cdots, x_n(\vec{Y})\right) \tag{1.31}$$

then

$$g(\vec{Y}) = f\left(x_1(\vec{Y}), x_2(\vec{Y}), \cdots, x_n(\vec{Y})\right) \left| \frac{\partial \vec{X}}{\partial \vec{Y}} \right| \mathbb{I}_{D_Y} \tag{1.32}$$

(Intuitively: $g\left(\vec{Y}\right) \mathrm{d}\vec{Y} = \mathrm{d}\mathbb{P} = f(\vec{X}) \mathrm{d}\vec{X}$)

Section 1.4 Properties of $\mathbb{E}$, var and cov

Expectation and Variance of common distributions see section. 1.1.

1.4.1 Expection $\mathbb{E}(\cdot)$

Expectation of r.v. $g(X)$ def.:

$$\mathbb{E}[g(X)] = \begin{cases} \int_\Omega g(x) f_X(x) \mathrm{d}x = \int_\Omega g(x) \mathrm{d}F(x) \\ \sum_\Omega g(X) f_X(x) \end{cases} \tag{1.33}$$

Sometimes when there are > 1 variables, say x, y, we would use $\mathbb{E}_X(g(X,Y))$ to avoid confusion.

☐ **Properties of expectation $E(\cdot)$:**

- Linearity of Expectation

$$\mathbb{E}(aX + bY) = a\mathbb{E}(X) + b\mathbb{E}(Y) \tag{1.34}$$

- Conditional Expectation

$$\mathbb{E}(X|A) = \frac{\mathbb{E}(X\mathbb{I}_A)}{\mathbb{P}(A)} \tag{1.35}$$

  Note: if take A as Y is also a r.v. then

$$\xi(Y) = \mathbb{E}(X|Y) = \int x f_{X|Y}(x) \mathrm{d}x \tag{1.36}$$

  is actually a function of Y

- Law of Total Expectation

$$\mathbb{E}_Y\{\mathbb{E}_X[g(X)|Y]\} = \mathbb{E}_X[g(X)] \tag{1.37}$$

- r.v.& Event

$$\mathbb{P}(A|X) = \mathbb{E}(\mathbb{I}_A|X) \Rightarrow \mathbb{E}[P(A|X)] = \mathbb{E}(\mathbb{I}_A) = \mathbb{P}(A) \tag{1.38}$$

- Conditional Expectation

$$\mathbb{E}\big[h(Y)g(X)|Y\big] = h(Y)\mathbb{E}[g(X)|Y] \tag{1.39}$$

1.4.2 Variance

Variance of r.v. X:

$$var(X) = \mathbb{E}\big[(X - \mathbb{E}(X))^2\big] = \mathbb{E}(X^2) - (\mathbb{E}(X))^2 \tag{1.40}$$

(sometimes denoted as σ_X^2.)

☐ **Properties:**

- Linear combination of Variance

$$var(aX + b) = a^2 var(X) \tag{1.41}$$

- Conditional Variance

$$var(X|Y) = \mathbb{E}[X - \mathbb{E}(X|Y)]^2|Y \tag{1.42}$$

- Law of Total Variance

$$var(X) = \mathbb{E}[var(X|Y)] + var[\mathbb{E}(X|Y)] \tag{1.43}$$

Standard Deviation def. as :

$$\sigma_X = \sqrt{var(X)} \tag{1.44}$$

Then can construct **Standardization** of r.v.

$$X_{\text{sd}} = \frac{X - \mathbb{E}(X)}{\sqrt{var(X)}} \tag{1.45}$$

1.4.3 Covariance and Correlation

Covariance of r.v. X and Y:

$$cov(X,Y) = \mathbb{E}\big[(X - \mu_X)(Y - \mu_Y)\big] = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y) \tag{1.46}$$

And (Pearson's) Correlation Coefficient

$$r = \rho_{X,Y} = corr(X,Y) = \frac{cov(X,Y)}{\sqrt{var(X)var(Y)}} \tag{1.47}$$

Remark: correlation $\not\Rightarrow$ cause and effect. Detail on causal effect topic see Chapter. 11.

Properties:

- Bilinear of Covariance

$$cov(X+Y,Z) = cov(X,Z) + cov(Y,Z)$$
$$cov(X,Y+Z) = cov(X,Y) + cov(X,Z)$$

- Variance and Covariance

$$var(X+Y) = var(X) + var(Y) + 2cov(X,Y) \tag{1.48}$$

- Covariance Matrix

Def $\Sigma = \mathbb{E}\big[(X-\mu)(X-\mu)^T\big] = \{\sigma_{ij}\}$ (where X should be considered as a column vector)

$$\Sigma = \begin{pmatrix} var(X_1) & cov(X_1,X_2) & \dots & cov(X_1,X_n) \\ cov(X_2,X_1) & var(X_2) & \dots & cov(X_2,X_n) \\ \vdots & \vdots & \ddots & \vdots \\ cov(X_n,X_1) & cov(X_n,X_2) & \dots & var(X_n) \end{pmatrix} \tag{1.49}$$

Attachment: Independence:

$$X_i \perp\!\!\!\perp X_j \Rightarrow \begin{cases} f(x_1,x_2,\cdots,x_n) = \prod f(x_i) \\ F(x_1,x_2,\cdots,x_n) = \prod F(x_i) \\ E(\prod X_i) = \prod E(X_i) \\ var(\sum X_i) = \sum var(X_i) \end{cases} \tag{1.50}$$

Section 1.5 PGF, MGF and C.F

Generating Function: Representation of P in function space. $P \Leftrightarrow$ Generating Function.

1.5.1 Probability Generating Function

PGF: used for non-negative, integer X

$$g(s) = \mathbb{E}(s^X) = \sum_{j=0}^{\infty} s^j \mathbb{P}(X = j), s \in [-1, 1] \tag{1.51}$$

☐ **Properties**

- $\mathbb{P}(X = k) = \dfrac{g^{(k)}(0)}{k!}$
- $\mathbb{E}(X) = g^{(1)}(1)$
- $var(X) = g^{(2)}(1) + g^{(1)}(1) - [g^{(1)}(1)]^2$
- For $X_1, X_2, \cdots, X_n$ independent with $g_i(s) = \mathbb{E}(s^{X_i})$, $Y = \sum_{i=1}^{n} X_i$, then

$$g_Y(s) = \prod_{i=1}^{n} g_i(s), s \in [-1, 1] \tag{1.52}$$

- For X_i i.i.d with $\psi(s) = \mathbb{E}(s^{X_i})$, Y with $G(s) \equiv \mathbb{E}(s^Y)$, $W = X_1 + X_2 + \cdots + X_Y$,then

$$g_W(s) = G[\psi(s)] \tag{1.53}$$

- 2-Dimensional PGF of (X, Y)

$$g(s, t) = \mathbb{E}(s^X t^Y) = \sum_{i=o}^{\infty} \sum_{j=0}^{\infty} \mathbb{P}_{(X,Y)}(X = i, Y = j) s^i t^j, \quad s, t \in [-1, 1] \tag{1.54}$$

1.5.2 Moment Generating Function

MGF:

$$M_X(s) = \mathbb{E}(e^{sX}) = \begin{cases} \sum_j e^{sx} \mathbb{P}(X = x_j) \\ \int_{-\infty}^{\infty} e^{sx} f_X(x) \mathrm{d}x \end{cases} \tag{1.55}$$

Properties

- MGF of $Y = aX + b$: $M_Y(s) = e^{sb} M(sa)$
- $\mathbb{E}(X^k) = M^{(k)}(0)$
- $\mathbb{P}(X = 0) = \lim_{s \to -\infty} M(s)$
- For $X_1, X_2, \cdots, X_n$ independent with $M_{X_i}(s) = \mathbb{E}(e^{sX_i})$, $Y = \sum_{i=1}^{n} X_i$, then

$$M_Y(s) = \prod_{i=1}^{n} M_{X_i}(s) \tag{1.56}$$

1.5.3 Characteristic Function

C.F is actually the Fourier Transform of f.

$$\phi(t)=\mathbb{E}(e^{itX})=\int_{-\infty}^{\infty}e^{itx}f_X(x)\mathrm{d}x \tag{1.57}$$

Properties

- if $E(|X|^k)<\infty$,then
$$\phi^{(k)}(t)=i^k\mathbb{E}(X^ke^{itX}) \qquad \phi^{(k)}(0)=i^k\mathbb{E}(X^k) \tag{1.58}$$
- For $X_1,X_2,\cdots,X_n$ independent with $\phi_{X_i}(t)=\mathbb{E}(e^{itX_i})$, $Y=\sum\limits_{i=1}^{n}X_i$, then
$$\phi_Y(t)=\prod_{i=1}^{n}\phi_{X_i}(t) \tag{1.59}$$
- Inverse (Fourier) Transform
$$f(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-itx}\phi(t)\mathrm{d}t \tag{1.60}$$

Section 1.6 Convergence and Limit Distribution

1.6.1 Convergence Mode

$$\begin{cases}\text{Convergence in Distribution} & X_n\xrightarrow{\mathscr{L}}X:\lim\limits_{n\to\infty}F_n(x)=F(x)\\ \text{Convergence in Probability} & X_n\xrightarrow{p}X:\lim\limits_{n\to\infty}\mathbb{P}(|X_n-X)\geq\varepsilon)=0\,,\forall\varepsilon>0\\ \text{Almost Sure Convergence} & X_n\xrightarrow{\text{a.s.}}X:\mathbb{P}(\lim\limits_{n\to\infty}X_n=X)=1\\ L_p\text{ Convergence} & X_n\xrightarrow{L_p}X:\lim\limits_{n\to\infty}\mathbb{E}(|X_n-X|^p)=0\end{cases} \tag{1.61}$$

Relations between convergence:

$$\begin{tikzcd}
\boxed{X_n\xrightarrow{\text{a.s.}}X} \arrow[dr] & & \\
& \boxed{X_n\xrightarrow{p}X} \arrow[r] & \boxed{X_n\xrightarrow{\mathscr{L}}X} \\
\boxed{X_n\xrightarrow{L_p}X} \arrow[ur] & &
\end{tikzcd}$$

Useful Thm.:

- Continuous Mapping Thm.: For continuous function $g(\cdot)$

  1. $X_n\xrightarrow{\text{a.s.}}X\Rightarrow g(X_n)\xrightarrow{\text{a.s.}}g(X)$

2. $X_n \xrightarrow{p} X \Rightarrow g(X_n) \xrightarrow{p} g(X)$
3. $X_n \xrightarrow{\mathscr{L}} X \Rightarrow g(X_n) \xrightarrow{\mathscr{L}} g(X)$

- Slutsky's Thm.: For $X_n \xrightarrow{\mathscr{L}} X, Y_n \xrightarrow{p} c$

1. $X_n + Y_n \xrightarrow{\mathscr{L}} X + c$
2. $X_n Y_n \xrightarrow{\mathscr{L}} cX$
3. $X_n / Y_n \xrightarrow{\mathscr{L}} X/c$

- Continuity Thm.

$$\lim_{n\to\infty} \phi_n(t) = \varphi(t) \Leftrightarrow X_n \xrightarrow{\mathscr{L}} X \tag{1.62}$$

1.6.2 Law of Large Number & Central Limit Theorem

- WLLN

$$\frac{1}{n}\sum X_i \xrightarrow{p} E(X_1) \tag{1.63}$$

- SLLN

$$\frac{1}{n}\sum X_i \xrightarrow{\text{a.s.}} C \tag{1.64}$$

- CLT

$$\frac{1}{\sigma\sqrt{n}}\sum(X_k - \mu) \xrightarrow{\mathscr{L}} N(0,1) \tag{1.65}$$

- de Moivre-Laplace Thm.

$$\mathbb{P}(k \le S_n \le m) \approx \Phi(\frac{m+0.5-np}{\sqrt{npq}}) - \Phi(\frac{k-0.5-np}{\sqrt{npq}}) \tag{1.66}$$

- Stirling Eqa.

$$\frac{\lambda^k}{k!}e^{-\lambda} \approx \frac{1}{\sqrt{\lambda}\sqrt{2\pi}}e^{-\frac{(k-\lambda)^2}{2\lambda}} \xrightarrow[\lambda=n]{k=n} n! \approx \sqrt{2\pi n}(\frac{n}{e})^n \tag{1.67}$$

Section 1.7 Inequalities

- Cauchy-Schwarz Inequality

$$|\mathbb{E}(XY)| \le \sqrt{\mathbb{E}(X^2)\mathbb{E}(Y^2)} \tag{1.68}$$

- Bonferroni Inequality

$$\mathbb{P}(\bigcup_{i=1}^{n} A_i) \ge \sum_{1\le i\le n}\mathbb{P}(A_i) + \sum_{1\le i<j\le n}\mathbb{P}(A_i \cap A_j) \tag{1.69}$$

- Markov Inequality

$$\mathbb{P}(|X| \ge \epsilon) \le \frac{\mathbb{E}(|X|^\alpha)}{\epsilon^\alpha} \tag{1.70}$$

- Chebyshev Inequality

$$\mathbb{P}(|X - E(X)| \ge \epsilon) \le \frac{var(X)}{\epsilon^2} \tag{1.71}$$

- Jensen Inequality: For convex function $g(x)$:

$$\mathbb{E}[g(X)] \ge g(\mathbb{E}(X)) \tag{1.72}$$

Section 1.8 Multivariate Normal Distribution

General Case and more discussion see section. 4.2.1.

Distribution of Normal $X \sim B(\mu, \sigma^2)$:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

For $X_1, X_2, \cdots, X_n$ independent and $X_k \sim N(\mu_k, \sigma_k^2)$, $k = 1, \cdots, n$, $T = \sum_{k=1}^{n} c_k X_k$, ($c_k$ const), then

$$T \sim N(\sum_{k=1}^{n} c_k \mu_k, \sum_{k=1}^{n} c_k^2 \sigma_k^2) \tag{1.73}$$

Deduction in some special cases:

- Given $\mu_1 = \mu_2 = \cdots = \mu_n = \mu$, $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_n^2 = \sigma^2$, i.e. X_k i.i.d., then

$$T \sim N(\mu \sum_{k=1}^{n} c_k, \sigma^2 \sum_{k=1}^{n} c_k^2) \tag{1.74}$$

- Further take $c_1 = c_2 = \cdots = c_n = \frac{1}{n}$, i.e. $T = \sum_{k=1}^{n} X_k/n = \bar{X}$, then

$$T = \bar{X} \sim N(\mu, \frac{\sigma^2}{n}) \tag{1.75}$$

1.8.1 Linear Transform

First consider $\epsilon_1, \epsilon_2, \cdots, \epsilon_m$ i.i.d. $\sim N(0, 1)$, $n \times 1$ const column vector $\vec{\mu}$, $n \times m$ const matrix $\boldsymbol{B} = \{b_{ij}\}$, def.$X_i = \sum_{j=1}^{m} b_{ij}\epsilon_j$, i.e.

$$\vec{X} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ b_{21} & b_{22} & \dots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nm} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_m \end{pmatrix} + \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix} = \boldsymbol{B}\vec{\varepsilon} + \vec{\mu} \tag{1.76}$$

We have: $\vec{X} \sim N(\vec{\mu}, \Sigma)$, where Σ, as defined in equation. 1.49 is

$$\Sigma = \mathbb{E}[(\vec{X} - \vec{\mu})(\vec{X} - \vec{\mu})^T] = \boldsymbol{B}\boldsymbol{B}^T = \begin{pmatrix} var(X_1) & cov(X_1, X_2) & \dots & cov(X_1, X_n) \\ cov(X_2, X_1) & var(X_2) & \dots & cov(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ cov(X_n, X_1) & cov(X_n, X_2) & \dots & var(X_n) \end{pmatrix} = \{\sigma_{ij}\} \tag{1.77}$$

Furthur Consider $\vec{Y} = (Y_1, \cdots, Y_n)^T$, $n \times n$ const square matrix $\mathbf{A} = \{\mathbf{a_{ij}}\}$ and def. $\vec{Y} = \mathbf{A}\vec{\mathbf{X}}$ i.e.

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{pmatrix} \tag{1.78}$$

Then $\vec{Y} \sim N(\boldsymbol{A}\vec{\mu}, \boldsymbol{A}\Sigma\boldsymbol{A}^T)$

Special case: $X_1, \cdots, X_n$ i.i.d. $\sim N(\mu, \sigma^2)$, $\vec{X} = (X_1, \cdots, X_n)^T$,

$$\begin{aligned}
\mathbb{E}(Y_i) =& \mu \sum_{k=1}^{n} a_{ik} \\
var(Y_i) =& \sigma^2 \sum_{k=1}^{n} a_{ik}^2 \\
cov(Y_i, Y_j) =& \sigma^2 \sum_{k=1}^{n} a_{ik} a_{jk}
\end{aligned}$$

Specially when $\boldsymbol{A} = \{a_{ij}\}$ orthonormal, we have $Y_1, \cdots, Y_n$ independent

$$Y_i \sim N(\mu \sum_{k=1}^{n} a_{ik}, \sigma^2) \tag{1.79}$$

1.8.2 Distributions of Function of Normal Variable: χ^2, t & F

Consider $X_1, X_2, \ldots, X_n$ i.i.d. $\sim N(0,1)$; $Y, Y_1, Y_2, \ldots, Y_m$ i.i.d. $\sim N(0,1)$

- χ^2 Distribution: Def. χ^2 distribution with degree of freedom n:

$$\xi = \sum_{i=1}^{n} X_i^2 \sim \chi_n^2 \tag{1.80}$$

  PDF of χ_n^2:

$$g_n(x) = \frac{1}{2^{n/2}\Gamma(n/2)} x^{n/2} e^{-x/2} I_{x>0} \tag{1.81}$$

  Properties

  – $\mathbb{E}$ and var of $\xi \sim \chi_n^2$

$$\mathbb{E}(\xi) = n \qquad var(\xi) = 2n \tag{1.82}$$

  – For independent $\xi_i \sim \chi_{n_i}^2$, $i = 1, 2, \ldots, k$:

$$\xi_0 = \sum_{i=1}^{k} \xi_i \sim \chi_{n_1+\ldots+n_k}^2 \tag{1.83}$$

  – Denoted as $\Gamma(\alpha, \lambda)$:

$$\xi = \sum_{i=1}^{n} X_i \sim \Gamma(\frac{n}{2}, \frac{1}{2}) = \chi_n^2 \tag{1.84}$$

- t Distribution: Def. t distribution with degree of freedom n:

$$T = \frac{Y}{\sqrt{\frac{\sum_{i=1}^{n} X_i^2}{n}}} = \frac{Y}{\sqrt{\xi/n}} \sim t_n \tag{1.85}$$

  (Usually take ν instead of n as degree of freedom for t distribution)

  PDF of t_ν:

$$t_\nu(x) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}} \left(1 + \frac{x^2}{\nu}\right)^{-\frac{\nu+1}{2}} \tag{1.86}$$

Denote: Upper α-fractile of t_ν, satisfies $\mathbb{P}(T \geq c) = \alpha$:

$$c = t_{\nu,\alpha} \tag{1.87}$$

(Similar for χ^2_n and $F_{m,n}$ etc.)

- F Distribution: Def. F distribution with degree of freedom m and n:

$$F = \frac{\sum_{i=1}^m Y_i}{\sum_{i=1}^n X_i} \sim F_{m,n} \tag{1.88}$$

PDF of $F_{m,n}$:

$$f_{m,n}(x) = \frac{\Gamma(\frac{m+n}{2}) m^{\frac{m}{2}} n^{\frac{n}{2}}}{\Gamma(\frac{m}{2})\Gamma(\frac{n}{2})} x^{\frac{m}{2}-1}(mx+n)^{-\frac{m+n}{2}} \mathbb{I}_{x>0} \tag{1.89}$$

Properties

  - If $Z \sim F_{m,n}$, then $\frac{1}{Z} \sim F_{n,m}$.
  - If $T \sim t_n$, then $T^2 \sim F_{1,n}$
  - $F_{m,n,1-\alpha} = \dfrac{1}{F_{n,m,\alpha}}$

☐ **Some useful Lemma (uesd in statistic inference, see section. 2.3.3):**

- For $X_1, X_2, \ldots, X_n$ independent with $X_i \sim N(\mu_i, \sigma_i^2)$, then

$$\sum_{i=1}^n \left(\frac{X_i - \mu_i}{\sigma_i}\right)^2 \sim \chi^2_n \tag{1.90}$$

- For $X_1, X_2, \ldots, X_n$ i.i.d.$\sim N(\mu, \sigma^2)$, then

$$T = \frac{\sqrt{n}(\bar{X} - \mu)}{S} \sim t_{n-1} \tag{1.91}$$

For $X_1, X_2, \ldots, X_m$ i.i.d.$\sim N(\mu_1, \sigma^2)$, $Y_1, Y_2, \ldots, Y_n$ i.i.d.$\sim N(\mu_2, \sigma^2)$, denote sample pooled variance $S_\omega^2 = \dfrac{(m-1)S_1^2 + (n-1)S_2^2}{m+n-2}$, then

$$T = \frac{(\bar{X} - \bar{Y}) - (\mu_1 - \mu_2)}{S_\omega} \cdot \sqrt{\frac{mn}{m+n}} \sim t_{m+n-2} \tag{1.92}$$

- For $X_1, X_2, \ldots, X_m$ i.i.d.$\sim N(\mu, \sigma^2)$, $Y_1, Y_2, \ldots, Y_n$ i.i.d.$\sim N(\mu_2, \sigma^2)$, then

$$T = \frac{S_1^2}{S_2^2}\frac{\sigma_2^2}{\sigma_1^2} \sim F_{m-1,n-1} \tag{1.93}$$

- For $X_1, X_2, \ldots, X_n$ i.i.d. $\sim \epsilon(\lambda)$, then

$$2\lambda n\bar{X} = 2\lambda\sum_{i=1}^n X_i \sim \chi^2_{2n} \tag{1.94}$$

Remark: for $X_i \sim \epsilon(\lambda) = \Gamma(1, \lambda) \Rightarrow 2\lambda\sum_{i=1}^n X_i \sim \Gamma(n, 1/2) = \chi^2_{2n}$.

Chapter. II 统计推断部分

Instructor: Jiangdian Wang

Statistical Inference: Given sample $X = (x_1, x_2, \dots, x_n)$, we want to estimate some features of the population. This part focus on parametric statistical inference, thus our task is to estimate/testing parameters.

☐ **Example of statistical inference**

- Sample item x_i, estimate its mean and variance
- Sample item $x_i = (\vec{x_i}, y_i)$, use multivariate linear model $Y \sim \vec{X}'\beta + \beta_0$, estimate slope & intercept β and variance σ^2

☐ **Two main tasks of Statistical Inference**

- Parameter Estimation
  - Point Estimation: section. 2.2
  - Interval Estimation: section. 2.3
- Hypothesis Testing: section. 2.4

Section 2.1 Statistical Model and Statistics

Random sample comes from population X. In parametric model case, we have population distribution family:

$$\mathscr{F} = \{f(x;\vec{\theta})|\vec{\theta} \in \Theta\} \tag{2.1}$$

where parameter $\vec{\theta}$ reflect some quantities of population (e.g. mean, variance, etc.), each $\vec{\theta}$ corresponds to a distribution of population X.

Sample space: Def. as $\mathscr{X} = \{\{x_1, x_2, \dots, x_n\}, \forall x_i\}$, then $\{X_i\} \in \mathscr{X}$ is random sample from population $X \sim f(x;\vec{\theta})$.

2.1.1 Statistics

Statistic(s): function of random sample $\vec{T}(X_1, X_2, \dots, X_n)$, **but not a function of parameter**.

Some useful statistics, e.g.

- Sample mean (Consider X_i i.i.d.)

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \tag{2.2}$$

- Sample variance

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2 \tag{2.3}$$

- Sample moments

- Origin moment

$$a_{n,k} = \frac{1}{n}\sum_{i=1}^{k} X_i^k \qquad k = 1, 2, 3, \dots \tag{2.4}$$

- Center moment

$$m_{n,k} = \frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^k \qquad k = 2, 3, 4, \dots \tag{2.5}$$

- Order statistics

$$(X_{(1)}, X_{(2)}, \dots, X_{(n)}),\ \text{for } X_{(1)} \le X_{(2)} \le \dots \le X_{(n)} \tag{2.6}$$

- Sample p-fractile

$$m_p = X_{(m)}, \quad m = \lfloor (n+1)p \rfloor \tag{2.7}$$

- Sample coefficient of variation

$$\hat{\nu} = \frac{S}{\bar{X}} \tag{2.8}$$

- Skewness and Kurtosis

$$\hat{g}_1 = \frac{m_{n,3}}{m_{n,2}^{3/2}} \qquad \hat{g}_2 = \frac{m_{n,4}}{m_{n,2}^2} - 3 \tag{2.9}$$

□ **Properties**

Statistic T is a function of random sample $\{X_i\}$, thus has distribution (say $g_T(t)$) called **Sampling Distribution**.

For X_i i.i.d. from $X \sim f(x)$ with population mean μ and variance σ^2

- Calculation of sample variance S^2

$$(n-1)S^2 = \sum_{i=1}^{n} x_i^2 - n\bar{x}^2 \tag{2.10}$$

- $\mathbb{E}$ and var of $\bar{X}$ and S^2

$$\mathbb{E}(\bar{X}) = \mu \qquad var(\bar{X}) = \frac{\sigma^2}{n} \qquad \mathbb{E}(S^2) = \sigma^2 \tag{2.11}$$

Further if X_i i.i.d. from $X \sim N(\mu, \sigma^2)$ where μ and σ^2 unknown.

- Independence of $\bar{X}$ and S^2

$$\bar{X} \perp\!\!\!\perp S^2 \tag{2.12}$$

  - Distribution of $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$

$$\bar{X} \sim N(\mu, \frac{\sigma^2}{n}) \tag{2.13}$$

  - Distribution of $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$

$$\frac{(n-1)S^2}{\sigma^2} \sim \chi^2_{n-1} \tag{2.14}$$

Comment: the independence here can explain the $n-1$ degree of freedom of χ^2_{n-1}

2.1.2 Exponential Family

Def. $\mathscr{F}_\Theta = \{f(x;\vec{\theta}|\vec{\theta}\in\Theta)\}$ is **Exponential Family** if $f(x;\vec{\theta})$ has the form as

$$f(x;\vec{\theta}) = C(\vec{\theta})h(x)\exp\left[\sum_{i=1}^{k} Q_i(\vec{\theta})T_i(x)\right] \quad \vec{\theta}\in\Theta \tag{2.15}$$

Or equivalently express $c(\vec{\theta}) = \ln C(\vec{\theta})$:

$$f(x;\vec{\theta}) = h(x)\exp\left[\sum_{i=1}^{k} Q_i(\vec{\theta})T_i(x) + c(\vec{\theta})\right] \quad \vec{\theta}\in\Theta \tag{2.16}$$

Canonical Form: Take $Q_i(\vec{\theta}) = \varphi_i$, then $\vec{\varphi} = (\varphi_1, \varphi_2, \ldots, \varphi_k)$ =$(Q_1(\vec{\theta}), Q_2(\vec{\theta}), \ldots, Q_k(\vec{\theta}))$ is a transform from Θ to Θ^*, s.t. $\mathscr{F}$ has canonical form, i.e.

$$f(x;\vec{\varphi}) = C^*(\vec{\varphi})h(x)\exp\left[\sum_{i=1}^{k} \varphi_i T_i(x)\right] \quad \vec{\varphi}\in\Theta^* \tag{2.17}$$

Θ^* is canonical parameter space.

□ **Why we need exponential family? It has some nice properties.**

2.1.3 Sufficient and Complete Statistics

Note: For simplification, the following parts denote $\vec{\theta}, \vec{T}, \ldots$ as $\theta, T, \ldots$ etc.

► A **Sufficient Statistic** $T(\vec{X})$ for θ contains all the information of sample when infer θ, i.e.

$$f(\vec{X};T(\vec{X})) = f(\vec{X};T(\vec{X}),\theta) \tag{2.18}$$

Properties

- **Factorization Thm.** $T(\vec{X})$ is sufficient **if and only if** $f_{\vec{X}}(\vec{x};\theta) = f(\vec{x};\theta)$ can be written as

$$f(\vec{x};\theta) = g[t(\vec{x});\theta]h(\vec{x}) \tag{2.19}$$

- If $T(\vec{X})$ sufficient, then $T'(\vec{X}) = g[T(\vec{X})]$ also.(require g single-valued and invertible)
- If $T(\vec{X})$ sufficient, then (T, T_1) also.
- Minimal sufficient statistic $T_\theta(\vec{X})$ satisfies

$$\forall \text{sufficient statistic } S,\ \exists\, q_S(\cdot),\ \text{s.t.} T_\theta = q_S(S) \tag{2.20}$$

  A minimal sufficient statistic not always exists.

  Sufficient & Complete $\Rightarrow$ Minimal sufficient.
- Usually dimension of $\vec{T}_\theta$ and θ equals.

Sufficient statistic is **not** unique.

- A **Complete Statistic** $T(\vec{X})$ for θ satisfies

$$\forall\theta \in \Theta\,;\, \forall\varphi \text{ satisfies } \mathbb{E}[\varphi(T(\vec{X}))] = 0, \text{ we have } \mathbb{P}[\varphi(T) = 0; \theta] = 1 \tag{2.21}$$

  Explanation: $T \sim g_T(t)$. Rewrite as

$$\int \varphi(t) g_T(t)\,\mathrm{d}t = 0 \;\Rightarrow \varphi(T) = 0 \text{ a.s. } \forall\,\theta \tag{2.22}$$

  i.e. span$\{g_T(t); \forall\theta\}$ is a complete space. Or to say that $\nexists$ none-zero $\varphi(t)$ so that $\mathbb{E}(\varphi(T)) = 0$ (unbiased estimation)

$$\varphi(T) \neq 0\ \forall\theta \Rightarrow \mathbb{E}[\varphi(T(\vec{X}))] \neq 0 \tag{2.23}$$

  So make sure the uniqueness of unbiased estimation of $\hat{\theta}$ using T.

  Properties

  - If $T(\vec{X})$ complete, then $T'(\vec{X}) = g[T(\vec{X})]$ also.(require g measurable)
  - A complete statistic not always exists.

- An **Ancillary Statistic** $S(\vec{X})$ is a statistic whose distribution does not depend on θ

  Basu Thm.: $\vec{X} = (X_1, X_2, \ldots, X_n)$ is sample from $\mathscr{F} = \{f(x;\theta), \theta \in \Theta\}$. $T(\vec{X})$ is a complete and minimal sufficient statistic, $S(\vec{X})$ is ancillary statistic, then $S(\vec{X}) \perp\!\!\!\perp T(\vec{X})$.

- Exponential family: For $\vec{X} = (X_1, X_2, \ldots, X_n)$ from exponential family with canonical form, i.e.

$$f(\vec{x};\theta) = C(\theta)h(\vec{x})\exp\left[\sum_{i=1}^{k}\theta_i T_i(\vec{x})\right], \quad \theta \in \Theta \tag{2.24}$$

  Then if $\Theta \in \mathbb{R}^k$ interior point exists, then $T(\vec{X}) = (T_1(\vec{X}), T_2(\vec{X}), \ldots, T_k(\vec{X}))$ is sufficient & complete statistic.

Section 2.2 Point Estimation

For parametric distribution family $\mathscr{F} = \{f(x,\theta), \theta \in \Theta\}$, random sample $\vec{X} = (X_1, X_2, \ldots, X_n)$ from $\mathscr{F}$. $g(\theta)$ is a function defined on Θ.

Mission: use sample $\{X_i\}$ to estimate $g(\theta)$, called **Parameter Estimation**.

$$\text{Parameter Estimation}\begin{cases}\text{Point Estimation} & \surd\\ \text{Interval Estimation}\end{cases} \tag{2.25}$$

Point estimation: when estimating θ or $g(\theta)$, denote the estimator (defined on sample space $\mathscr{X}$) as

$$\hat{\theta}(\vec{X}) \qquad \hat{g}(\vec{X}) \tag{2.26}$$

Estimator is a statistic, with sampling distribution.

2.2.1 Optimal Criterion

Some nice properties of estimators (that we expect)

- Unbiasedness

$$\mathbb{E}(\hat{\theta}) = \theta \quad \text{or} \quad \mathbb{E}(\hat{g}(\vec{X})) = g(\theta) \tag{2.27}$$

  Otherwise, say $\hat{\theta}$ or $\hat{g}$ biased. Def. **Bias**: $\mathbb{E}(\hat{\theta}) - \theta$

  Asymptotically unbiasedness with n as sample size

$$\lim_{n\to\infty} E(\hat{g}_n(\vec{X})) = g(\theta) \tag{2.28}$$

- Efficiency: say $\hat{g}_1(\vec{X})$ is more efficient than $\hat{g}_2(\vec{X})$, if

$$var(\hat{g}_1) \leq var(\hat{g}_2) \quad \forall \theta \in \Theta \tag{2.29}$$

- Mean Squared Error (MSE): Bias-Variance Trade-Off

$$\text{MSE} = \mathbb{E}[(\hat{\theta} - \theta)^2] = var(\hat{\theta}) + [Bias(\hat{\theta})]^2 \tag{2.30}$$

  For unbiased estimator, i.e. $Bias(\hat{\theta}) = 0$, we have

$$\text{MSE} = \mathbb{E}[(\hat{\theta} - \theta)^2] = var(\hat{\theta}) \tag{2.31}$$

- (Weak) Consistency

$$\lim_{n\to\infty} \mathbb{P}(|\hat{g}_n(\vec{X}) - g(\theta)| \geq \varepsilon) = 0 \quad \forall \varepsilon > 0 \tag{2.32}$$

- Asymptotic Normality

2.2.2 Method of Moments

Review: Population moments & Sample moments

$$\alpha_k = \mathbb{E}(X^k) \qquad\qquad \mu_k = \mathbb{E}[(X - \mathbb{E}(X))^k]$$

$$a_{n,k} = \hat{\alpha}_k = \frac{1}{n}\sum_{i=1}^n X_i^k \qquad\qquad m_{n,k} = \hat{\mu}_k = \frac{1}{n}\sum_{i=1}^n (X_i - \bar{X})^k$$

Property: $a_{n,k}$ is the unbiased estimator of α_k.(while $m_{n,k}$ unually biased for μ_k)

For sample $\vec{X} = (X_1, X_2, \ldots, X_n)$ from $\mathscr{F} = \{f(x; \theta, \theta \in \Theta)\}$, unknown parameter (or its function) $g(\theta)$ can be written as

$$g(\theta) = G(\alpha_1, \alpha_2, \ldots, \alpha_k; \mu_2, \mu_3, \ldots, \mu_l) \tag{2.33}$$

Then its **Moment Estimate** $\hat{g}(\vec{X})$ is

$$\hat{g}(\vec{X}) = G(a_{n,1}, a_{n,2}, \ldots, a_{n,k}; m_{n,2}, m_{n,3}, \ldots, m_{n,l}) \tag{2.34}$$

Example: coefficient of variance & skewness

$$\hat{\nu} = \frac{S}{\bar{X}} \qquad \hat{\beta}_1 = \frac{m_{n,3}}{m_{n,2^{3/2}}} = \sqrt{n}\frac{\sum_{i=1}^{n}(X_i - \bar{X})^3}{\left[\sum_{i=1}^{n}(X_i - \bar{X})^2\right]^{\frac{3}{2}}} \tag{2.35}$$

☐ **Note:**

- G may not have explicit expression.
- Moment estimate may not be unique.
- If $G = \sum_{i=1}^{k} c_i \alpha_i$ (linear combination of α, without μ), then $\hat{g}(\vec{X}) = \sum_{i=1}^{k} c_i a_{n,i}$ unbiased.

  Usually $\hat{g}(\vec{X})$ is asymptotically unbiased.
- For small sample, not so accurate.
- May not contain all the information about θ, i.e. may not be sufficient statistic.
- Do not require a statistic model.

2.2.3 Maximum Likelihood Estimation

For sample $\vec{X} = (X_1, X_2, \ldots, X_n)$ with distribution $f(\vec{x};\theta)$ from $\mathscr{F} = \{f(x;\theta), \theta \in \Theta\}$, def. **Likelihood Function** $L(\theta;\vec{x})$, defined on Θ (as a function of θ)

$$L(\theta;\vec{x}) = f(\vec{x};\theta) \qquad \theta \in \Theta,\, \vec{x} \in \mathscr{X} \tag{2.36}$$

Also def. log-likelihood function $l(\theta;\vec{x}) = \ln L(\theta;\vec{x})$.

If estimator $\hat{\theta} = \hat{\theta}(\vec{X})$ satisfies

$$L(\hat{\theta};\vec{x}) = \sup_{\theta\in\Theta} L(\theta;\vec{x}), \quad \vec{x} \in \mathscr{X} \tag{2.37}$$

Or equivalently take $l(\theta;\vec{x})$ instead of $L(\theta;\vec{x})$.

Then $\hat{\theta} = \hat{\theta}(\vec{X})$ is a **Maximum Likelihood Estimate**(MLE) of $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$

How to identify MLE?

- Differentiation: Fermat Lemma

$$\left.\frac{\partial L}{\partial \theta_i}\right|_{\theta=\hat{\theta}} = 0 \qquad \left.\frac{\partial^2 L}{\partial \theta_i \partial \theta_j}\right|_{\theta=\hat{\theta}} \text{negative definite} \qquad \forall i, j = 1, 2, \ldots, k \tag{2.38}$$

- Graphing method.
- Numerically compute maximum.

☐ **Some properties of MLE**

- (Depend on the case, not always) unbiased.

- Invariance of MLE: If $\hat{\theta}$ is MLE of θ, invertible function $g(\theta)$, then $g(\hat{\theta})$ is MLE of $g(\theta)$.

- MLE and Sufficiency: $T = T(X_1, X_2, \ldots, X_n)$ is a sufficient statistic of θ, if MLE of θ exists, say $\hat{\theta}$, then $\hat{\theta}$ is a function of T, i.e.
$$\hat{\theta} = \hat{\theta}(\vec{X}) = \hat{\theta}^*(T(\vec{X})) \tag{2.39}$$

- Asymptotic Normality:
$$\sqrt{n}(\hat{\theta}_n - \theta) \xrightarrow{d} N(0, \sigma_\theta^2), \quad \sigma_\theta^2 = \frac{1}{\mathbb{E}_\theta[\frac{\partial}{\partial\theta} \ln f(\vec{X};\theta)]^2} \tag{2.40}$$
i.e.
$$\hat{\theta}_n \xrightarrow{d} N(\theta, \frac{\sigma_\theta^2}{n}) \tag{2.41}$$

□ **Comparison: MoM and MLE**

- MoM do not require statistic model; MLE need to know PDF.

- MoM is more robust than MLE.

MLE in Exponential Family:

For sample $\vec{X} = (X_1, X_2, \ldots, X_n)$ from canonical exponential family $\mathscr{F} = \{f(x;\theta), \theta \in \Theta\}$
$$f(x;\theta) = C(\theta)h(x)\exp\left[\sum_{i=1}^k \theta_i T_i(x)\right] \quad \theta = (\theta_1, \ldots, \theta_k) \in \Theta \tag{2.42}$$

Likelihood function $L(\theta, \vec{x}) = \prod_{j=i}^n f(x_j;\theta)$ and log-likelihood function $l(\theta, \vec{x})$
$$L(\theta, \vec{x}) = C^n(\theta)\prod_{j=1}^n h(x_j)\exp\left[\sum_{i=1}^k \theta_i \sum_{j=1}^n T_i(x_j)\right]$$
$$\ell(\theta, \vec{x}) = n\ln C(\theta) + \sum_{j=1}^n \ln h(x_j) + \sum_{i=1}^k \theta_i \sum_{j=1}^n T_i(x_j)$$

Solution of MLE: (Require $\hat{\theta} \in \Theta$)
$$\frac{n}{C(\theta)}\frac{\partial C(\theta)}{\partial\theta_i}\bigg|_{\theta=\hat{\theta}} = -\sum_{j=1}^n T_i(x_j), \quad i = 1, 2, \ldots, k \tag{2.43}$$

2.2.4 Uniformly Minimum Variance Unbiased Estimator

MSE: For $\hat{g}(\vec{X})$ is estimate of $g(\theta)$,then MSE
$$\text{MSE}(\hat{g}(\vec{X})) = \mathbb{E}[(\hat{g}(\vec{X}) - g(\theta))^2] = var(\hat{g}) + [Bias(\hat{g})]^2 \tag{2.44}$$

Note: Unbiased estimator (i.e. $Bias(\hat{g}) = 0$) is not unique; ang not always exists.

Now only consider unbiased estimators of $g(\theta)$ exists, say $\hat{g}(\vec{X})$, then
$$\text{MSE}(\hat{g}(\vec{X})) = var(\hat{g}(\vec{X})) \tag{2.45}$$

If $\forall$ unbiased estimate $\hat{g}\prime(\vec{X})$, $\hat{g}$ satisfies

$$var[\hat{g}(\vec{X})] \leq var[\hat{g}\prime(\vec{X})] \tag{2.46}$$

☐ **Then $\hat{g}(\vec{X})$ is Uniformly Minimum Variance Unbiased Estimator(UMVUE) of $g(\theta)$**

How to determine UMVUE? (Not an easy task)

- Zero Unbiased Estimate Method
- Sufficient and Complete Statistic Method
- Cramer-Rao Inequality

1. **Zero Unbiased Estimate Method**

   Let $\hat{g}(\vec{X})$ be an unbiased estimate with $var(\hat{g}) < \infty$. If $\forall\ \mathbb{E}(\hat{l}(\vec{X})) = 0$, $\hat{g}$ holds that

   $$cov(\hat{g}, \hat{l}) = \mathbb{E}(\hat{g} \cdot \hat{l}) = 0, \quad \forall \theta \in \Theta \tag{2.47}$$

   Then $\hat{g}$ is a UMVUE of $g(\theta)$ (sufficient & necessary).

2. **Sufficient and Complete Statistic Method**

   For $T(\vec{X})$ sufficient statistic, $\hat{g}(\vec{X})$ unbiased estimate of $g(\theta)$, then

   $$h(T) = \mathbb{E}(\hat{g}(\vec{X})|T) \tag{2.48}$$

   is an unbiased estimate of $g(\theta)$ and $var(h(T)) \leq var(\hat{g})$.

   Remark:

   - A method to improve estimator.
   - A UMVUE has to be a function of sufficient statistic.

   Lehmann-Scheffé Thm.: For $\vec{X} = (X_1, X_2, \ldots, X_n)$ from population $X \sim \mathscr{F} = \{f(x;\theta) : \vec{\theta} \in \Theta\}$. $T(\vec{X})$ sufficient and complete, and $\hat{g}(T(\vec{X}))$ be an unbiased estimator, then $\hat{g}(T(\vec{X}))$ is the unique UMVUE.

   Can be used to construct UMVUE: given $T(\vec{X})$ sufficient and complete and some unbiased estimator $\hat{g}\prime(\theta)$ then

   $$\hat{g}(T) = \mathbb{E}(\hat{g}\prime|T) \tag{2.49}$$

   is the unique UMVUE.

3. **Cramer-Rao Inequality**

   Core idea: determine a lower bound of $var(\hat{g})$.

   Consider $\theta = \theta$ (One dimension parameter); For $\{X_i\}$ i.i.d. $f(x, \theta)$: def.

- **Score function**: Reflects the steepness/slope of likelihood function.

$$S(\vec{x};\theta)=\frac{\partial \ln f(\vec{x};\theta)}{\partial \theta}=\frac{\partial \ell(\theta;\vec{x})}{\partial \theta}=\sum_{i=1}^{n}\frac{\partial \ln f(x_i;\theta)}{\partial \theta} \tag{2.50}$$

  Property:[1]

$$\mathbb{E}[S(\vec{X};\theta)]=0 \tag{2.51}$$

- **Fisher Information**: Variance of $S(\vec{x};\theta)$, reflects the accuracy to conduct estimation, i.e. reflects information of statistic model that sample brings.[2]

$$I(\theta)=\mathbb{E}\left[\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial \theta}\right)^2\right]=-\mathbb{E}\left[\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial \theta^2}\right] \tag{2.52}$$

Consider $\mathscr{F}$ satisfies some regularity conditions(in most cases, regularity conditions do hold), then the lower bound of $var(\hat{g})$ satisfies **Cramer-Rao Inequality**:

$$var(\hat{g}(\vec{X}))\geq\frac{[g'(\theta)]^2}{nI(\theta)} \tag{2.53}$$

Special case: $g(\theta)=\theta$ then

$$var(\hat{\theta})\geq\frac{1}{nI(\theta)} \tag{2.54}$$

note:

- C-R Inequality determine a lower bound, not the infimum(i.e. UMVUE$\nRightarrow$ $var(\hat{g}(\vec{X}))=\frac{[g'(\theta)]^2}{nI(\theta)}$).
- Take '=': Only some cases in Exponential family.
- **Efficiency**: How good the estimator is.

$$e_{\hat{g}(\vec{X})}(\theta)=\frac{[g'(\theta)]^2/(nI(\theta))}{var(\hat{g}(\vec{X}))} \tag{2.55}$$

---

[1] Proof of $\mathbb{E}(S(\vec{x};\theta))=0$:

$$\begin{aligned}\mathbb{E}(S|\theta)&=\int f(\vec{x};\theta)\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}\,\mathrm{d}\vec{x}\\&=\int f(\vec{x};\theta)\frac{1}{f(\vec{x};\theta)}\frac{\partial f(\vec{x};\theta)}{\partial\theta}\,\mathrm{d}\vec{x}\\&=\frac{\partial}{\partial\theta}\int f(\vec{x};\theta)\,\mathrm{d}\vec{x}=\frac{\partial}{\partial\theta}1=0\end{aligned}$$

[2] Proof of $I(\theta)=\mathbb{E}\left[\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial \theta}\right)^2\right]=-\mathbb{E}\left[\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial \theta^2}\right]$:

$$\begin{aligned}0&=\frac{\partial}{\partial\theta^T}\mathbb{E}(S|\theta)\\&=\int\frac{\partial}{\partial\theta^T}\left\{\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}f(\vec{x};\theta)\right\}\mathrm{d}\vec{x}\\&=\int\left\{\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial\theta\partial\theta^T}f(\vec{x};\theta)+\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}\frac{\partial f(\vec{x};\theta)}{\partial\theta^T}\right\}\mathrm{d}\vec{x}\\&=\int\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial\theta\partial\theta^T}f(\vec{x};\theta)\,\mathrm{d}\vec{x}+\int\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta^T}f(\vec{x};\theta)\,\mathrm{d}\vec{x}\\&=\mathbb{E}\left(\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial\theta\partial\theta^T}\right)+\mathbb{E}\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta^T}\right)\\\Rightarrow\mathbb{E}\left(\frac{\partial^2 \ln f(\vec{x};\theta)}{\partial\theta\partial\theta^T}\right)&=-\mathbb{E}\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta}\frac{\partial \ln f(\vec{x};\theta)}{\partial\theta^T}\right)\end{aligned}$$

4. **Multi-Dimensional Cramer-Rao Inequality** ReDef. Fisher Information:

$$\mathbf{I}(\theta) = \{I_{ij}(\theta)\} = \{\mathbb{E}\left[\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial \theta_i}\right)\left(\frac{\partial \ln f(\vec{x};\theta)}{\partial \theta_j}\right)\right]\} \tag{2.56}$$

Then covariance matrix $\Sigma(\theta)$ satisfies **Cramer-Rao Inequality**

$$\Sigma(\theta) \succeq (n\mathbf{I}(\theta))^{-1} \tag{2.57}$$

Note: '$\succeq$' holds for all diagonal elements, i.e.

$$var(\hat{\theta}_i) \geq \frac{I^*_{ii}(\theta)}{n}, \quad \forall\, i = 1, 2, \ldots, k \tag{2.58}$$

2.2.5 MoM and MLE in Linear Regression

Note: More detailed knowledge see Chapter. 3 Linear Regression Analysis.

☐ **Linear Regression Model(1-dimension case):**

$$y_i = \beta_0 + \beta_1 x_0 + \epsilon_i \tag{2.59}$$

where β_0, β_1 are regression coefficient, and ϵ_i are unknown random **error**.

Basic Assumptions (Guass-Markov Assumption):

$$\text{Zero-Mean: } \epsilon_i \text{ are i.i.d.}$$
$$\text{Homogeneity of Variance: } \mathbb{E}(\epsilon_i|x_i) = 0$$
$$\text{Independent: } var(\epsilon_i) = \sigma^2$$

Mission: use data $\{(x_i, y_i)\}$ to estimate β_0, β_1(i.e. regression line), and error ϵ_i.

1. OLS (Ordinary Least Squares): Take β_0, β_1 so that MSE min, i.e. SSE min

$$(\hat{\beta}_0, \hat{\beta}_1) = \arg\min \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 \tag{2.60}$$

(Express in Matrix Notation equation. 2.75, so that it can be generalized to multidimensional case) SSE can be expressed as the **Euclean Distance** between $\{y_i\}$ and $\{\hat{\beta}_0 + \hat{\beta}_1 x_i\}$, i.e.

$$\arg\min D(y, X\hat{\beta}) \tag{2.61}$$

i.e. $\hat{\beta}$ is the Projection of y onto hyperplane X, then

$$(X\hat{\beta})^T (y - X\hat{\beta}) = 0 \Rightarrow \hat{\beta} = (X^T X)^{-1} X^T y \tag{2.62}$$

Solution for 1-D case:

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \begin{bmatrix} \bar{y} - \hat{\beta}_1 \bar{x} \\ \dfrac{\sum\limits_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum\limits_{i=1}^{n} (x_i - \bar{x})^2} \end{bmatrix} \tag{2.63}$$

So get regression line:$y = \hat{\beta}_0 + \hat{\beta}_1 x$

Def. Residuals

$$e_i = \hat{\epsilon}_i = y_i - \hat{y}_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i) \tag{2.64}$$

Residuals can be used to estimate ϵ_i: $E[(\epsilon_i)^2] = \sigma^2$

$$\hat{\sigma^2} = \frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \tag{2.65}$$

2. MoM: Consider r.v. $\epsilon \sim f(\varepsilon; x, y, \beta_0, \beta_1)$, sample $\{\epsilon_i | \epsilon_i = y_i - \beta_0 - \beta_1 x_i\}$, then obviously

$$\bar{\epsilon} = \bar{y} - \beta_0 - \beta_1 \bar{x} \tag{2.66}$$

Take moment estimate of ϵ, we have

$$\mathbb{E}(\epsilon_i) = 0 \qquad \mathbb{E}(\epsilon_i x_i) = 0 \text{ (note that } \mathbb{E}(\epsilon|x) = 0) \tag{2.67}$$

$$\text{i.e.} \begin{cases} \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) = 0 \\ \frac{1}{n}\sum_{i=1}^{n} x_i(y_i - \beta_0 - \beta_1 x_i) = 0 \end{cases} \tag{2.68}$$

Solution:

$$\begin{cases} \hat{\beta}_0 & = \bar{y} - \beta_1 \bar{x} \\ \hat{\beta}_1 & = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \end{cases} \tag{2.69}$$

(the same as OLS)

Moment estimate of σ^2

$$\hat{\sigma}_n^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \tag{2.70}$$

3. MLE: Assume $\epsilon_i \sim N(0, \sigma^2)$, then $y_i | x_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$. Get likelihood function:

$$L(\beta_0, \beta_1, \sigma^2; x_1, \ldots, x_n, y_1, \ldots, y_n) = (2\pi\sigma^2)^{-\frac{n}{2}} \exp\left[-\frac{\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)}{2\sigma^2}\right] \tag{2.71}$$

Log-likelihood:

$$\ell(\beta_0, \beta_1, \sigma^2; x_1, \ldots, x_n, y_1, \ldots, y_n) = -\frac{n}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2 \tag{2.72}$$

MLE, use Fermat Lemma:

$$\begin{cases} \frac{\partial l}{\partial \beta_0} = 0 & \Rightarrow -\frac{1}{\sigma^2}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) = 0 \\ \frac{\partial l}{\partial \beta_1} = 0 & \Rightarrow -\frac{1}{\sigma^2}\sum_{i=1}^{n} x_i(y_i - \beta_0 - \beta_1 x_i) = 0 \\ \frac{\partial l}{\partial \sigma^2} = 0 & \Rightarrow -\frac{n}{2}\frac{1}{\sigma^2} + \frac{1}{2(\sigma^2)^2}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) = 0 \end{cases} \tag{2.73}$$

Solution:

$$\hat{\beta}_0 = \bar{y} - \beta_1 \bar{x}$$
$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
$$\hat{\sigma}_n^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)$$

☐ **Linear Regression Model(Multi-dimension case):**

Detailed derivation see section. 3.3

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \epsilon_i \tag{2.74}$$

Denote: $\vec{\beta} = (\beta_0, \beta_1, \ldots, \beta_p)$, $\vec{x}_i = (1, x_{i1}, x_{i2}, \ldots, x_{ip})$, then for each i: $y_i = x_i^T \beta + \epsilon_i$

Further denote: Matrix form:

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \ldots & x_{1p} \\ 1 & x_{21} & \ldots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{np} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix} = X\vec{\beta} + \vec{\epsilon} \tag{2.75}$$

Basic Assumptions: Gauss-Markov Assumptions

- OLS unbiased

$$\mathbb{E}(\epsilon_i | x_i) = 0 \qquad \mathbb{E}(y_i | x_i) = x_i^T \beta \tag{2.76}$$

- Homogeneity of ϵ_i

$$var(\epsilon_i) = \sigma^2 \tag{2.77}$$

- Independent of ϵ

- (For MLE) ϵ_i i.i.d. $\sim N(0, \sigma^2)$

Residuals:

$$e_i = \hat{\epsilon}_i = y_i - \hat{y}_i = y_i - x_i^T \hat{\beta} \tag{2.78}$$

Def. Error Sum of Squares (SSE)

$$\text{SSE} = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2 \tag{2.79}$$

Estimator exists and unique:($\hat{\sigma}^2$ is after bias correction)

$$\hat{\beta} = (X^T X)^{-1} X^T y$$
$$\hat{\sigma}_n^2 = \frac{1}{n} \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2$$
$$\hat{\sigma}^2 = \frac{1}{n-p-1} \sum_{i=1}^n (y_i - x_i^T \hat{\beta})^2 \tag{2.80}$$

2.2.6 Kernel Density Estimation

Given random sample $\{X_i\}$. Def. Empirical CDF.

$$\hat{F}_n(x) = \frac{1}{n}\sum_{i=1}^{n} I_{(-\infty,x]}(X_i) \tag{2.81}$$

Problem: Overfitting when getting $\hat{f}$. Solution: Using **Kernel Estimate**, replace $I_{(-\infty,x]}(\cdot)$ with Kernel function $K(\cdot)$, then

$$\hat{f}_n(x) = \frac{F_n(x+h_n) - F - n(x-h_n)}{2h_n} = \frac{1}{nh_n}\sum_{i=1}^{n} K(\frac{x-X_i}{h_n}) \tag{2.82}$$

where h_n is **bandwidth**. Take proper kernel function K to get estimate of f.

Can be considered as a convolution of sample $\{X_i\}$ and kernel function K.

Useful Kernel Functions:

$$K(x) := \begin{cases} \mathbb{I}_{[-\frac{1}{2},\frac{1}{2}]}, & \text{Square Kernel} \\ (1-|x|)\mathbb{I}_{[-1,1]}, & \text{Triangle Kernel} \\ \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}, & \text{Gaussian Kernel} \\ \frac{1}{\pi(1+x^2)}, & \text{Cauchy Kernel} \\ \frac{1}{2\pi}\text{sinc}^2\frac{x}{2} = \frac{1}{2\pi}\left(\frac{\sin x/2}{x/2}\right)^2, & \text{sinc Kernel} \end{cases}$$

Section 2.3 Interval Estimation

$$\text{Parameter Estimation} \begin{cases} \text{Point Estimation} \\ \text{Interval Estimation} \quad \checkmark \end{cases} \tag{2.83}$$

Interval Estimation: to estimate $g(\theta)$, give **two** estimators $\hat{g}_1(\vec{X})$, $\hat{g}_2(\vec{X})$ defined on $\mathscr{X}$ as the two ends of interval (i.e. give an interval $[\hat{g}_1(\vec{X}),\ \hat{g}_2(\vec{X})]$), then random interval $[\hat{g}_1(\vec{X}),\ \hat{g}_2(\vec{X})]$ is an **Interval Estimation** of $g(\theta)$.

2.3.1 Confidence Interval

How to judge an interval estimation?

- Reliability

$$\mathbb{P}(g(\theta) \in [\hat{g}_1, \hat{g}_2]) \tag{2.84}$$

- Precision

$$\mathbb{E}(\hat{g}_2 - \hat{g}_1) \tag{2.85}$$

Trade off: (in most cases)

Given a level of reliability, find an interval with the highest precision above the level

☐ **For a given** $0 < \alpha < 1$**, if**

$$\mathbb{P}(\hat{g}_1 \leq g(\theta) \leq \hat{g}_2) \geq 1 - \alpha \tag{2.86}$$

then $[\hat{g}_1, \hat{g}_2]$ is a **Confidence Interval** for $g(\theta)$, with **Confidence Level** $1 - \alpha$.

Confidence Coefficient:

$$\inf_{\forall \theta \in \Theta} \mathbb{P}(\theta \in \mathrm{CI}) \tag{2.87}$$

Other cases:

- **Confidence Limit**: (One-way) Upper/Lower Confidence Limit

$$\mathbb{P}(g \leq \hat{g}_U) \geq 1 - \alpha$$
$$\mathbb{P}(\hat{g}_L \leq g) \geq 1 - \alpha$$

- **Confidence Region**: For high dimensional parameters $\vec{g} = (g_1, g_2, \ldots, g_k)$

$$\mathbb{P}(\vec{g} \in S(\vec{X})) \geq 1 - \alpha \quad \forall \theta \in \Theta \tag{2.88}$$

Mission: Determine $\hat{g}_1, \hat{g}_2$.

2.3.2 Pivot Variable Method

Idea: Based on point estimation, construct a new variable and thus find the interval estimation.

Def. **Pivot Variable** T, satisfies:

- Expression of T contains θ (thus T is not a statistic).
- Distribution of T independent of θ.[3]

In different cases, construct different pivot variable, usually base on sufficient statistics and transform.

Knowing a proper pivot variable $T = T(\hat{\varphi}, g(\theta)) \sim f$, ($f$ is some distribution independent of θ), $\hat{\varphi}$ is a sufficient statistic), then we can take T satisfies:

$$\mathbb{P}(f_{1-\frac{\alpha}{2}} \leq T \leq f_{\frac{\alpha}{2}}) = 1 - \alpha \tag{2.89}$$

Construct the inverse mapping of $T = T(\hat{\varphi}, g(\theta)) \rightleftarrows g(\theta) = T^{-1}(T, \hat{\varphi})$, we get

$$\mathbb{P}[T^{-1}(f_{1-\frac{\alpha}{2}}, \hat{\varphi}) \leq \hat{g} \leq T^{-1}(f_{\frac{\alpha}{2}}, \hat{\varphi})] = 1 - \alpha \tag{2.90}$$

Thus get a confidence interval for θ with confidence coefficient $1 - \alpha$.

[3]Comment: $T(X, \theta)$ is both function of sample X an parameter in statistics model. Note that X also depends on θ, but is fixed once we complete a sample.

2.3.3 Confidence Interval for Common Distributions

Some important properties of χ^2, t and F see section. 1.8.2.

1. Single normal population: $\vec{X} = \{X_1, X_2, \ldots, X_n\} \in \mathscr{X}$ i.i.d from Normal Distribution population $N(\mu, \sigma^2)$. Denote sample mean and sample variance:

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \qquad S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2 \qquad S_\mu = \frac{1}{n}\sum_{i=1}^{n}(X_i - \mu)^2, \text{(for } \mu \text{ known)} \tag{2.91}$$

Estimating μ & σ^2: construction of pivot variable under different circumstances:

Estimation	Pivot Variable	Confidence Interval
σ^2 known, estimate μ	$T = \dfrac{\sqrt{n}(\bar{X} - \mu)}{\sigma} \sim N(0,1)$	$\left[\bar{X} - \dfrac{\sigma}{\sqrt{n}} N_{\frac{\alpha}{2}}, \bar{X} + \dfrac{\sigma}{\sqrt{n}} N_{\frac{\alpha}{2}}\right]$
σ^2 unknown, estimate μ	$T = \dfrac{\sqrt{n}(\bar{X} - \mu)}{S} \sim t_{n-1}$	$\left[\bar{X} - \dfrac{S}{\sqrt{n}} t_{n-1,\frac{\alpha}{2}}, \bar{X} + \dfrac{S}{\sqrt{n}} t_{n-1,\frac{\alpha}{2}}\right]$
μ known, estimate σ^2	$T = \dfrac{nS_\mu^2}{\sigma^2} \sim \chi_n^2$	$\left[\dfrac{nS_\mu^2}{\chi^2_{n,\frac{\alpha}{2}}}, \dfrac{nS_\mu^2}{\chi^2_{n,1-\frac{\alpha}{2}}}\right]$
μ unknown, estimate σ^2	$T = \dfrac{(n-1)S^2}{\sigma^2} \sim \chi^2_{n-1}$	$\left[\dfrac{(n-1)S^2}{\chi^2_{n-1,\frac{\alpha}{2}}}, \dfrac{(n-1)S^2}{\chi^2_{n-1,1-\frac{\alpha}{2}}}\right]$

2. Double normal population: $\vec{X} = \{X_1, X_2, \ldots, X_m\}$ i.i.d. from $N(\mu_1, \sigma_1^2)$; $\vec{Y} = \{Y_1, Y_2, \ldots, Y_n\}$ i.i.d. from $N(\mu_2, \sigma_2^2)$

   Denote sample mean, sample variance and pooled sample variance:

$$\bar{X} = \frac{1}{m}\sum_{i=1}^{n} X_i \qquad S_X^2 = \frac{1}{m-1}\sum_{i=1}^{m}(X_i - \bar{X})^2 \qquad S_{\mu_1}^2 = \frac{1}{m}\sum_{i=1}^{m}(X_i - \mu_1)^2, (\mu_1 \text{ known})$$

$$\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i \qquad S_Y^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \bar{Y})^2 \qquad S_{\mu_2}^2 = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \mu_2)^2, (\mu_2 \text{ known})$$

$$S_\omega^2 = \frac{(m-1)S_X^2 + (n-1)S_Y^2}{m+n-2}$$

   Estimating $\mu_1 - \mu_2$:

   When $\sigma_1^2 \neq \sigma_2^2$ unknown, estimate $\mu_1 - \mu_2$: Behrens-Fisher Problem, remain unsolved, but can deal with simplified cases.

Estimation	Pivot Variable	Confidence Interval
σ_1^2 & σ_2^2 known, estimate $\mu_1-\mu_2$	$T=\dfrac{\bar{X}-\bar{Y}-(\mu_1-\mu_2)}{\sqrt{\dfrac{\sigma_1^2}{m}+\dfrac{\sigma_2^2}{n}}}\sim N(0,1)$	$\left[\bar{X}-\bar{Y}-N_{\frac{\alpha}{2}}\sqrt{\dfrac{\sigma_1^2}{m}+\dfrac{\sigma_2^2}{n}},\ \bar{X}-\bar{Y}+N_{\frac{\alpha}{2}}\sqrt{\dfrac{\sigma_1^2}{m}+\dfrac{\sigma_2^2}{n}}\right]$
$\sigma_1^2=\sigma_2^2$ unknown, estimate $\mu_1-\mu_2$	$T=\dfrac{\bar{X}-\bar{Y}-(\mu_1-\mu_2)}{S_\omega\sqrt{\dfrac{1}{m}+\dfrac{1}{n}}}\sim t_{m+n-2}$	$\left[\bar{X}-\bar{Y}-S_\omega t_{m+n-2,\frac{\alpha}{2}}\sqrt{\dfrac{1}{m}+\dfrac{1}{n}},\ \bar{X}-\bar{Y}+S_\omega t_{m+n-2,\frac{\alpha}{2}}\sqrt{\dfrac{1}{m}+\dfrac{1}{n}}\right]$
Welch's t-Interval (when m, n large enough)	$T=\dfrac{\bar{X}-\bar{Y}-(\mu_1-\mu_2)}{\sqrt{\dfrac{S_X^2}{m}+\dfrac{S_Y^2}{n}}}\xrightarrow{\mathscr{L}}N(0,1)$	$\left[\bar{X}-\bar{Y}-N_{\frac{\alpha}{2}}\sqrt{\dfrac{S_1^2}{m}+\dfrac{S_2^2}{n}},\ \bar{X}-\bar{Y}+N_{\frac{\alpha}{2}}\sqrt{\dfrac{S_1^2}{m}+\dfrac{S_2^2}{n}}\right]$

Estimating $\dfrac{\sigma_1^2}{\sigma_2^2}$:

Estimation	Pivot Variable	Confidence Interval
μ_1,μ_2 known, estimate $\dfrac{\sigma_1^2}{\sigma_2^2}$	$T=\dfrac{S_{\mu_2}^2}{S_{\mu_1}^2}\dfrac{\sigma_1^2}{\sigma_2^2}\sim F_{n,m}$	$\left[\dfrac{S_{\mu_1}^2}{S_{\mu_2}^2}\dfrac{1}{F_{m,n,\frac{\alpha}{2}}},\dfrac{S_{\mu_1}^2}{S_{\mu_2}^2}\dfrac{1}{F_{m,n,1-\frac{\alpha}{2}}}\right]$ or $\left[\dfrac{S_{\mu_1}^2}{S_{\mu_2}^2}F_{m,n,\frac{\alpha}{2}},\dfrac{S_{\mu_1}^2}{S_{\mu_2}^2}F_{n,m,\frac{\alpha}{2}}\right]$
μ_1,μ_2 unknown, estimate $\dfrac{\sigma_1^2}{\sigma_2^2}$	$T=\dfrac{S_Y^2}{S_X^2}\dfrac{\sigma_1^2}{\sigma_2^2}\sim F_{n-1,m-1}$	$\left[\dfrac{S_X^2}{S_Y^2}\dfrac{1}{F_{m-1,n-1,\frac{\alpha}{2}}},\dfrac{S_X^2}{S_Y^2}\dfrac{1}{F_{m-1,n-1,1-\frac{\alpha}{2}}}\right]$ or $\left[\dfrac{S_X^2}{S_Y^2}\dfrac{1}{F_{m-1,n-1,\frac{\alpha}{2}}},\dfrac{S_X^2}{S_Y^2}F_{n-1,m-1,\frac{\alpha}{2}}\right]$

3. Non-normal population:

Estimation	Pivot Variable	Confidence Interval
Uniform Distribution: $\vec{X}$ i.i.d. from $U(0,\theta)$	$T=\dfrac{X_{(n)}}{\theta}\sim U(0,1)$	$\left[X_{(n)},\dfrac{X_{(n)}}{\sqrt[n]{\alpha}}\right]$
Exponential Distribution: $\vec{X}$ i.i.d. from $\epsilon(\lambda)$	$T=2n\lambda\bar{X}\sim\chi_{2n}^2$	$\left[\dfrac{\chi^2_{2n,1-\frac{\alpha}{2}}}{2n\bar{X}},\dfrac{\chi^2_{2n,\frac{\alpha}{2}}}{2n\bar{X}}\right]$
Bernoulli Distribution: $\vec{X}$ i.i.d. from $B(1,\theta)$	$T=\dfrac{\sqrt{n}(\bar{X}-\theta)}{\sqrt{\bar{X}(1-\bar{X})}}\xrightarrow{\mathscr{L}}N(0,1)$	$\left[\bar{X}-N_{\frac{\alpha}{2}}\sqrt{\dfrac{\bar{X}(1-\bar{X})}{n}},\bar{X}+N_{\frac{\alpha}{2}}\sqrt{\dfrac{\bar{X}(1-\bar{X})}{n}}\right]$
Poisson Distribution: $\vec{X}$ i.i.d. from $P(\lambda)$	$T=\dfrac{\sqrt{n}(\bar{X}-\lambda)}{\sqrt{\bar{X}}}\xrightarrow{\mathscr{L}}N(0,1)$	$\left[\bar{X}-N_{\frac{\alpha}{2}}\sqrt{\dfrac{\bar{X}}{n}},\bar{X}+N_{\frac{\alpha}{2}}\sqrt{\dfrac{\bar{X}}{n}}\right]$

4. General Case: Use asymptotic normality of MLE to construct CLT for large sample. MLE of θ satisfies:

$$\sqrt{n}(\hat{\theta}^* - \theta) \xrightarrow{\mathscr{L}} N(0, \frac{1}{I(\theta)}) \tag{2.92}$$

where $\hat{\theta}^*$ is MLE of θ. Replace $\dfrac{1}{I(\theta)}$ by $\sigma^2(\hat{\theta}^*)$, then

$$T = \frac{\sqrt{n}(\hat{\theta}^* - \theta)}{\sigma(\hat{\theta}^*)} \xrightarrow{\mathscr{L}} N(0,1) \tag{2.93}$$

confidence interval:

$$\left[\hat{\theta}^* - \frac{N_{\frac{\alpha}{2}}}{\sqrt{n}}\sigma(\hat{\theta}^*), \hat{\theta}^* + \frac{N_{\frac{\alpha}{2}}}{\sqrt{n}}\sigma(\hat{\theta}^*)\right] \tag{2.94}$$

2.3.4 Fisher Fiducial Argument*

Idea: When sample is known, we can get '**Fiducial Probability**' of θ, thus can find an interval estimation based on fiducial distribution.(Similar to the idea of MLE)

Remark: Fiducial probability (denoted as $\tilde{\mathbb{P}}(\theta)$) is 'probability of parameter', in the case that sample is known. **Fiducial probability is different from Probability**.

Thus get

$$\tilde{\mathbb{P}}(\hat{g}_1 \leq g(\theta) \leq \hat{g}_2) = 1 - \alpha \tag{2.95}$$

Section 2.4 Hypothesis Testing

Hypothesis is a statement about the characteristic of population, e.g. distribution form, parameters, etc.

Mission: Use sample to test the hypothesis, i.e. judge whether population has some characteristic.

2.4.1 Basic Concepts

Parametric hypothesis testing.

For random sample $\vec{X} = (X_1, X_2, \ldots, X_n) \in \mathscr{X}$ i.i.d. from $\mathscr{F} = \{f(x;\theta); \theta \in \Theta\}$

- Null Hypothesis H_0 & Alternative Hypothesis H_1: Wonder whether a statement is true. Def. **Null Hypothesis**: $H_0 : \theta \in \Theta_0 \subset \Theta$, **a statement that we try to reject based on sample**; $H_1 : \theta \in \Theta_1 = \Theta/\Theta_0$ is **Alternative Hypothesis**.

  ☐ **Note: Cannot exchange H_0 and H_1, because when the evidence is ambiguity, we have to accept H_0, regardless of what H_0 is. So it is very important to pick the proper H_0.**

  Thus Hypothesis Testing:

  $$H_0 : \theta \in \Theta_0 \longleftrightarrow H_1 : \theta \in \Theta_1 \tag{2.96}$$

- Rejection Region R & Acceptance Region R^C: Judge whether to reject H_0 from sample, Def. **Rejection Region**:

  $$R \subset \mathscr{X}: \text{reject } H_0 \text{ if } \vec{X} \in R \tag{2.97}$$

  Acceptance Region: accept H_0 if $\vec{X} \in R^C$

- Test Function: Describe how to make a decision.
  - Continuous Case:

$$\varphi(\vec{X}) = \begin{cases} 1, & \vec{X} \in R \\ 0, & \vec{X} \in R^{\complement} \end{cases} \tag{2.98}$$

i.e. $R = \{\vec{X} : \varphi(\vec{X}) = 1\}$. Where R to be determined.

  - Discrete Case: Randomized Test Function

$$\varphi(\vec{X}) = \begin{cases} 1, & \vec{X} \in R - \partial R \\ r, & \vec{X} \in \partial R \\ 0, & \vec{X} \in R^{\complement} \end{cases} \tag{2.99}$$

Where R and r to be determined. ∂R means the boundary of R

- Type I Error & Type II Error: Sample is random, possible to make a wrong judge.
  - Type I Error (弃真): H_0 is true but sample falls in R, thus H_0 is rejected.

$$\mathbb{P}(\text{type I error}) = \mathbb{P}(\vec{X} \in R | H_0) = \alpha(\theta) \tag{2.100}$$

  - Type II Error (取伪): H_0 is wrong but sample falls in R^C, thus H_0 is accepted.

$$\mathbb{P}(\text{type II error}) = \mathbb{P}(\vec{X} \notin R | H_1) = \beta(\theta) \tag{2.101}$$

		Judgement	
		Accept H_0	Reject H_0
Real Case	H_0	$\surd$	Type I Error
	H_1	Type II Error	$\surd$

表 1: 'Confusion Matrix'

Impossible to make probability of Type I & II Error small simultaneously, how to pick a proper test $\varphi(\vec{x})$?

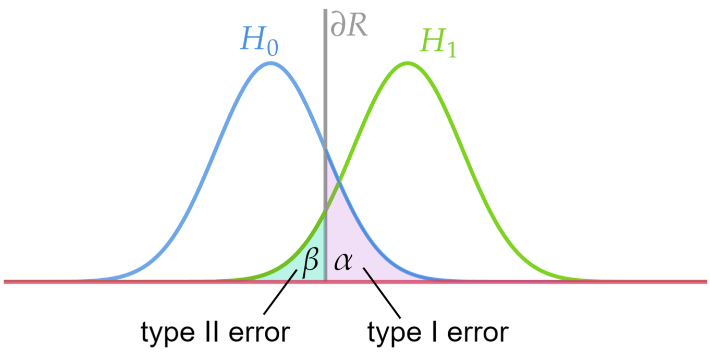


图 1: Illustration of type I&II error

☐ **Neyman-Pearson Principle: First control $\alpha \le \alpha_0$, then take $\min \beta$.**

How to determine α_0? Depend on specific problem.[4]

[4] In most cases, take $\alpha_0 = 0.05$.

- p-value: probability to get larger bias than observed $\vec{x}_0$ under H_0.

  e.g. For reject region $R = \{\vec{X}|T(\vec{X}) \geq C\}$, p-value:

$$p_{H_0}(\vec{x}) = \mathbb{P}[T(\vec{X}) \geq t(\vec{x}_0)|H_0] \tag{2.102}$$

  Remark: We believe that sample should reflect the property of model parameter, and p-value is that under H_0, the probability to get a **worse** result than $\vec{x}$.

  Rule: Reject H_0 if $p(\vec{x}_0) \leq \alpha_0$.

  Note: p-value is **different from** α or type I error. p-value is generated before we make decision while α arises after we decide how to make decisions. (But they do target the same result.)

- Power Function: (when H_0 is given), probability to reject H_0 by sampling.

$$\pi(\theta) = \begin{cases} \mathbb{P}(\text{type I error}), & \theta \in \Theta_0 \\ 1 - \mathbb{P}(\text{type II error}), & \theta \in \Theta_1 \end{cases} = \begin{cases} \alpha(\theta), & \theta \in \Theta_0 \\ 1 - \beta(\theta), & \theta \in \Theta_1 \end{cases} \tag{2.103}$$

  Express as test function:

$$\pi(\theta) = \mathbb{E}[\varphi(\vec{X})|\theta] \tag{2.104}$$

  A nice test: $\pi(\theta)$ small under H_0, large under H_1 (and grows very fast at the boundary of H_0 and H_1).

☐ **General Steps of Hypothesis Testing:**

1. Propose H_0 & H_1.
2. Determine R (usually in the form of a statistic, e.g. $R = \{\vec{X} : T(\vec{X}) \geq c\}$).
3. Select a proper α (to determine c).
4. Sampling, get sample (as well as $t(\vec{x})$), then
   - compare with R and determine whether to reject/accept H_0, or
   - calculate p-value and determine whether to reject/acceptH_0

2.4.2 Hypothesis Testing of Common Distributions

For some common distribution populations, determine rejection region R under certain H_0 with confidence coefficient α.

Definition of necessary statistics see section section. 2.3.3.

1. Single normal population:

Condition	H_0	H_1	Testing Statistic T	Rejection Region R
σ^2 known, test μ	$\mu = \mu_0$ $\mu \leq \mu_0$ $\mu \geq \mu_0$	$\mu \neq \mu_0$ $\mu > \mu_0$ $\mu < \mu_0$	$T = \frac{\sqrt{n}(\bar{X} - \mu_0)}{\sigma} \sim N(0,1)$	$\|T\| > N_{\frac{\alpha}{2}}$ $T > N_\alpha$ $T < -N_\alpha$
σ^2 unknown, test μ	$\mu = \mu_0$ $\mu \leq \mu_0$ $\mu \geq \mu_0$	$\mu \neq \mu_0$ $\mu > \mu_0$ $\mu < \mu_0$	$T = \frac{\sqrt{n}(\bar{X} - \mu_0)}{S} \sim t_{n-1}$	$\|T\| > t_{n-1,\frac{\alpha}{2}}$ $T > t_{n-1,\alpha}$ $T < -t_{n-1,\alpha}$
μ known, test σ^2	$\sigma^2 = \sigma_0^2$ $\sigma^2 \leq \sigma_0^2$ $\sigma^2 \geq \sigma_0^2$	$\sigma^2 \neq \sigma_0^2$ $\sigma^2 > \sigma_0^2$ $\sigma^2 < \sigma_0^2$	$T = \frac{nS_\mu^2}{\sigma_0^2} \sim \chi_n^2$	$T < \chi^2_{n,1-\frac{\alpha}{2}} \cup T > \chi^2_{n,\frac{\alpha}{2}}$ $T > \chi^2_{n,\alpha}$ $T < \chi^2_{n,1-\alpha}$
μ unknown, test σ^2	$\sigma^2 = \sigma_0^2$ $\sigma^2 \leq \sigma_0^2$ $\sigma^2 \geq \sigma_0^2$	$\sigma^2 \neq \sigma_0^2$ $\sigma^2 > \sigma_0^2$ $\sigma^2 < \sigma_0^2$	$T = \frac{(n-1)S^2}{\sigma_0^2} \sim \chi_{n-1}^2$	$T < \chi^2_{n-1,1-\frac{\alpha}{2}} \cup T > \chi^2_{n-1,\frac{\alpha}{2}}$ $T > \chi^2_{n-1,\alpha}$ $T < \chi^2_{n-1,1-\alpha}$

2. Double normal population:

Condition	H_0	H_1	Testing Statistic T	Rejection Region R
σ_1^2, σ_2^2 known, test $\mu_1 - \mu_2$	$\mu_1 - \mu_2 = \mu_0$ $\mu_1 - \mu_2 \leq \mu_0$ $\mu_1 - \mu_2 \geq \mu_0$	$\mu_1 - \mu_2 \neq \mu_0$ $\mu_1 - \mu_2 > \mu_0$ $\mu_1 - \mu_2 < \mu_0$	$T = \frac{\bar{X} - \bar{Y} - \mu_0}{\sqrt{\frac{\sigma_1^2}{m} + \frac{\sigma_2^2}{n}}} \sim N(0,1)$	$\|T\| > N_{\frac{\alpha}{2}}$ $T > N_\alpha$ $T < -N_\alpha$
σ_1^2, σ_2^2 unknown, test $\mu_1 - \mu_2$	$\mu_1 - \mu_2 = \mu_0$ $\mu_1 - \mu_2 \leq \mu_0$ $\mu_1 - \mu_2 \geq \mu_0$	$\mu_1 - \mu_2 \neq \mu_0$ $\mu_1 - \mu_2 > \mu_0$ $\mu_1 - \mu_2 < \mu_0$	$T = \frac{\bar{X} - \bar{Y} - \mu_0}{S_\omega}\sqrt{\frac{mn}{m+n}}$ $\sim t_{m+n-2}$	$\|T\| > t_{m+n-2,\frac{\alpha}{2}}$ $T > t_{m+n-2,\alpha}$ $T < -t_{m+n-2,\alpha}$
μ_1, μ_2 known, test $\frac{\sigma_1^2}{\sigma_2^2}$	$\sigma_1^2 = \sigma_2^2$ $\sigma_1^2 \geq \sigma_2^2$ $\sigma_1^2 \leq \sigma_2^2$	$\sigma_1^2 \neq \sigma_2^2$ $\sigma_1^2 < \sigma_2^2$ $\sigma_1^2 > \sigma_2^2$	$T = \frac{S_{\mu_2}^2}{S_{\mu_1}^2} \sim F_{n,m}$	$T < F_{n,m,1-\frac{\alpha}{2}}$ $\cup T > F_{n,m,\frac{\alpha}{2}}$ $T > F_{n,m,\alpha}$ $T < F_{n,m,1-\alpha}$
μ_1, μ_2 unknown, test $\frac{\sigma_1^2}{\sigma_2^2}$	$\sigma_1^2 = \sigma_2^2$ $\sigma_1^2 \geq \sigma_2^2$ $\sigma_1^2 \leq \sigma_2^2$	$\sigma_1^2 \neq \sigma_2^2$ $\sigma_1^2 < \sigma_2^2$ $\sigma_1^2 > \sigma_2^2$	$T = \frac{S_2^2}{S_2^2} \sim F_{n-1,m-1}$	$T < F_{n-1,m-1,1-\frac{\alpha}{2}}$ $\cup T > F_{n-1,m-1,\frac{\alpha}{2}}$ $T > F_{n-1,m-1,\alpha}$ $T < F_{n-1,m-1,1-\alpha}$

3. None normal population:

4. More than two normal population: Analysis of Variance.

Condition	H_0	H_1	Testing Statistic T	Rejection Region R
$\vec{X}$ from $B(1,p)$, test p	$p=p_0$	$p\neq p_0$	$T=\dfrac{\sqrt{n}(\bar{X}-p_0)}{\sqrt{p_0(1-p_0)}}\xrightarrow{\mathscr{L}}N(0,1)$	$\lvert T\rvert>N_{\frac{\alpha}{2}}$
$\vec{X}$ from $P(\lambda)$, test λ	$\lambda=\lambda_0$	$\lambda\neq\lambda_0$	$T=\dfrac{\sqrt{n}(\bar{X}-\lambda_0)}{\sqrt{\lambda_0}}\xrightarrow{\mathscr{L}}N(0,1)$	$\lvert T\rvert>N_{\frac{\alpha}{2}}$

2.4.3 Likelihood Ratio Test

Idea: To test $H_0:\theta\in\Theta_0\longleftrightarrow H_1:\theta\in\Theta_1$ known $\vec{x}$, examine the likelihood function $L(\theta;\vec{x})$ and **compare** $L_{\theta\in\Theta_0}$ and $L_{\theta\in\Theta}$ to see the likelihood that H_0 is true.

Def. **Likelihood Ratio** (LR):

$$\Lambda(\vec{x})=\frac{\sup\limits_{\theta\in\Theta_0}L(\theta;\vec{x})}{\sup\limits_{\theta\in\Theta}L(\theta;\vec{x})}\tag{2.105}$$

Reject H_0 if $\Lambda(\vec{x})<\Lambda_0$. Or equivalently: Reject H_0 if $-2\ln\Lambda(\vec{x})>C(=-2\ln\Lambda_0)$.

where Λ_0 (or equivalently $C=-2\ln\Lambda_0$) satisfies:

$$\mathbb{E}_{\Theta_0}[\varphi(\vec{X})]\leq\alpha,\quad\forall\theta\in\Theta_0\tag{2.106}$$

LR and sufficient statistic: $\Lambda(\vec{x})$ can be expressed as $\Lambda(\vec{x})=\Lambda^*(T(\vec{x}))$, where $T(\vec{X})$ is sufficient statistic.

□ **LRT for one-sample t-test: For $X_1,X_2,\ldots,X_n$ i.i.d. $\sim N(\mu,\sigma^2)$, test**

$$H_0:\mu=\mu_0\longleftrightarrow H_1:\mu\neq\mu_0\quad\textbf{when } \sigma^2 \textbf{ unknown}$$

Can prove:

$$\Lambda^{2/n}=\frac{\sum\limits_{i=1}^{n}(x_i-\bar{x})^2}{\sum\limits_{i=1}^{n}(x_i-\mu_0)^2}$$

Denote $T=\dfrac{\sqrt{n}(\bar{x}-\mu_0)}{S}$, then LRT is

$$\Lambda=\left(1+\frac{T^2}{n-1}\right)^{-n/2}$$

The Multivariate case see section. 4.2.4, where T^2 itself is the Hotelling's T^2 statistic.

□ **Limiting Distribution of LRT: Wilks' Thm.**

If $\dim\Theta=k>\dim\operatorname{span}\{\Theta_0\}=s$[5], then under $H_0:\theta\in\Theta_0$:

$$\Lambda_{\theta\in\Theta_0}(\vec{x})=-2\ln\lambda(\vec{x})\xrightarrow{\mathscr{L}}\chi^2_{k-s}\tag{2.107}$$

2.4.4 Uniformly Most Powerful Test

Idea: Neyman-Pearson Principle: control α, find min β. i.e. control α, find max $\pi(\theta)$

[5] Here 'dimension' refers to 'degree of freedom'.

Def. **Uniformly Most Powerful Test** (UMP) φ_{UMP} with level of significance α satisfies

$$\pi_{\text{UMP}}(\theta) \geq \pi(\theta),\ \forall\theta \in \Theta_1 \tag{2.108}$$

Neyman-Pearson Lemma: For $\vec{X} = (X_1, X_2, \ldots, X_n)$ i.i.d. from $f(\vec{x}; \theta)$.

Test hypothesis $H_0 : \theta = \theta_0 \longleftrightarrow H_1 : \theta = \theta_1$. Def. test function φ as:

$$\varphi(\vec{x}) = \begin{cases} 1, & \dfrac{f(\vec{x};\theta_1)}{f(\vec{x};\theta_0)} > C \\ r, & \dfrac{f(\vec{x};\theta_1)}{f(\vec{x};\theta_0)} = C \\ 0, & \dfrac{f(\vec{x};\theta_1)}{f(\vec{x};\theta_0)} < C \end{cases} \tag{2.109}$$

Then there exists C and r such that

- $\mathbb{E}[\varphi(\vec{x})|\theta_0] = \mathbb{P}(\dfrac{f(\vec{x};\theta_1)}{f(\vec{x};\theta_0)} > C) + r\mathbb{P}(\dfrac{f(\vec{x};\theta_1)}{f(\vec{x};\theta_0)} = C) = \alpha$
- This φ is UMP of level of significance α

Actually kind of 1-dimensional case of LRT.

Note: UMT exist for **simple** H_0, H_1, otherwise may not exist.

UMP and sufficient statistics: Test function $\varphi(\vec{X})$ given by equation. 2.109 is function of sufficient statistics $T(\vec{X})$, i.e. $\varphi(\vec{X}) = \varphi^*(T(\vec{X}))$.

UMP and Exponential Family: For sample $\vec{X} = (X_1, X_2, \ldots, X_n)$ from exponential family:

$$f(\vec{x};\theta) = C(\theta)h(\vec{x})\exp\{Q(\theta)T(\vec{x})\} \tag{2.110}$$

Test single hypothesis $H_0 : \theta = \theta_0 \longleftrightarrow H_1 : \theta = \theta_1$, (where $\theta_0 < \theta_1$). If

- θ_0 is inner point of Θ
- $Q(\theta)$ monotone increase with θ

Then UMP exists, in the form of:

$$\varphi(\vec{x}) = \begin{cases} 1, & T(\vec{x}) > C \\ r, & T(\vec{x}) = C \\ 0, & T(\vec{x}) < C \end{cases} \tag{2.111}$$

where C and r satisfies $\mathbb{E}[\varphi(\vec{x})|\theta_0] = \alpha$.

Note: or take $Q(\theta)$ mono decreased, then in equation. 2.111, take opposite inequality operators.

☐ **General Steps of UMP:**

1. Find a point $\theta_0 \in \Theta_0$ and a point $\theta_1 \in \Theta_1$. (Note: **one** point)
2. Construct test function in the form of equation. 2.109, use $\mathbb{E}[\varphi(\vec{x})|\theta_0] = \alpha$ to determine C and r.
3. Get R and $\varphi(\vec{x})$.
4. If φ does **not** depend on θ_1, then H_1 can be generalized to $H_1 : \theta \in \Theta_1$.
5. If φ satisfies $\mathbb{E}_{\theta\in\Theta_0}(\varphi) \leq \alpha$, then H_0 an be generalized to $H_0 : \theta \in \Theta_0$.

2.4.5 Duality of Hypothesis Testing and Interval Estimation

- Thm.: $\forall \theta_0 \in \Theta$ there exists hypothesis testing $H_0 : \theta = \theta_0 \longleftrightarrow H_1 : \theta \neq \theta_0$ of level α with rejection region R_{θ_0}. Then

$$C(\vec{X}) = \{\theta : \vec{X} \in R_\theta^C\} \tag{2.112}$$

  is a $1 - \alpha$ confidence region for θ

- Thm.: $C(\vec{X})$ is a $1 - \alpha$ confidence region for θ. Then $\forall \theta_0 \in C(\vec{X})$, the rejection region of hypothesis testing $H_0 : \theta = \theta_0 \longleftrightarrow H_1 : \theta \neq \theta_0$ of level α satisfies

$$R_{\theta_0}^{\complement} = \{\vec{X} : \theta_0 \in C(\vec{X})\} \tag{2.113}$$

☐ **Idea:**

$$H_0 : \theta = \theta_0 \longleftrightarrow H_1 : \theta \neq \theta_0$$

$$\updownarrow \tag{2.114}$$

$$\mathbb{P}(R^{\complement}(\vec{X})|H_0) = \mathbb{P}(R^{\complement}(\vec{X})|\theta_0) = 1 - \alpha$$

$$\updownarrow \tag{2.115}$$

$$\text{Confidence Interval: } \theta_0 \in R^{\complement}(\vec{X})$$

Similar for Confidence Limit and One-Sided Testing.

2.4.6 Introduction to Non-Parametric Hypothesis Testing

Motivation: Usually distribution form unknown, cannot use parametric hypothesis testing.

Useful Method:

- Sign Test: Used for paired comparison $\vec{X} = (X_1, X_2, \ldots, X_n)$, $\vec{Y} = (Y_1, Y_2, \ldots, Y_n)$.

  Take $Z_i = Y_i - X_i$ i.i.d., denote $E(Z) = \mu$. Test $H_0 : \mu = 0 \longleftrightarrow H_1 : \mu \neq 0$.

  Denote $n_+ = \#(\text{positive } Z_i)$ and $n_- = \#(\text{negative } Z_i)$, $n_0 = n_+ + n_-$. Then $n_+ \sim B(n_0, \theta)$, test $H_0 : \theta = \frac{1}{2} \longleftrightarrow H_1 : \theta \neq \frac{1}{2}$

  Then use Binomial Testing or large sample CLT Normal Testing.

  Remark:

  - Also can test $H_0 : \theta \leq \frac{1}{2} \longleftrightarrow H_1 : \theta > \frac{1}{2}$
  - Drawback: ignores magnitudes.

- Wilcoxon Signed Rank Sum Test: Improvement of Sign Test. Base on order statistics.

  Order Statistics of Z_i: $Z_{(1)} < Z_{(2)} < \ldots < Z_{(n)}$, where each $Z_{(j)}$ corresponds to some Z_i, denote as $Z_i = Z_{(R_i)}$, then R_i is the rank of Z_i.[6]

[6] If some $X_i, X_j, \ldots$ equal, then take same rank $R = \text{mean}\{R_i, R_j, \ldots\}$.

Def. $\vec{R} = (R_1, R_2, \ldots, R_n)$ is **Rank Statistics** of $(Z_1, Z_2, \ldots, Z_n)$

Def. **Sum of Wilcoxon Signed Rank**:

$$W^+ = \sum_{i=1}^{n_0} R_i \mathbb{I}_{Z_i > 0} \tag{2.116}$$

Distribution of W^+ is complex. E and var of W^+ under H_0:

$$\mathbb{E}(W^+) = \frac{n_0(n_0+1)}{4} \qquad var(W^+) = \frac{n_0(n_0+1)(2n_0+1)}{24} \tag{2.117}$$

Usually consider large sample CLT, construct normal approximation:

$$T = \frac{W^+ - \mathbb{E}(W^+)}{\sqrt{var(W^+)}} \xrightarrow{\mathscr{L}} N(0,1) \tag{2.118}$$

Rejection Region: $R = \{|T| > N_{\frac{\alpha}{2}}\}$

- Wilcoxon Two-Sample Rank Sum Test: Used for two independent sample comparison.

  Assume $\vec{X} = (X_1, \ldots, X_m)$ i.i.d. $\sim f(x)$; $\vec{Y} = (Y_1, \ldots, Y_n)$ i.i.d. $\sim f(x-\theta)$, test $H_0 : \theta = 0 \longleftrightarrow H_1 : \theta \neq 0$.

  Rank X_i and Y_i as:

$$Z_1 \leq Z_2 \leq \ldots \leq Z_{m+n} \tag{2.119}$$

  in which denote rank of Y_i as R_i, and def. **Wilcoxon two-sample rank sum**:

$$W = \sum_{i=1}^{n} R_i \tag{2.120}$$

  $\mathbb{E}$ and var of W under H_0:

$$\mathbb{E}(W) = \frac{n(m+n+1)}{2} \qquad var(W) = \frac{mn(n+m+1)}{12} \tag{2.121}$$

  Use large sample approximation, construct CLT:

$$T = \frac{W - \mathbb{E}(W)}{\sqrt{var(W)}} \xrightarrow{\mathscr{L}} N(0,1) \tag{2.122}$$

- Goodness-of-Fit Test: For $\vec{X} = (X_1, X_2, \ldots, X_n)$ i.i.d. from some certain population X. Test $H_0 : X \sim F(x)$. where F is theoretical distribution, can be either parametric or non-parametric.

  Idea: Define some *quantity* $D = D(X_1, \ldots, X_n; F)$ to measure the difference between F and sample. And def. *Goodness-of-fit* when observed value of D (say d_0) is given:

$$p(d_0) = \mathbb{P}(D \geq d_0 | H_0) \tag{2.123}$$

  Goodness-of-Fit Test: Reject H_0 if $p(d_0) < \alpha$.

  Pearson χ^2 Test: Usually used for discrete case.

  Test $H_0 : \mathbb{P}(X_i = a_i) = p_i$, $i = 1, 2, \ldots, r$. Denote $\#(X_j = a_i) = \nu_i$, take D as:

$$K_n = K_n(X_1, \ldots, X_n; F) = \sum_{i=1}^{r} \frac{(\nu_i - np_i)^2}{np_i} \tag{2.124}$$

Pearson Thm.: For K_n defined as equation. 2.124, then under H_0:

$$K_n \xrightarrow{\mathscr{L}} \chi^2_{r-1-s} \tag{2.125}$$

Here s is number of unknown parameter, $r-1-s$ is the degree of freedom.

Note:

- a_i must **not** depend on sample.
- For continuous case, construct division:

$$\mathbb{R} \to (-\infty, a_1, a_2, \dots, a_{r-1}, \infty = a_r) \tag{2.126}$$

  and test $H_0 : \mathbb{P}(X \in I_j) = p_j$

  Criterion: Pick proper interval so that np_i and ν_i both ≥ 5.

• Contingency Table Independence & Homogeneity Test

- Independence Test:

  Test a two-parameter sample and to see whether these two parameters(features) are independent. Denote $Z = (X, Y)$ are some 'level' of sample, n_{ij} is number of sample with level (i, j)

  Contingency Table:

X \ Y	1	$\dots$	j	$\dots$	s	$\sum$
1	n_{11}	$\dots$	n_{1j}	$\dots$	n_{1s}	$n_{1\cdot}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
i	n_{i1}	$\dots$	n_{ij}	$\dots$	n_{is}	$n_{i\cdot}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
r	n_{r1}	$\dots$	n_{rj}	$\dots$	n_{rs}	$n_{r\cdot}$
$\sum$	$n_{\cdot 1}$	$\dots$	$n_{\cdot j}$	$\dots$	$n_{\cdot s}$	n

  Test $H_0 : X$ & Y are independent. i.e. $H_0 : P(X = i, Y = j) = P(X = i)P(Y = j) = p_{i\cdot}p_{\cdot j}$.

  Construct χ^2 test statistic:

$$K_n = \sum_{i=1}^{r}\sum_{j=1}^{s} \frac{[n_{ij} - n(\frac{n_{i\cdot}}{n})(\frac{n_{\cdot j}}{n})]^2}{n(\frac{n_{i\cdot}}{n})(\frac{n_{\cdot j}}{n})} = n\left(\sum_{i=1}^{r}\sum_{j=1}^{s} \frac{n_{ij}^2}{n_{i\cdot}n_{\cdot j}} - 1\right) \tag{2.127}$$

  Then under H_0, $K_n \xrightarrow{\mathscr{L}} \chi^2_{rs-1-(r+s-2)} = \chi^2_{(r-1)(s-1)}$

  Reject H_0 if $p(k_0) = P(K_n \geq k_0) < \alpha$

- Homogeneity Test:

  Test R groups of sample with category rank, to see whether these groups has similar rank distribution.

Group \ Category	Category 1	$\dots$	Category j	$\dots$	Category C	$\sum$
Group 1	n_{11}	$\dots$	n_{1j}	$\dots$	n_{1C}	$n_{1\cdot}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Group i	n_{i1}	$\dots$	n_{ij}	$\dots$	n_{iC}	$n_{i\cdot}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
Group R	n_{R1}	$\dots$	n_{Rj}	$\dots$	n_{RC}	$n_{R\cdot}$
$\sum$	$n_{\cdot 1}$	$\dots$	$n_{\cdot j}$	$\dots$	$n_{\cdot C}$	n

Denote $P(\text{Category } j|\text{Group } i) = p_{ij}$. Test $H_0 : p_{ij} = p_j,\ \forall 1 \le i \le R$.

Construct χ^2 test statistic:

$$D = \sum_{i=1}^{R}\sum_{j=1}^{C} \frac{[n_{ij} - n(\frac{n_{i\cdot}}{n})(\frac{n_{\cdot j}}{n})]^2}{n(\frac{n_{i\cdot}}{n})(\frac{n_{\cdot j}}{n})} = n\left(\sum_{i=1}^{R}\sum_{j=1}^{C}\frac{n_{ij}^2}{n_{i\cdot}n_{\cdot j}} - 1\right) \tag{2.128}$$

Then under H_0, $D \xrightarrow{\mathscr{L}} \chi^2_{R(C-1)-(C-1)} = \chi^2_{(R-1)(C-1)}$

- Test of Normality: normality is a good & useful assumption.

  For $\vec{Y} = (Y_1, Y_2, \dots, Y_n)$,

  Test H_0 : exists μ & σ^2 such that Y_i i.i.d. $\sim N(\mu, \sigma^2)$.

  – Kolmogorov-Smirnov Test: Assume $\vec{X}$ form population CDF $F(x)$, test $H_0 : F(x) = F_0(x)$(where can take $F_0 = \Phi$ or some other known CDF).

    use $F_n(x)$ (as defined in equation. 2.81) as approx. to $F(x)$, test

$$D_n = \sum_{-\infty<x<+\infty} |F_n(x) - F_0(x)| \tag{2.129}$$

    Reject H_0 if $D_n > c$

    or use goodness-of-fit: denote observed value of D_n as d_n. Reject H_0 if

$$p(d_n) = \mathbb{P}(D_n > d_n|H_0) < \alpha \tag{2.130}$$

  – Shapiro-Wilk Test:

    Test H_0 : exists μ & σ^2 such that X_i i.i.d. $\sim N(\mu, \sigma^2)$.

    Denote $Y_{(i)} = \dfrac{X_{(i)} - \mu}{\sigma}$, $m_i = \mathbb{E}(Y_{(i)})$

    Under H_0, $(X_{(i)}, m_i)$ falls close to straight line. Test Statistic: Correlation

$$R^2 = \frac{\left(\sum_{i=1}^{n}(X_{(i)} - \bar{X})(m_i - \bar{m})\right)^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2 \sum_{i=1}^{n}(m_i - \bar{m})^2} = corr(X_{(i)}, m_i) \tag{2.131}$$

    Reject H_0 if $R^2 < c$

    Shapiro-Wilk correction:

$$W = \frac{\left(\sum_{i=1}^{[n/2]} a_i(X_{(n+1-i)} - X_{(i)})\right)^2}{\sum_{i=1}^{n}(X_{(i)} - \bar{X})^2} \tag{2.132}$$

☐ **Summary: Useful Non-Parameter Hypothesis Testing.**

- Non-Parameter Hypothesis Testing
  - One Population Sample
    - χ^2 Test
    - Binomial Test
    - One-Sample K-S Test
    - Wilcoxon Sign Test
    - Runs Test
  - Two Population Sample
    - Independent Sample
      - Mann-Whitney Test
      - K-S Test
      - Wald-Wolfowitz Test
      - Moses Test of Extreme Reactions
    - Relative Sample
      - Sign Test
      - McNemar Test
      - Wilcoxon Rank Sum Test
      - Marginal Homogeneity Test
  - Multi-Population Sample
    - Independent Sample
      - Median Test
      - K-W One-Way ANOVA Test
      - Jonckheere-Terpstra Test
    - Relative Sample
      - Friedman Rank Sum Test
      - Kendall's Coefficient of Concordance Test
      - Cochran Q Test

Chapter. III 线性回归分析部分

Instructor: Zaiying Zhou

☐ **Steps in Regression Analysis**

1. Statement of the problem;
2. Selection of potentially relevant **variables**;
3. Data collection;
4. Exploratory Data Analysis (**EDA**)
5. **Model** specification;
6. Choice of fitting method;
7. Model fitting;
8. Model validation and criticism;
9. Using the chosen model(s) for the solution of the posed problem;
10. **Explain** the result.

R. Code for EDA

```
libaray('GGally')
head(df)
ggpairs(df)
str(df)
summary(df)
```

☐ **Used Packages in** R.

```
library('ggplot2')
libaray('GGally')
library('car')
library('moments')
library('lmtest')
library('nortest')
library('MASS')
library('tseries')

source('package.r')
```

Section 3.1 Regression Model

In regression model, we will observe pairs of variables, called 'cases'(样本点). A sample is $(X_1; Y_1), \dots, (X_n; Y_n)$, where X_i can be multivariate $X_i = \vec{X}_i = (X_{i1}, X_{i2}, \dots, X_{ip})$.

If X is continuous `numeric` variable, use Regression Model(s), else if X is discrete `factor` variable, use Factor Model(s).

▷ R. **Code**

Example data import:

```
df <- read.table('dataset/testdata.txt', header=FALSE, sep=',', col.names
    = c('y','x1','x2'))
```

3.1.1 Linear Regression Model

Regression Model focuses on how Y changes with continuous variables $X \in \mathbb{R}$. As a basic situation, we use **Linear Regression**, i.e. $Y \sim X$ in linear relation.

□ **Sample Geometry Notation**

For most general case, in sample matrix notation:

$$Y = X\beta + \varepsilon \leftrightharpoons Y_j = X\beta_j + \varepsilon_j, \forall j = 1, 2, \dots, q \tag{3.1}$$

in Einstein Summation Convention:

$$Y_{ij} = X_{ij'}\beta_{j'j} + \varepsilon_{ij} \tag{3.2}$$

Why we need ε as 'random error term'?

- It represents the intrinsic random property of the model.
- Based on ε, we can take r.v. into our statistic model.

where

$$\underset{n\times q}{Y} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1q} \\ y_{21} & y_{22} & \cdots & y_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nq} \end{bmatrix} = \begin{bmatrix} y_1, y_2, \dots, y_q \end{bmatrix} \qquad y_j = \begin{bmatrix} y_{1j} \\ y_{2j} \\ \vdots \\ y_{nj} \end{bmatrix} \tag{3.3a}$$

$$\underset{n\times(p+1)}{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{bmatrix} \qquad x_i = \begin{bmatrix} 1 \\ x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix} \tag{3.3b}$$

$$\underset{(p+1)\times q}{\beta} = \begin{bmatrix} \beta_{01} & \beta_{02} & \dots & \beta_{0q} \\ \beta_{11} & \beta_{12} & \dots & \beta_{1q} \\ \beta_{21} & \beta_{22} & \dots & \beta_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{p1} & \beta_{p2} & \dots & \beta_{pq} \end{bmatrix} = \begin{bmatrix} \beta_1, \beta_2, \dots, \beta_q \end{bmatrix} \qquad \beta_j = \begin{bmatrix} \beta_{j0} \\ \beta_{j1} \\ \vdots \\ \beta_{jp} \end{bmatrix} \tag{3.3c}$$

$$\underset{n\times q}{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \dots & \varepsilon_{1q} \\ \varepsilon_{21} & \varepsilon_{22} & \dots & \varepsilon_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ \varepsilon_{n1} & \varepsilon_{n2} & \dots & \varepsilon_{nq} \end{bmatrix} = \begin{bmatrix} \varepsilon_1, \varepsilon_2, \dots, \varepsilon_q \end{bmatrix} \qquad \varepsilon_j = \begin{bmatrix} \varepsilon_{1j} \\ \varepsilon_{2j} \\ \vdots \\ \varepsilon_{nj} \end{bmatrix} \tag{3.3d}$$

with Guass-Markov Assumption:

$$\begin{aligned} \text{Zero-Mean: } & \mathbb{E}(\epsilon_i|X_i) = 0 \\ \text{Homogeneity of Variance: } & var(\epsilon_i) = \sigma^2 \\ \text{Independent: } & \epsilon_i \text{ i.i.d. } \sim \varepsilon \end{aligned} \tag{3.4}$$

and Normality Error Assumption:

$$\text{Normality: } \varepsilon_i \text{ i.i.d. } \sim N(0, \sigma^2) \tag{3.5}$$

Under matrix notation, model and assumptions equation. 3.4(equation. 3.5) can be expressed in condensed notation:

$$Y_j = X\beta_j + \varepsilon_j \sim N_n(X\beta_j, \sigma_j^2 I_n), \quad j = 1, 2, \dots, q \tag{3.6}$$

△ **Note:** In this section we only focus on $q = 1$, i.e.

$$\underset{n\times 1}{Y} = \underset{n\times(p+1)}{X} \underset{(p+1)\times 1}{\beta} + \underset{n\times 1}{\varepsilon} \tag{3.7}$$

3.1.2 Factor Analysis Model

Regression Model focuses on continuous variables $X \in \mathbb{R}$ while factor model focus on discrete variable. More specifically, the 'value' of X is just a label, not necessarily a 'numeric value'.

Here only introduce one-way factor analysis,(single factor analysis) i.e. Y with only one factor with r levels: fac $= 1, 2, \dots, r$. Re-denote Y_{ij} = the observation outcome of the j^{th} item labelled the i^{th} level.

Model:

$$Y_{ij} = \mu + \tau_i + \varepsilon_{ij},\ i = 1, \dots, r,\ j = 1, \dots, n_i \tag{3.8}$$

where μ is the average effect of all r factor levels, τ_i is the level effect of the i^{th} factor level, and ε i.i.d. $\sim N(0, \sigma^2)$ is noise error.

In matrix notation:

$$Y = \begin{bmatrix} y_{11} & \dots & y_{1n_1} & y_{21} & \dots & y_{2n_2} & \dots \end{bmatrix}^T \tag{3.9a}$$

$$X = \begin{bmatrix} 1 & 1 & 0 & \dots \\ 1 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \\ 1 & 0 & 1 & \dots \\ 1 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{1}_{n_1} & 0 & \dots & 0 \\ \mathbf{1}_{n_2} & 0 & \mathbf{1}_{n_2} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_{n_r} & 0 & 0 & \dots & \mathbf{1}_{n_r} \end{bmatrix} \tag{3.9b}$$

$$\tau = \begin{bmatrix} \mu & \tau_1 & \tau_2 & \dots \end{bmatrix}^T \tag{3.9c}$$

$$\varepsilon = \begin{bmatrix} \varepsilon_{11} & \dots & \varepsilon_{1n_1} & \varepsilon_{21} & \dots & \varepsilon_{2n_2} & \dots \end{bmatrix}^T \tag{3.9d}$$

For more factor model e.g. two-way factor analysis with k denoting item and i, j denoting factor:

$$Y_{ijk} = \mu + \alpha_i + \beta_j + \varepsilon_{ij} \tag{3.10}$$

cannot be simply expressed in matrix notation $\longrightarrow$ use index notation.

Assumption: Normal, Equal variance, independent

- One-way: $Y_{j|i}$ i.i.d. $\sim N(\mu + \tau_i, \sigma^2), \forall i$
- Two-way: $Y_{k|ij}$ i.i.d. $\sim N(\mu + \alpha_i + \beta_j, \sigma^2), \forall i, j$

Section 3.2 Monovariate Linear Regression Model

First focus on the simpliest monovariate case $\vec{X}_i = X_i$. Monovariate Linear Model[7] with Gauss-Markov assumption & Normal Error assumption:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i,\ \varepsilon_i \text{ i.i.d.} \sim N(0, \sigma^2) \tag{3.11}$$

What does Linear Regression do? Try to estimate

- β_0 (intercept) ;
- β_1 (slope) ;
- σ^2 (variance of error).

(Thus Linear Regression is also a Statistics Inference process: deduce properties of model from data)

3.2.1 The Ordinary Least Square Estimation

Aim: use (x_i, y_i) to estimate $\beta_0, \beta_1, \sigma^2$. The idea is to define a 'loss function' to reflect the 'distance' from sample point to estimation point.

[7] Here in linear regression, we consider X_i only as real number, **without** randomness. So here Y_i can be considered as an r.v. with X_i as parameter, i.e. $Y_i|_{X_i=x_i}$

Estimate Principle: [8]

- Ordinary Least Squares:

$$(\hat{\beta}_0, \hat{\beta}_1) = \arg\min \sum_{i=1}^{n} (y - \beta_0 - \beta_1 x_i)^2 \tag{3.12}$$

- MLE or MoM Estimation.

And get $\hat{\beta}_1, \hat{\beta}_0$ as well as $\hat{\sigma^2}$(see equation. 3.17:[9]

$$\begin{aligned}\hat{\beta}_1 &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\sigma^2} &= \frac{1}{n-p-1}\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2\end{aligned} \tag{3.14}$$

Def. **Residual**: distance from sample point to estimate point, to reflect how the sample points fit the model.

$$e_i = y_i - \hat{y}_i = \text{observed value of } \varepsilon_i \tag{3.15}$$

Note: under least square estimation, we have[10]

$$\sum e_i = 0 \qquad \sum x_i e_i = 0 \tag{3.16}$$

Then use e_i to estimate σ^2 (because it is ε_0 that are i.i.d., not Y_i), where $(n-p-1)$ is Degree of Freedom (df or dof)[11]

$$\begin{aligned}\hat{\sigma^2_n} &= \frac{1}{n}\sum e_i^2 \quad \text{(use MLE or MoM)} \\ \hat{\sigma^2} &= \frac{1}{n-p-1}\sum e_i^2 = \frac{1}{n-2}\sum e_i^2 \quad \text{(use OLS, unbiased)}\end{aligned} \tag{3.17}$$

Degree of Freedom of a Quadric Form:

- Intuitively: the number of independent variable;
- Rigorously: for quadric SS $= x'Ax$:

$$dof_{SS} = \text{rank}(A) \tag{3.18}$$

▷ `R.` **Code**

[8]Detailed Definition and Derivation see section. 2.2.5 or section. 3.3.

[9]A memory trick: use $\frac{Y}{\sqrt{s_Y}} = r_{XY}\frac{X}{\sqrt{s_X}}$ to get formular of $Y \sim X$:

$$\hat{\beta}_1 = r_{XY}\frac{\sqrt{s_Y}}{\sqrt{s_X}} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2} \tag{3.13}$$

[10]Intuitively, they each means '$E(\varepsilon) = 0$' and '$X \parallel \varepsilon$'.

[11]Generally, MLE and OLSE are different.

Comment from R.A.Fisher: $\sum e_i^2$ should be divided by 'number of e_i^2 that contribute to variance'. Here $(n-p-1)$ corresponds to 'degree of freedom' $= (n-2)$, $p = 1$ corresponds to 'one' variable (see section. 2.2.5, equation. 2.80), and correponds to the two equations of e_i, equation. 3.16

```
lmfit <- lm(formula,df)
summary(lmfit,cor=TRUE)
ggcoef(lmfit)
```

`lmfit` includes parameters `lmfit$coefficient` and `lmfit$residuals`

Example `lm()` output:

```
    Call:
    lm(formula = y ~ x, data = df)

    Residuals:
         Min        1Q    Median        3Q       Max
    -16.1368   -6.1968   -0.5969    6.7607   23.4731

    Coefficients:
                Estimate Std. Error t value Pr(>|t|)
    (Intercept) 156.3466     5.5123   28.36   <2e-16 ***
    x            -1.1900     0.0902  -13.19   <2e-16 ***
    ---
    Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

    Residual standard error: 8.173 on 58 degrees of freedom
    Multiple R-squared:  0.7501,    Adjusted R-squared:  0.7458
    F-statistic: 174.1 on 1 and 58 DF,  p-value: < 2.2e-16
```

3.2.2 Statistical Inference to β_0, β_1, σ^2, e_i

☐ **Sampling Distribution of $\hat{\beta}_1, \hat{\beta}_0$**

Consider $\hat{\beta}_1, \hat{\beta}_0$ as statistics of sample, then we can examine the sampling distribution of $\hat{\beta}_1, \hat{\beta}_0$. Their randomness comes from

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i \tag{3.19}$$

(The following part treats $\hat{\beta}_1, \hat{\beta}_0$ as r.v., and note that X_i are **not** r.v.. And for convenience and conciseness, denote $S_{XX} = \sum_{i=1}^{n}(X_i - \bar{X})^2$)

$$\hat{\beta}_1 = \beta_1 + \sum_{i=1}^{n} \frac{X_i - \bar{X}}{S_{XX}} \varepsilon_i$$

$$\hat{\beta}_0 = \beta_0 + \sum_{i=1}^{n} \left(\frac{1}{n} - \frac{(X_i - \bar{X})\bar{X}}{S_{XX}} \right) \varepsilon_i$$

Denote corresponding variance as $\sigma^2_{\hat{\beta}_1}$ and $\sigma^2_{\hat{\beta}_0}$, using equation. 1.74 to get:

$$\sigma^2_{\hat{\beta}_1} = \frac{\sigma^2}{S_{XX}} \qquad \sigma^2_{\hat{\beta}_0} = \sigma^2(\frac{1}{n} + \frac{\bar{X}^2}{S_{XX}}) \tag{3.20}$$

And under normal error assumption, distribution of $\hat{\beta}_1, \hat{\beta}_0$ are

$$\hat{\beta}_1 \sim N(\beta_1, \sigma^2_{\hat{\beta}_1}) = N(\beta_1, \frac{\sigma^2}{S_{XX}})$$
$$\hat{\beta}_0 \sim N(\beta_0, \sigma^2_{\hat{\beta}_0}) = N(\beta_0, \sigma^2(\frac{1}{n} + \frac{\bar{X}^2}{S_{XX}}))$$

Based on sampling distribution of $\hat{\beta}_1, \hat{\beta}_0$, we can conduct statistical inference, including CI and HT.[12]

Note: In linear regression model, we usually focus more on β_1. And note that when 0 is **not** within the fitting range,β_0 is not so important.[13]

☐ **Sampling Distribution of e_i** Consider e_i as r.v. satisfies

$$e_i = Y_i - \hat{Y}_i = Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i \tag{3.21}$$

and get the expression of $\hat{e}_i$

$$\hat{e}_i = \varepsilon_i - \sum_{k=1}^{n} \left(\frac{1}{n} + \frac{(X_i - \bar{X})^2}{S_{XX}} \right) \varepsilon_k \tag{3.22}$$

$$\mathbb{E}(e_i) = 0 \qquad \sigma^2_{e_i} = \sigma^2 \left(1 - \frac{1}{n} - \frac{(X_i - \bar{X})^2}{S_{XX}} \right) \tag{3.23}$$

Under normal assumption:

$$\varepsilon_i \sim N(0, \sigma^2 \left(1 - \frac{1}{n} - \frac{(X_i - \bar{X})^2}{S_{XX}} \right)) \tag{3.24}$$

Further we can get $\hat{\sigma}^2 = \mathbb{E}(\frac{1}{n-2} \sum_{i=1}^{n} e_i^2)$ where $e_i^2 \sim \sigma^2 \left(1 - \frac{1}{n} - \frac{(X_i - \bar{X})^2}{S_{XX}} \right) \chi^2$

$$\hat{\sigma}^2 = \frac{1}{n-2} \sigma^2 \sum_{i=1}^{n} (1 - \frac{1}{n} - \frac{(X_i - \bar{X})^2}{S_{XX}}) = \sigma^2 \tag{3.25}$$

More definition of refined residuals see section. 3.4.3 in page 3.4.3.

☐ **Why we choose OLS to get regression coefficients?**

Gauss - Markov Thm.: the OLS estimator has the lowest sampling variance within the class of linear unbiased estimators, i.e. OLS is the Best Linear Unbiased Estimator(BLUE).[14]

---

[12]Detail see section. 2.4, estimating/testing $\hat{\beta}_1, \hat{\beta}_0$ usually corresponds to 'estimate μ, with σ^2 unknown'.

[13]Two reason:

- The etimation error of Y from $\hat{\beta}_1$ increases with $X_h - \bar{X}$;
- $\beta_1 == 0$ is important: decides whether linear model can be used.

[14]This Thm. does **not** require normal error assumption.

3.2.3 Prediction to Y_h

For a new X_h at which we wish to **predict** the corresponding Y_h (based on other known point (X_i, Y_i)), denote the estimator as $\hat{\mu}_h$:

$$\hat{\mu}_h = \hat{\beta}_1 X_h + \hat{\beta}_0 = \beta_1 X_h + \beta_0 + \sum_{i=1}^{n} \left(\frac{1}{n} + \frac{(X_i - \bar{X})(X_h - \bar{X})}{S_{XX}} \right) \varepsilon_i \tag{3.26}$$

Thus we can get[15]

$$\mathbb{E}(\hat{\mu}_h) = \beta_1 X_h + \beta_0 \qquad \sigma^2_{\hat{\mu}_h} = \left(\frac{1}{n} + \frac{(X_h - \bar{X})^2}{S_{XX}} \right) \sigma^2 \tag{3.27}$$

Under Normal assumption:

$$\hat{\mu}_h \sim N(\beta_1 X_h + \beta_0, \left(\frac{1}{n} + \frac{(X_h - \bar{X})^2}{S_{XX}} \right) \sigma^2) \tag{3.28}$$

Base on distribution we can give CI and HT.

Note: We can either consider

- Y_h **itself as an r.v.** : Confidence Interval of Y_h;

  And we can just use $\sigma^2_{\hat{\mu}_h}$ to construct CI;

  ▷ `R.` **Code**

```
predict(lmfit,newdata = 40),
    interval="confidence",level=0.95)
```

- **predicted Y_h from other sample points**: Prediction Interval of Y_h

  Need to have the randomness of $\hat{\beta}_0, \hat{\beta}_1$ considered(if they are unknown).

  Def. Prediction Error: Y_h itself is an Y of the linear model, i.e. $Y_i = \beta_0 + \beta_1 X_h + \varepsilon_h$, we can and define **Prediction Error**:

$$d_h = Y_h - \hat{\mu}_h \tag{3.29}$$

$$\mathbb{E}(d_h) = 0 \qquad \sigma^2_{d_h} = var(Y_h - \hat{\mu}_h) = \sigma^2 \left[1 + \frac{1}{n} + \frac{(X_h - \bar{X})}{S_{XX}} \right] > \sigma^2_{\hat{\mu}_h} \tag{3.30}$$

  ▷ `R.` **Code**

```
predict(lmfit,newdata = 40),
    interval="prediction",level=0.95)
```

☐ **Simultaneous Confidence Band(SCB)**

Confidence Band is **not** the CI at each point, but really a **band** for the **entire** regression line.[16]

Aim: Find lower and upper function $L(x)$ and $U(x)$ such that

$$\mathbb{P}[L(x) < (\beta_0 + \beta_1 x) < U(x), \forall x \in I_x] = 1 - \alpha \tag{3.31}$$

[15] So $\sigma^2(\hat{\mu}_h)$ increases with $X_h - \bar{X}$. Intuitively it make sense, because $(\bar{X}, \bar{Y})$ must falls on regression line.

[16] Why they are different? We require the confidence band have a **simultaneous** converage probability. For the same band $(L(x), U(x))$, P(the whole line) $<$ P(each point), so Confidence Band is wider than $\bigcup$CIs to hold the same $1 - \alpha$.

Also, we will see that for linear model, the boundary of SCB forms hyperbola, which make sense considering its asymptotic line.

and get **Confidence Band**:

$$\{(x,y)|L(x)<y<U(x)|\forall x\in I_x\} \tag{3.32}$$

Where $(L(x),U(x))$ can be derived as

$$(L(x),U(x))=\hat{\mu}_x\pm s_{\hat{\mu}_x}W_{2,n-2,1-\alpha} \tag{3.33}$$

Where W correponds to W distribution: $W_{m,n}=\sqrt{2F_{m,n}}$

Small sample case: Bonferroni correction.

▷ R. **Code**

```
library(ggplot2)
ggplot(df,aes(x,y))+geom_point()+geom_smooth(method='lm',formula=y~x)
```

3.2.4 Analysis of Variance: Monovariate

ANalysis **O**f **VA**riance (ANOVA): One-sample t test ⇝ Two sample t test ⇝ More-sample: ANOVA

☐ **Key Idea Of ANOVA: Test whether the mean of some groups are the same, i.e.** $\mu_1=\mu_2=\ldots=\mu_r$

In linear regression model, modified as testing $\beta_1 == 0$. Conduction: Take Partition of Total Sum of Square To Examine **Variation**. Because Y_i are not i.i.d. (different mean value $X\beta$), so has different parts of variation from Regression Model/Error Term.

Measure of Variation: Sum of Square (SS) & Mean Sum of Square (MS).

MS: Divide each SS by corresponding dof. Definition of dof see equation. 3.18.

$$\text{MS}=\frac{\text{SS}}{dof} \tag{3.34}$$

- SST: Total Sum of Squares

$$\text{SST}=\sum_{i=1}^{n}(Y_i-\bar{Y})^2 \qquad dof_{\text{SST}}=n-1 \tag{3.35}$$

- SSRegression: Variation due to Regression Model (which is explained by regression line);[17]

$$\text{SSR}=\sum_{i=1}^{n}(\hat{Y}_i-\bar{Y})^2 \qquad dof_{\text{SSR}}=1 \tag{3.36}$$

- SSError: Variation attribtes to ε (which is reflected by residuals).

$$\text{SSE}=\sum_{i=1}^{n}(Y_i-\hat{Y}_i) \qquad dof_{\text{SSE}}=n-2 \tag{3.37}$$

△ **IMPORTANT:** In some books

- SSRegression → SSExplained or SSModel;
- SSError → SSResidual.

And Cause **Confusion**! In this summary we take the former.

[17] $\text{SSR}=\hat{\beta}_1^2\sum_{i=1}^{n}(X_i-\bar{X})^2$, so $dof_R=1$

Idea: take partition of SST. i.e.

$$Y_i - \bar{Y} = (Y_i - \hat{Y}) + (\hat{Y} - \bar{Y}) = e_i \tag{3.38}$$

And we can prove that

$$\text{SST} = \sum_{i=1}^{n}(Y_i - \bar{Y})^2 = \sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2 + \sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 = \text{SSR} + \text{SSE} \tag{3.39}$$

That is: we **partition** SST into two parts, so that we can examine them seperately.

☐ **ANOVA Table**

Source	dof	SS	MS	F-Statistic
SSRegression	1	$\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2$	SSR/dof_R	MSR/MSE
SSError	$n-2$	$\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$	SSE/dof_E	
SSTotal	$n-1$	$\sum_{i=1}^{n}(Y_i - \bar{Y})^2$	SST/dof_T	

▷ R. **Code**

```
anova(lmfit)
```

Properties:

$$\mathbb{E}(\text{MSE}) = \sigma^2 \qquad \mathbb{E}(\text{MSR}) = \sigma^2 + \beta_1^2 S_{XX} \tag{3.40}$$

Section 3.3 Multivariate Linear Regression Model

As a more general case of $\vec{X}_i = (X_{i1}, X_{i2}, \ldots, X_{ip})$, Multivariate Linear Model is expressed as in EqaMultivarite-LinearModel:

$$Y = X\beta + \varepsilon,\ \varepsilon \sim N_p(0, \sigma^2 I) \tag{3.41}$$

3.3.1 The Ordinary Least Estimation

To conduct OLS

$$\hat{\beta} = \underset{\beta\in\mathbb{R}^{p+1}}{\arg\min}(Y - X\beta)^T(Y - X\beta) \tag{3.42}$$

Here we introduce two approaches:

- Analytical: Take matrix differciation (See section. 4.1.2 equation. 4.29)

$$\begin{aligned} 0 &= \frac{\partial (Y - X\beta)^T(Y - X\beta)}{\partial \beta} = \frac{\partial}{\partial \beta}(Y^TY - Y^TX\beta - \beta^TX^TY + \beta^TX^TX\beta) \\ &= -X^TY - X^TY + (X^TX + XX^T)\beta = -2X^T(Y - X\beta) \end{aligned}$$

Thus we get OLS:

$$\hat{\beta} = (X'X)^{-1}X'Y \tag{3.43}$$

- Geometric/Algebraical: Use hyper-projection.

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^{p+1}} d(Y, X\beta) \tag{3.44}$$

i.e. $\hat{\beta}$ is the (hyper-)projection of Y onto X (within Euclidean Space), naturally we have

$$(X\beta)^T (Y - X\beta) = 0 \Rightarrow \hat{\beta} = (X'X)^{-1}X'Y \tag{3.45}$$

☐ **Matrix Notation of OLS Estimator:**

$$\hat{\beta} = (X'X)^{-1}X'Y \tag{3.46}$$

3.3.2 Statistical Inference to β, σ^2, e

Properties & Extrapolation

- Sampling Distribution of $\hat{\beta}$: (Here consider normal case $Y \sim N(X\beta, \sigma^2 I_n)$, and use equation. 4.40)

$$\hat{\beta} = (X'X)^{-1}X'Y \sim N_p(\beta, \sigma^2 (X'X)^{-1}) \tag{3.47}$$

Comment: $cov(\beta_i, \beta_j)$ are generally not 0, $\Rightarrow \beta_i, \beta_j$ dependent.

- Predicted Response & Hat Matrix H:

$$\hat{Y} = X\hat{\beta} = X(X'X)^{-1}X'Y \equiv HY = P_X Y \tag{3.48}$$

where **Hat Matrix**/Influence matrix/Projection matrix $H = P_X = X(X'X)^{-1}X'$, with properties

  – Symmertric: $H^T = H$;

  – Idempotence: $H^2 = H$

  – Rank: $\text{rk}(H) = tr(H) = \text{rk}(X)$

  – H and self-influene factor h_{ii}: Note the linearity of $\hat{Y}$ on Y

$$\hat{Y} = HY \Rightarrow H = \frac{\partial \hat{Y}}{\partial Y} \tag{3.49}$$

The diagonal elements of H is

$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = X_i (X'X)^{-1} X_i' \tag{3.50}$$

Comment on h_{ii}: $var(e_i) = \sigma^2(1 - h_{ii})$, for $h_{ii} \to 1$, i.e. the regression line always pass y_i, thus it's 'influential'.

- Residual:

$$e = Y - \hat{Y} = (I - H)Y \sim N_n\left(0, \sigma^2 (I - H)\right) \tag{3.51}$$

where $I - H$ is the complementary projection of X

Covariance Matrix of Residual:

$$cov(e) = \sigma^2 (I - H) = \sigma^2 \begin{bmatrix} 1 - h_{11} & -h_{12} & \dots & -h_{1n} \\ -h_{21} & 1 - h_{22} & \dots & -h_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -h_{n1} & -h_{n2} & \dots & 1 - h_{nn} \end{bmatrix} \tag{3.52}$$

- Estimator and Distribution of σ^2:

  First use equation. 4.41 to get [18]

$$\mathbb{E}(\text{SSE}) = \mathbb{E}(e'e) = \mathbb{E}(Y'(I-H)Y) = (X\beta)'(I-H)X\beta + tr((I-H)\sigma^2 I_n) = \sigma^2(n-p-1) \tag{3.54}$$

  dof of Residual e (use definition equation. 3.18):

$$dof_e = dof_{(I-H)Y} = \text{rank}(I-H) = n-p-1 \tag{3.55}$$

  Thus the unbiased estimator of σ^2 is

$$\hat{\sigma}^2 = \text{MSE} = \frac{e'e}{n-p-1} = \frac{Y'(I-H)Y}{n-p-1} \tag{3.56}$$

  Distribution (under normal assumption):

$$\frac{(n-p-1)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p-1} \tag{3.57}$$

- Gauss-Markov Thm.: OLS Estimator of β is the BLUE Estimator.

More hypothesis testing to β see section. 4.2.4.

3.3.3 Prediction to Y_h

For a new $\vec{X}_h$ at which we wish to **predict** the corresponding Y_h (based on other known point (X_i, Y_i)), denote the estimator as $\hat{\mu}_h$:

$$\hat{\mu}_h = X_h'\hat{\beta} = X_h'(X'X)^{-1}X'Y \tag{3.58}$$

thus we get

$$\mathbb{E}(\hat{\mu}_h) = X_h'\beta \qquad \sigma^2_{\hat{\mu}_h} = \sigma^2(1 + X_h'(X'X)^{-1}X_h) \tag{3.59}$$

under normal assumption:

$$\hat{\mu}_h \sim N(X'\beta, \sigma^2(1 + X_h'(X'X)^{-1}X_h)) \tag{3.60}$$

3.3.4 Analysis of Variance: Multivariate

Sampling Notation see equation. 3.3, still consider $(p+1)$ -dim $(\mathbf{1}_n, X_i)$ v.s. 1-dim Y, and $\beta = (\beta_0, \beta_1, \beta_2, \dots, \beta_p)$

- SST:

$$\text{SST} = (Y - \bar{Y}\mathbf{1}_n)'(Y - \bar{Y}\mathbf{1}_n) \qquad dof_{\text{SST}} = n-1 \tag{3.61}$$

[18] Also we need the property of idmpotnet matrix

$$\lambda_i = 0 \text{ or } 1 \Rightarrow tr(H) = \text{rank}(H) = \sum_{i=1}^{n} \lambda_i = \#(\lambda = 1) \tag{3.53}$$

- SSR:

$$\text{SSR} = (\hat{Y} - \bar{Y}\mathbf{1}_n)'(\hat{Y} - \bar{Y}\mathbf{1}_n) \qquad dof_{\text{SSR}} = p \tag{3.62}$$

Denoted in hat matrix H and $\mathcal{J}$ in equation. 4.9

$$\text{SSR} = Y'(H - \frac{1}{n}\mathcal{J})Y \tag{3.63}$$

- SSE:

$$\text{SSE} = (Y - \hat{Y})'(Y - \hat{Y}) \qquad dof_{\text{SSE}} = n - p - 1 \tag{3.64}$$

Denoted in residual e and hat matrix H:

$$\text{SSE} = e'e = Y'(I - H)Y \tag{3.65}$$

More knowledge about multivariate ANOVA see section. 3.4.5.

☐ **ANOVA Table**

Source	dof	SS	MS	F-Statistic
SSRegression	p	$\sum_{i=1}^n(\hat{Y}_i - \bar{Y})^2$	SSR/dof_R	MSR/MSE
SSError	$n-p-1$	$\sum_{i=1}^n(Y_i - \hat{Y}_i)^2$	SSE/dof_E	
SSTotal	$n-1$	$\sum_{i=1}^n(Y_i - \bar{Y})^2$	SST/dof_T	

▷ `R.` **Code**

```
anova(lmfit)
```

Section 3.4 Diagnostics

To apply OLS, we need the basic Gauss-Markov Assumption equation. 3.4; or we further need better properties of the model, e.g. take Normal Assumption.

Assumptions:

$$\begin{aligned}
\text{Zero-Mean: } & \mathbb{E}(\epsilon_i|X_i) = 0 \\
\text{Homogeneity of Variance: } & var(\epsilon_i) = \sigma^2 \\
\text{Independent: } & \epsilon_i \text{ i.i.d. } \sim \varepsilon \\
\text{Normal: } & \varepsilon \sim N(0, \sigma^2)
\end{aligned} \tag{3.66}$$

Or sum up as

$$Y \sim N_n(X\beta, \sigma^2 I_n) \tag{3.67}$$

Thus we need to conduct Diagnostics and Remedies to

- examine whether these assumptions are satisfies;
- perform correction to regression method.

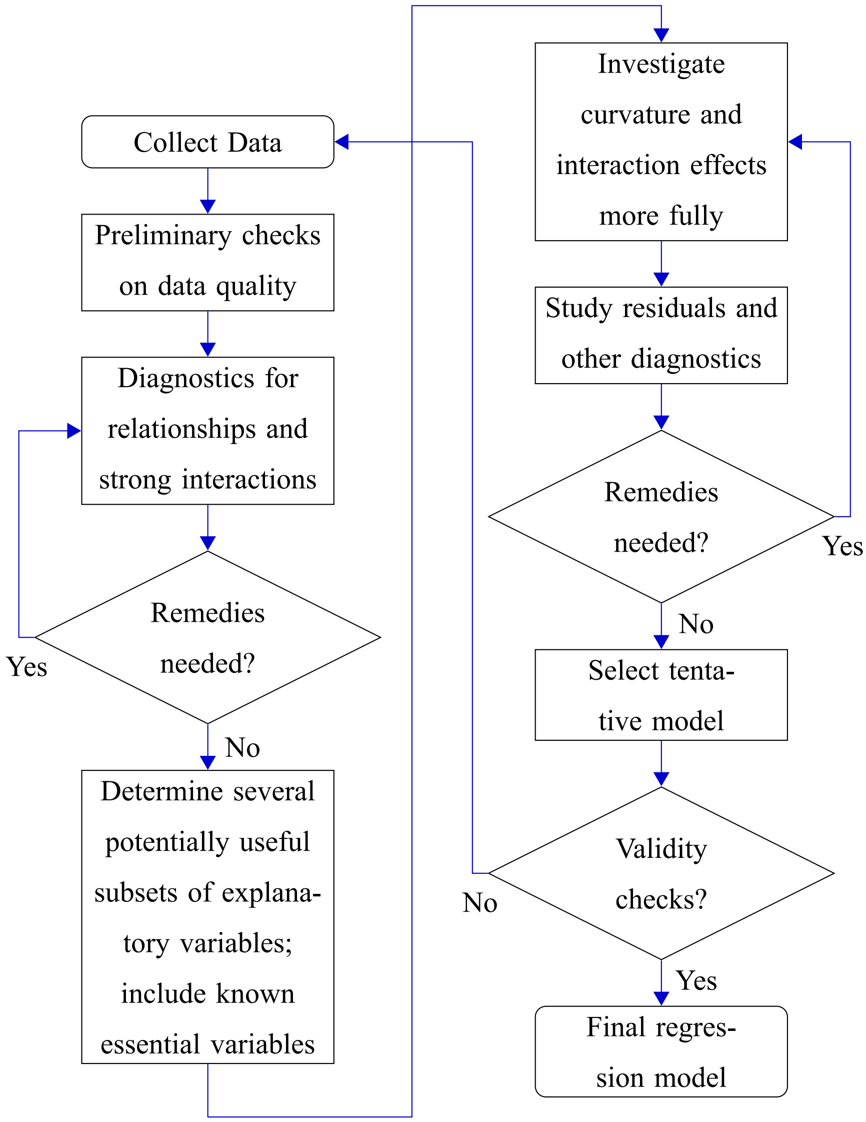


图 2: Diagnostics and Remedies for Regression Model

Preliminary Diagnostics:

▷ R. **Code**

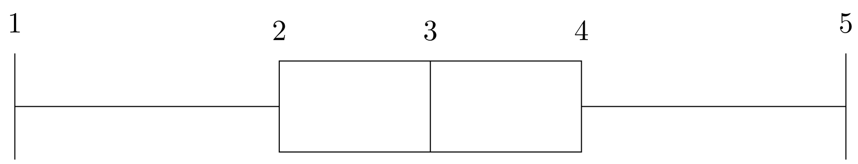
```
lmfit <- lm(y~x,lmfit)
par(mfrow = c(2, 2))
plot(lmfit)
```

3.4.1 Useful Diagnostics Plots

- BoxPlot: to examine the similarity of distribution.

  Notation:

  1. min point above 25% quartile-1.5IQR;
  2. 25% quartile;
  3. median;
  4. 75% quartile;
  5. max point below 75% quartile+1.5IQR.



- Histogram Plots: Frequency distribution (can deal with many-peak)
- Quartile-Quartile Plots: Examine the similarity between distribution.

  For two CDF $q = F(x)$ and $q = G(x)$(where q for quartile), with $x = F^{-1}(q)$, $x = G^{-1}(q)$. And Plot $F^{-1}(q)$-$G^{-1}(q)$.

  Usually test normality, take $G = \Phi$
- Partial Regression Plot: Test non-linearity/heterogeneous-variance.

  For each X_i variable:

  - Use other $X_{(\wedge i)}$ to predict Y, get residual $e_Y|X_{(\wedge i)}$;
  - Use other $X_{(\wedge i)}$ to predict X_i, get residual $e_{X_i}|X_{(\wedge i)}$

  Plot $(e_Y|X_{(\wedge i)})$-$(e_{X_i}|X_{(\wedge i)})$ as Added Variable Plot (AV Plot). Used for testing non-linearity/heterogeneous-variance.

▷ R. **Code**

```
boxplot(df$x)

hist(df$x)
```

```r

hist(df$x,freq=FALSE)
lines(density(df$x))

stem(df$x)

qqnorm(df$x)
qqline(df$x,col='red')

library(car)
avPlots(lmfit)
```

3.4.2 Diagnostics to X Distribution

Considering the dependence of Y_i on X_i, to get a more reliable $\hat{\beta}_1$, we cannot just focus on the (marginal) distribution of Y_i, we would also need a better 'distribution' of X_i

- Plots: BoxPlot/QQPlot
- 4 statistics(parameters);[19]
  - Mean: Location;

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \tag{3.68}$$

  - Standard Deviation: Variability;

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2 \tag{3.69}$$

  - Skewness: Lack of Symmertry;

$$\hat{g}_1 = \frac{m_{n,3}}{m_{n,2}^{3/2}} = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^3}{\left(\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})\right)^{3/2}} \tag{3.70}$$

    Adjusted Skewness (Least MSE):

$$\frac{\sqrt{n(n-1)}}{n-2}\hat{g}_1 \tag{3.71}$$

    * $\hat{g}_1 > 0$: Right skewness, longer right tail;
    * $\hat{g}_1 < 0$: Left skewness, longer left tail.

    Fisher-Pearson coefficient of skewness: $\dfrac{3(\text{mean} - \text{median})}{\sigma}$.

  - Kurtosis: Heavy/Light Tailed.

$$\hat{g}_2 = \frac{m_{n,4}}{m_{n,2}^2} - 3 = \frac{\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^4}{\left(\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2\right)^2} - 3 \tag{3.72}$$

[19] See section. 2.1.1

$\hat{g}_2 = 0 \Rightarrow$ similar to normal.

* $\hat{g}_2 > 0$: Leptokurtic, heavy tail, slender;
* $\hat{g}_2 < 0$: Platykurtic, light tail, broad.

Note: In expression of $\hat{g}_1$ and $\hat{g}_2$, we already divide the variance. So Skewness and Kurtosis only reflect the difference from normal, but **not** related to variance.

Best tool to determine Kurtosis: QQ-Plot.

▷ R. **Code**

```
summary(df$x)
```

Other moments use package `moments`

- Bias: Inspect the design methodology
  - Selection Bias: Not completely random sampling;
  - Information Bias: Difference between 'designed' and 'get', e.g. no response;
  - Confounding: Exist another important variable, while the model actually focuses on a less important variable, or even reverse the causality.

3.4.3 Diagnostics to Residual

☐ **Residual Reflects the properties of ε**

- **Linearity** : use Residual Plot/AV Plot to Reflect the linearity and variance assumption.

▷ R. **Code**

```
lmfit <- lm(y~x,df)
scatter(df$x,lmfit$residuals)
abline(h=0)

library(car)
avPlots(lmfit)
```

- The Assumption of **Equal Variances** :
  - AV Plot , e.g. test the R^2 of $(e_Y|X_{(\wedge i)})$-$(e_{X_i}|X_{(\wedge i)})$ relation.
  - Bartlett's test:

    Idea: divide the sample into groups g, and get each MSE

$$\mathrm{MSE}_g = \frac{1}{n_g}\sum_{i=1}^{n_g}(Y_{gi} - \hat{Y}_g)^2 \tag{3.73}$$

and take statistic

$$S = -\frac{(N-g)\ln\left[\sum_g \frac{n_g}{N-n_g}\mathrm{MSE}_g\right] - \sum_g (n_g-1)\ln\frac{n_g}{N-n_g}\mathrm{MSE}_g}{1+\frac{1}{3(G-1)}\sum_g\left(\frac{1}{n_g-1}-\frac{1}{N-G}\right)} \sim \chi^2 \tag{3.74}$$

to conduct test.

Note: **sensitive** to normal assumption, not robust. Used when normal assumption is satisfied.

– Levene's test: Divide the sample into G groups. Denote **mean** of residual within each group as $\tilde{e}_g$, and in each group compute

$$d_{ig} = |e_{ig} - \tilde{e}_g| \Rightarrow \bar{d}_g = \frac{1}{n_g}\sum_{j=1}^{n_g} d_{ig} \tag{3.75}$$

Then conduct ANOVA to d_{ig}.

If $G = 2$: 2-sample t-test,

$$T = \frac{\bar{d}_1 - \bar{d}_2}{s\sqrt{\frac{1}{n_1}+\frac{1}{n_2}}} \xrightarrow{\mathscr{L}} t_{n-2} \qquad s^2 = \frac{\sum(d_{i1}-\bar{d}_1)^2 + \sum(d_{i2}-\bar{d}_2)^2}{n-2} \tag{3.76}$$

– Brown-Forsythe's Test (Modified Levene's test): For skewed sample, take the **mean** as **median**, more robust.

⋆ Breusch-Pagan Test:

Assume variance of ε_i dependent on X_i as m^{th} polynomial:

$$\sigma_i^2 = \alpha_0 + \sum_{k=1}^{m} \alpha_k X_i^k \tag{3.77}$$

and test

$$H_0 : \alpha_k = 0\,\forall k = 1, 2, \ldots, m \longleftrightarrow H_1 \tag{3.78}$$

Method: First conduct OLS to get regression line $\hat{l}_1$ and residuals e_i and SSE, and conduct regression of e_i^2 over X_i to get another regression line $\hat{l}_2$ and corresponding SSR*.

Then statistic

$$S = \frac{\mathrm{SSR}^*/2}{(\mathrm{SSE}/n)^2} \xrightarrow{\mathscr{L}} \chi_m^2 \tag{3.79}$$

▷ `R`. **Code**

Example for $G = 2$:

```
group <-factor(rep(c(1,2),length.out=length(df$x),
    each=(ceiling(length(df$x)/2))))

bartlett.test(lmfit$residuals~group,group)

library(car)
leveneTest(lmfit$residuals~group,group,center=mean)
leveneTest(lmfit$residuals~group,group,center=median)
```

```
library(lmtest)
bptest(lmfit)
```

- The Assumption of **Normality** :

  In most case we use S-W Test($n < 2000$) and K-S Test($n > 2000$):

  - QQ-plot of ordered residuals.
  - ⋆ Shapiro-Wilk Test (Most Powerful)[20]: To test $H_0 : \exists\sigma^2,\ s.t.\ \varepsilon \sim N_n(0, \sigma^2 I_n)$, denote

$$m_i = E(\frac{\varepsilon_{(i)}}{\sigma}) \tag{3.80}$$

    then under H_0, $\varepsilon_{(i)} \sim m_i \rightarrow$ linear, thus test correlation

$$R^2 = \frac{\left(\sum_{i=1}^{n}(e_{(i)} - \bar{e})(m_i - \bar{m})\right)^2}{\sum_{i=1}^{n}(e_i - \bar{e})^2 \sum_{i=1}^{n}(m_i - \bar{m})^2} = corr(e_{(i)}, m_i) \tag{3.81}$$

  - Kolmogorov-Smirnov Test:

$$D_n = \sum_e |F_n(e) - \Phi(e)| \tag{3.82}$$

  - Cramér-von Mises Test:

$$T = n \int_{-\infty}^{\infty} (F_n(e) - \Phi(e))^2 \,\mathrm{d}\Phi(e) \tag{3.83}$$

  - Anderson-Darling Test:

$$A^2 - n \int_{-\infty}^{\infty} (F_n(e) - \Phi(e))^2 \frac{1}{\Phi(e)(1 - \Phi(e))} \,\mathrm{d}\Phi(e) \tag{3.84}$$

  - Jarque-Bera Test , using skewness $\hat{g}_1$ and kurtosis $\hat{g}_2$ of $\vec{e}$

$$\mathrm{JB} = \frac{n}{6}(\hat{g}_1^2 + \frac{1}{4}\hat{g}_2^2) \xrightarrow{\mathscr{L}} \chi_2^2 \tag{3.85}$$

▷ R. **Code**

```
qqnorm(lmfit$residuals)
qqline(lmfit$residuals)

qqp <- qqnorm(lmfit$residuals)
cor(qqp$x,qqp$y)

shapiro.test(lmfit$residuals)

ks.test(jitter(lmfit$residuals), pnorm,mean(lmfit$residuals), sd(
    lmfit$residuals))

```

[20]Detail of S-W Test and K-S Test see Test of Normality in section. 2.4.6

```
library(nortest)
cvm.test(lmfit$residuals)

ad.test(lmfit$residuals)

library(tseries)
jarque.bera.test(lmfit$residuals)
```

- The Assumption of **Independence** :
  - Durbin-Watson Test:
$$d = \frac{\sum_{j=2}^{n}(e_j - e_{j-1})^2}{\sum_{j=1}^{n} e_j^2} \tag{3.86}$$
    $d \in (1.5, 2.5)$ is fine.
  - Ljung-Box Test:
$$Q = n(n+2)\sum_{k=1}^{n}\frac{\hat{\rho}_k^2}{n-k} \tag{3.87}$$

▷ R. **Code**

```
dwtest(lmfit)
```

3.4.4 Diagnostics to Influentials

An intuitive explanation to extreme values:

- Outliers: Extreme case for Y;
- High Leverage: Extreme case for X;
- Influentials: Cases that influence the regression line.

☐ **Influentials = Outliers ∩ High Leverage**

In section. 3.3, we got the $\hat{\beta}$ as $\hat{\beta} = (X'X)^{-1}X'Y = HY$ and got $\hat{Y}$ as
$$\hat{Y} = X\hat{\beta} = X(X'X)^{-1}X'Y = \hat{H}Y \tag{3.88}$$
where hat matrix $H \equiv X(X'X)^{-1}X' = \dfrac{\partial \hat{Y}}{\partial Y}$

Also we got statistical inference to β, σ^2, e

$$\hat{\beta} = (X'X)^{-1}X'Y \sim N(\beta, \sigma^2(X'X)^{-1}) \tag{3.89}$$
$$e = Y - \hat{Y} = (I-H)Y \sim N(0, \sigma^2(I-H)) \tag{3.90}$$
$$\hat{\sigma}^2 = \text{MSE} = \frac{e'e}{n-p-1} = \frac{Y'(I-H)Y}{n-p-1} \tag{3.91}$$
$$\frac{(n-p-1)\hat{\sigma^2}}{\sigma^2} \sim \chi^2_{n-p-1} \tag{3.92}$$

The diagonal elements of $\hat{H}$ is self-sensitivity h_{ii}

$$h_{ii} = X_i'(X'X)^{-1}X_i \tag{3.93}$$

☐ **Some refined residuals to help conduct Diagnostics:**

- Standardized Residual:

$$e_{\text{sd}i} = \frac{e_i}{\sigma_{e_i}} = \frac{e_i}{\sigma\sqrt{1-h_{ii}}} \tag{3.94}$$

- (Internal) Studentized Residual: replace σ with $s = \hat{\sigma}$

$$r_i = \frac{e_i}{\hat{\sigma}\sqrt{1-h_{ii}}} = \frac{e_i}{\sqrt{\text{MSE}}\sqrt{1-h_{ii}}} \tag{3.95}$$

- Deleted Residual:[21]

$$d_i = Y_i - \hat{Y}_{i(\wedge i)} = \frac{e_i}{1-h_{ii}} \tag{3.98}$$

---

[21] *Proof*:

Lemma: $(A+B)^{-1} = A^{-1} - \dfrac{1}{1+tr(BA^{-1})}A^{-1}BA^{-1}$, where $\text{rk}(B) = 1$.

$$\hat{\beta}_{(\wedge i)} = (X'_{(\wedge i)}X_{(\wedge i)})^{-1}X'_{(\wedge i)}Y_{(\wedge i)} \tag{3.96}$$

Using the above lemma: (here for aesthetic purpose, treat X_i as row vector)

$$\begin{aligned}
(X'_{(\wedge i)}X_{(\wedge i)})^{-1} =&(X'X - X_i'X_i)^{-1}\\
=&(X'X)^{-1} + \frac{1}{1-tr[X_i'X_i(X'X)^{-1}]}(X'X)^{-1}X_i'X_i(X'X)^{-1}\\
=&(X'X)^{-1} + \frac{1}{1-h_{ii}}(X'X)^{-1}X_i'X_i(X'X)^{-1}\\
X_{(\wedge i)}Y_{(\wedge i)} =&X'Y - X_i'Y_i
\end{aligned}$$

then calaulate $\hat{\beta}_{(\wedge i)}$:

$$\begin{aligned}
\hat{\beta}_{(\wedge i)} =&(X'_{(\wedge i)}X_{(\wedge i)})^{-1}X'_{(\wedge i)}Y_{(\wedge i)}\\
=&\left[(X'X)^{-1} + \frac{(X'X)^{-1}X_i'X_i(X'X)^{-1}}{1-h_{ii}}\right](X'Y - X_i'Y_i)\\
=&\hat{\beta} + \frac{(X'X)^{-1}X_i'X_i(X'X)^{-1}X'Y}{1-h_{ii}} - (X'X)^{-1}X_i'Y_i - \frac{(X'X)^{-1}X_i'X_i(X'X)^{-1}X_i'Y_i}{1-h_{ii}}\\
=&\hat{\beta} + \frac{(X'X)^{-1}X_i'\hat{Y}_i}{1-h_{ii}} - \frac{(X'X)^{-1}X_i'Y_i(1-h_{ii})}{1-h_{ii}} - \frac{(X'X)^{-1}X_i'Y_i}{1-h_{ii}}h_{ii}\\
=&\hat{\beta} + \frac{(X'X)^{-1}X_i'}{1-h_{ii}}(\hat{Y}_i - Y_i)\\
\Rightarrow&\hat{\beta} - \hat{\beta}_{(\wedge i)} = (X'X)^{-1}X_i'\frac{e_i}{1-h_{ii}}
\end{aligned} \tag{3.97}$$

Then

$$\begin{aligned}
Y_i - \hat{Y}_{i(\wedge i)} =&Y_i - \hat{Y}_i + \hat{Y}_i - \hat{Y}_{i(\wedge i)}\\
=&e_i + X_i(\hat{\beta} - \hat{\beta}_{(\wedge i)})\\
=&e_i + X_i(X'X)^{-1}X_i'\frac{e_i}{1-h_{ii}}\\
=&\frac{e_i}{1-h_{ii}}
\end{aligned}$$

where $\hat{Y}_{i(\wedge i)}$ is predicted Y value at X_i obtained from the regression of dataset with the i case (X_i, Y_i) removed:

$$\hat{\beta}_{(\wedge i)} = (X'_{(\wedge i)} X_{(\wedge i)})^{-1} X'_{(\wedge i)} Y_{(\wedge i)} \qquad \hat{Y}_{i(\wedge i)} = X'_i \hat{\beta}_{(\wedge i)} \tag{3.99}$$

- (External) Studentized Residual: To avoid self-influence, take deleted residual in equation. 3.95

$$t_i = \frac{d_i}{\hat{\sigma}_{(\wedge i)}\sqrt{1-h_{ii}}} = \frac{d_i}{\sqrt{\text{MSE}_{(\wedge i)}}\sqrt{1-h_{ii}}} \sim t_{n-p-2} \tag{3.100}$$

Relation between MSE and $\text{MSE}_{(\wedge i)}$:

$$(n-p-1)\text{MSE} = (n-p-2)\text{MSE}_{(\wedge i)} + \frac{e_i^2}{1-h_{ii}} \tag{3.101}$$

- Diagnostics to **Outlier**: use external studentized residual for t-test with Bonferroni adjustment. Declare the i^{th} case an outlier if:

$$|t_i| > t_{\alpha/2n, n-p-2} \tag{3.102}$$

- Diagnostics to **Leverage**: use hat matrix H/self-sensitivity h_{ii}.

$$\sum_{i=1}^{n} h_{ii} = tr(H) = p+1 \Rightarrow \bar{h} = \frac{p+1}{n} \tag{3.103}$$

Declare the i^{th} case a leverage if:

$$h_{ii} > \kappa \bar{h} = \kappa \frac{p+1}{n} \tag{3.104}$$

where usually take $\kappa = 2$ or 3.

- Diagnostics to **Influential**: Studentized DIFference caused to FITted values (DIFFITS)

DIFFIT:

$$\text{DIFFIT}_i = \hat{Y}_i - \hat{Y}_i(\wedge i) = e_i \frac{h_{ii}}{1-h_{ii}} \tag{3.105}$$

DIFFITS:

$$\text{DIFFITS}_i = \frac{\text{DIFFIT}_i}{s(\hat{Y}_i)} = t_i \sqrt{\frac{h_{ii}}{1-h_{ii}}} \tag{3.106}$$

Declare the i^{th} case an influential if:

$$\begin{cases} \text{DIFFITS}_i > 1 & \text{small/medium data} \\ \text{DIFFITS}_i > 2\sqrt{\dfrac{p+1}{n}} & \text{large data} \end{cases} \tag{3.107}$$

- Diagnostics to **Influential**: Cook's Distance, by quantifying the 'influence' to $\hat{\beta}$.

Using equation. 3.47(equation. 3.57) we could construct the following Cook's Distance[22]

$$D_i = \frac{\left\| X(\hat{\beta} - \hat{\beta}_{(\wedge 1)}) \right\|^2}{(p+1)\hat{\sigma}^2} = \frac{e_i^2}{(p+1)\hat{\sigma}^2} \frac{h_{ii}}{(1-h_{ii})^2} \qquad \frac{1-h_{ii}}{h_{ii}} D_i \sim F_{p+1, n-p-1} \tag{3.108}$$

[22] Proof uses EqaProofOfDeleteedResidual.

Comment:

$$D_i = \frac{e_i^2}{(p+1)\hat{\sigma}^2}\left[\frac{h_{ii}}{(1-h_{ii})^2}\right] = \frac{1}{p+1}\frac{h_{ii}}{1-h_{ii}} \times r_i^2 \tag{3.109}$$

where $\frac{1}{p+1}\frac{h_{ii}}{1-h_{ii}}$ correponds to hige leverage, and r_i^2 correponds to outliers, multiply to get influentials.

Declare the i^{th} case an influential if

$$D_i > \frac{4}{n} \tag{3.110}$$

Or conduct F-test using the distribution of D_i, with $\alpha \sim 20\%$.

- Diagnostics to **Influential**: Studentized DiFference in BETA estimates (DFBETAS). Use equation. 3.47, define

$$var(\hat{\beta}_k) = \sigma^2 (X'X)^{-1}_{kk} := \sigma^2 c_{kk} \tag{3.111}$$

And studentize difference in $\hat{\beta}$ with i^{th} case removed: $\hat{\beta}_k - \hat{\beta}_{k(\wedge i)}$

$$\text{DFBETAS}_{k(\wedge i)} = \frac{\hat{\beta}_k - \hat{\beta}_{k(\wedge i)}}{\sqrt{\text{MSE}_{(\wedge i)} c_{kk}}},\ k = 1, 2, \ldots, p \tag{3.112}$$

Declare the i^{th} case an influential if

$$\begin{cases} \text{DFBETAS}_i > 1 & \text{small/medium data} \\ \text{DFBETAS}_i > \frac{2}{\sqrt{n}} & \text{large data} \end{cases} \tag{3.113}$$

▷ R. **Code**

```
rstudent(lmfit)
library(car)
outlierTest(lmfit)

hatvalues(lmfit)

cooks.distance(lmfit)
plot(lmfit,which=4)

dfbetas(lmfit)
```

Leverage and Mahalanobis Distance:

Mahalanobis Distance between X and Y as defined in equation. 4.19

$$d_M(\vec{x}) = \sqrt{(\vec{x}-\vec{\mu})^T S^{-1} (\vec{x}-\vec{\mu})} \tag{3.114}$$

And we can proof d_M of a case item $X_{i\cdot} = (1, X_{i1}, X_{i2}, \ldots, X_{ip})$ is

$$d_M^2(X_{i\cdot}) = (n-1)(h_{ii} - \frac{1}{n}) \tag{3.115}$$

3.4.5 Extra Sum Of Square

Def. Extra SS: the part of SSE explained by a new X_2 when adding to model $Y \sim X_1$:

$$\mathrm{SSR}(X_2|X_1) = \mathrm{SSE}(X_1) - \mathrm{SSE}(X_1, X_2) = \mathrm{SSR}(X_1, X_2) - \mathrm{SSR}(X_1) \tag{3.116}$$

where $\mathrm{SS}(\cdot)$ represents the SS when the model contains variable $\cdot$.[23]

(The following part use model (Y, X_1, X_2) as example.)

We could use extra SS to examine the proper regression model: examine the `F value` and `Pr(>F)` in the output.

▷ `R.` **Code**

```
lm(y~x1+x2+x1:x2) %>% anova
```

Note: Three types of SS

Term	Type I SS[24]	Type II SS	Type III SS
X_1	$\mathrm{SSR}(X_1)$	$\mathrm{SSR}(X_1\|X_2)$	$\mathrm{SSR}(X_1\|X_2, X_1X_2)$
X_2	$\mathrm{SSR}(X_2\|X_1)$	$\mathrm{SSR}(X_2\|X_1)$	$\mathrm{SSR}(X_2\|X_1, X_1X_2)$
X_1X_2	$\mathrm{SSR}(X_1X_2\|X_1, X_2)$	Assume no interaction term	$\mathrm{SSR}(X_1X_2\|X_1, X_2)$
Language.Function	`R.anova`	`python.`	`SPSS,SAS,R.lm`

To get Type II and III anova, use `Anova(lmfit,type='III')` in `'car'` package.

Hierarchical Principle: the interaction term X_1X_2 should always come in **after** marginal term X_1 and X_2.

▷ `R.` **Code**

```
libaray('car')
Anova(lmfit,type='II')
Anova(lmfit,type='III')
```

3.4.6 Hypotheses Testing to Slope

Main focus: whether the linear relation exist:

$$H_0 : \beta_1 = \beta_2 = \ldots = \beta_p = 0 \longleftrightarrow H_1 : \exists \beta_i \neq 0,\ i = 1, 2, \ldots, p \tag{3.117}$$

As for general case $H_0 : \underset{q\times(p+1)}{C} \beta - \underset{(p+1)\times 1}{t} = 0$, use General Linear Test.

- ANOVA F-Test:

  We can examine

$$F = \frac{\mathrm{MSR}}{\mathrm{MSE}} \sim F_{p,n-p-1} \tag{3.118}$$

- General Linear Test (GLT)

  First we introduce the examine models:

[23] $\mathrm{SSE}(1) = \mathrm{SST}$, where 1 correponds to intercept.

- Full model: Include all variable/parameters to be examined, with p variables.

$$Y = X\beta + \varepsilon \tag{3.119}$$

  And define $\mathrm{SSE_F}$ with $dof_\mathrm{F} = n - p - 1$ under Full Model.

- Reduced model: Apply the Null Hypothesis to Full Model, with $\tilde{p}$ variables

$$Y_i = \tilde{X}\tilde{\beta} + \varepsilon \tag{3.120}$$

  And define $\mathrm{SSE_R}$ with $dof_\mathrm{R} = n - \tilde{p} - 1$ under Reduced Model.

Then conduct test to the difference between Full model and Reduced model through $\mathrm{SSE_F}$ and $\mathrm{SSE_R}$.

- One dimensional case: $H_0 : \beta_1 = 0$

  Examine

$$F = \frac{(\mathrm{SSE_R} - \mathrm{SSE_F})/(dof_\mathrm{R} - dof_\mathrm{F})}{\mathrm{SSE_F}/dof_F} \sim F_{1,n-2} \tag{3.121}$$

  ▷ R. **Code**

```
fullmodel <- lmfit
nullmodel <- lm(y ~ 1,df)
anova(nullmodel,fullmodel)
```

- General case: Test $H_0 : \underset{q\times(p+1)}{C}\beta - \underset{(p+1)\times 1}{t} = 0$, construct F statistics as

$$F = \frac{(C\hat{\beta} - t)' \left[C(X'X)^{-1}C'\right]^{-1} (C\hat{\beta} - t)}{q\hat{\sigma}^2} \sim F_{q,n-q} \tag{3.122}$$

• Pearson Correlation Coefficient r and Coefficient of Multiple Determination R^2:

Pearson's r:

$$r = \hat{cov}(Y, \hat{Y}) = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(\hat{Y}_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}\sqrt{\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2}} = \sqrt{\frac{\sum_{i=1}^{n}(\hat{Y} - \bar{Y})^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}} \tag{3.123}$$

CMD R^2:

$$R^2 = \frac{\mathrm{SSR}}{\mathrm{SST}} = 1 - \frac{\mathrm{SSE}}{\mathrm{SST}} \tag{3.124}$$

Adjusted R^2:

$$R^2_\mathrm{a} = 1 - \frac{\mathrm{MSE}}{\mathrm{MST}} = 1 - \frac{n-1}{n-p-1}\frac{\mathrm{SSE}}{\mathrm{SST}} \tag{3.125}$$

- Relation between r and R^2: Under Simple Linear Model, we have

$$R^2 = r^2 \tag{3.126}$$

- Relation between R^2 and F-Statistic:

$$F = \frac{R^2}{1 - R^2}\frac{n-p-1}{n-1} \tag{3.127}$$

Hypothesis testing for r:

$$t = \frac{r}{\sqrt{1-r^2}}\sqrt{n-2} \sim t_{n-2} \tag{3.128}$$

▷ R. **Code**

```
cor.text(df$x,df$y)
```

- Coefficient of Partial Determination $R^2_{Yk|\wedge X_k}$ and Coefficient of Multiple Determination R^2: CMD reflects the interpretability of the model, to examine the interpretability of each variable, use coef. partial determination

$$R^2_{YX_k|X_1,\ldots,X_{k-1},X_{k+1},\ldots,X_p} = R^2_{YX_k|\wedge X_k} = \frac{\text{SSR}(X_k|X_1,\ldots,X_{k-1},X_{k+1},\ldots,X_p)}{\text{SSE}(X_1,\ldots,X_{k-1},X_{k+1},\ldots,X_p)} = \frac{\text{SSR}(X_k|\wedge X_k)}{\text{SSE}(\wedge X_k)} \tag{3.129}$$

Note: Coef. Partial determination can also be used for X_i, X_j: $R^2_{X_iX_j|\wedge X_i,X_j}$

Sometimes we use $\eta_k^2 = R^2_{YX_k|\wedge k} = R^2_{Yk.\wedge k}$

- Coefficient of Partial Correlation: Measures the strength of linear relation, $\pm$ sign depend on posi./nega. correction.

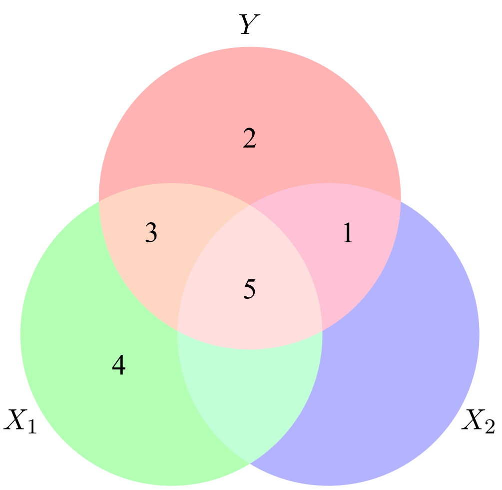
$$\eta_k = \pm\sqrt{\eta_k^2} \tag{3.130}$$

▷ R. **Code**

```
library('heplots')
etasq(lmfit)
```

3.4.7 Diagnostics to Multi-collinearity

- Venn Diagram for Multi-Linear Regression: Used to show the interpretability of variables.



Explanation of each region:

- 1/3: Variation in Y uniquely attributes to X_2/X_1;
- 2: Variation in Y that cannot be explained by regression to X_1, X_2, corresponds to ε;

- 5: Cross term of X_1, X_2, **cannot** verify the orientation, corresponds to **Multi-colinearity**.

In the presence of multi-colinearity, i.e. X is column singular ($\dfrac{S_5}{S_1 \text{ or } S_3}$ large), the regression parameter

$$\hat{\beta} = (X'X)^{-1}X'Y \tag{3.131}$$

Issue of multi-collinearity:

- Statistically:'better' prediction, worse interpretability;
- Numerically: Calculation of $(X'X)^{-1}$ becomes unstable/ill-posed/NAN.

☐ **Use Variance Inflation Factor (VIF) to detect multi-collinearity.**

First construct R_k^2, $k = 1, 2, \dots p$: Regress X_k against other $p-1$ variable X_is and get corresponding R_k^2, and

$$\mathrm{VIF}_k = (1 - R_k^2)^{-1} \tag{3.132}$$

$$\overline{\mathrm{VIF}} = \frac{1}{p}\sum_{k=1}^{p} \mathrm{VIF}_k \tag{3.133}$$

If $\|\mathrm{VIF}_i\|_\infty > 10$ or $\overline{\mathrm{VIF}} > 1$, then we identify an excessive multi-colinearity.[25]

▷ R. **Code**

```
library('car')
vif(lmfit)
```

3.4.8 Diagnostics to Model Variable Selection

In Multi-variate regression, proper explanatory variables form a subset of all available variables.

Aim: Avoid over-fitting, get a simple explanatory model.

Comment: If we consider the model with all p_{max} variables as full, unbiased model, then model selection is a kind of **Bias-Variance Trade-Off**.

☐ **Model Validation: k-Fold Cross Validation(CV):**

1. **Separate the dataset size n into k parts;**
2. **pick the i^{th} part as test set y_i, and the other $k-1$ part as train set $y_{\wedge i}$(to conduct regression, etc); then conduct prediction of model $y_{\wedge i}$ to part y_i ane get MSE_i;**
3. **Take average of MSE_i as the measure of validity.**

☐ **Evaluation Criteria**

Useful model validation approach: To check a model with $p-1$ variable (this part p for 1+# variable)

[25] Why $\mathrm{VIF}_k = \dfrac{1}{R_k^2}$ is called 'variance inflation factor'? We can prove that

$$var(\hat{\beta}_k) = \frac{\sigma^2}{(n-1)S_{x_k}^2} \cdot \frac{1}{R_k^2} = \frac{\sigma^2}{(n-1)S_{x_k}^2} \cdot \mathrm{VIF}_k \tag{3.134}$$

- Traditional way: Test R^2, R_a^2, p-value, etc.
- Mallow's C_p: For a model with p variable:

$$\hat{Y}^p = X_p(X_p'X_p)^{-1}X_p'Y = H_pY \tag{3.135}$$

Denote:

$$\mathbb{E}(\hat{Y}^p) = H_pE(Y) \equiv H_p\mu \qquad var(\hat{Y}^p) = H_p\sigma^2 I_n H_p' = \sigma^2 H_p \tag{3.136}$$

Recall the MSE expansion of bias-variance trade-off in equation. 2.30[26]

$$\begin{aligned}\sum_{i=1}^n \mathbb{E}[(\hat{Y}_i^p - \mu_i)^2] = &\sum_{i=1}^n \mathbb{E}(\hat{Y}_i^p) - \mu_i]^2 + \sum_{i=1}^n var(\hat{Y}_i^p) \\ \Rightarrow = &\mathbb{E}(\text{SSE}(p)) - (n-2p)\sigma^2\end{aligned}$$

Sum Squared Prediction Error (SSPE):

$$\Gamma_0 \equiv \frac{\sum_{i=1}^n \mathbb{E}[(\hat{Y}_i^p - \mu_i)^2]}{\sigma^2} = \frac{\mathbb{E}(\text{SSE}(p))}{\sigma^2} - (n-2p) \tag{3.138}$$

And construct Mallow's $C-p$: Estimation of Γ_p

$$C_p = \hat{\Gamma}_p = \frac{\mathbb{E}(\text{SSE}(p))}{\hat{\sigma}^2} - (n-2p) \tag{3.139}$$

where SSE(p) $= Y'(I-H_p)Y$.

When the model is unbiased, then $\mathbb{E}(\text{SSE}(p)) \to n-p$, use C_p-p plot to pick proper p:

- $C_p \approx p$: Model unbiased, then choose model with smaller C_p;
- $C_p \gg p$: Significant biased, miss some important predictors;
- $C_p \ll p$: Overfitting.

---

[26]Derivtion:

- Bias part: (Here use equation. 4.41 in 3rd line; use equation. 3.54 in 4th line.)

$$\begin{aligned}\sum_{i=1}^n [e(\hat{Y}_i^p - \mu_i)]^2 = &\mu'(H_p - I)'(H_p - I)\mu \\ = &\mu(I-H_p)\mu' \\ = &E(Y'(I-H_p)Y) - tr[(I-H_p)\sigma^2] \\ = &E(\text{SSE}(p)) - (n-p)\sigma^2\end{aligned}$$

- Variance part:

$$\sum_{i=1}^n var(\hat{Y}_i^p) = tr(var(\hat{Y}^p)) = \sigma^2 tr(H_p) = p\sigma^2$$

Then

$$\frac{\sum_{i=1}^n \mathbb{E}[(\hat{Y}_i^p - \mu_i)^2]}{\sigma^2} = \frac{\mathbb{E}(\text{SSE}(p))}{\sigma^2} - (n-2p) \tag{3.137}$$

- Akaike Information Criterion (AIC): Euivalent to Mallow's C_p for gaussion regression model.

$$\mathrm{AIC}(p) = -2\log(\hat{L}) + 2p \tag{3.140}$$

where $\hat{L}$ is the maximum likelihood, for linear regression case

$$\mathrm{AIC}(p) = n\log\left(\frac{\mathrm{SSE}(p)}{n}\right) + 2p \tag{3.141}$$

Select the model that minimizes $\mathrm{AIC}(p)$.

- Bayesian Information Criterion (BIC)/Schwarz's Bayesian Criterion (SBC):

$$\mathrm{BIC}(p) = -2\log(\hat{L}) + p\log n \tag{3.142}$$

where $\hat{L}$ is the maximum likelihood, for linear regression case

$$\mathrm{BIC}(p) = n\log\left(\frac{\mathrm{SSE}(p)}{n}\right) + p\log n \tag{3.143}$$

Select the model that minimizes $\mathrm{BIC}(p)$.

- PRESS Creterion (Predictive Residual Error Sum of Squares): A kind of within-model cross validation

$$\mathrm{PRESS}(p) = \sum_{i=1}^{n}(Y_i - \hat{Y}_{i(\wedge i)})^2 \tag{3.144}$$

where

$$\begin{aligned}\hat{Y}_{i(\wedge i)} =& (1, X_{i1}, \ldots, X_{ip})\hat{\beta}_{(\wedge i)}\\ \hat{\beta}_{(\wedge i)} =& (X'_{(\wedge i)}X_{(\wedge i)})^{-1}X'_{(\wedge i)}Y_{(\wedge i)}\end{aligned}$$

where $\hat{\beta}_{(\wedge i)}$ as in EqaEstimatorWithWedgeX, is the estimated β with (X_i, Y_i) removed from X.[27]

Select the model that minimizes $\mathrm{PRESS}(p)$.

▷ R. **Code**

```
library('leaps')
predictor <- df[,c('...','...',...)]
response <- df[,...]
leapSet <- leaps(x=predictor, y=response, nbest = ...)
# method=c('Cp','adjr2','r2')
leapSet$which[which.min(leapSet$Cp),]
```

nbest for NUMBER_OF_BEST_MODELS

[27] A useful thm.: Deleted Residual

$$d_i := Y_i - \hat{Y}_{i(\wedge i)} = \frac{e_i}{1-h_{ii}} \tag{3.145}$$

Section 3.5 Remedies

3.5.1 Variable Transformation

The goal of Transformation:

- Stablize Variance;
- Improve Normality;
- Simplify the Model.

☐ **Transformation Methods:**

- Variance Stabilizing Transformations: For $E(Y_X) = \mu_X$, $var(Y_X) = h(\mu_X)$, take transformation $f(Y)$ such that $var(f(Y)) =$ const, satisfies
$$f(\mu) = \int \frac{c\,\mathrm{d}\mu}{\sqrt{h(\mu)}} \tag{3.146}$$
Examples:
$$\begin{aligned} h(\mu) =& \mu^2 \Rightarrow f(\mu) = \ln \mu \\ h(\mu) =& \mu^{2\nu} \Rightarrow f(\mu) = \mu^{1-\nu} \end{aligned}$$

- Box-Cox Transformation: Take
$$Y^* = \frac{Y^\lambda - 1}{\lambda} \tag{3.147}$$
Examples:
$$\begin{aligned} \lambda = 1 &\Rightarrow Y^* \sim Y \\ \lambda = 0.5 &\Rightarrow Y^* \sim \sqrt{Y} \\ \lambda = 0 &\Rightarrow Y^* \sim \ln Y \\ \lambda = -1 &\Rightarrow Y^* \sim 1/Y \end{aligned}$$
And conduct regression to model
$$Y^* = \beta_0 + \beta_1 X + \varepsilon_i \tag{3.148}$$
Likelihood Function
$$L(\beta, \sigma^2; \lambda) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (Y_i^* - \beta_0 - \beta_1 X_i)^2 \right) J(\frac{\partial Y^*}{\partial Y}) \tag{3.149}$$
where the Jacobi Matrix denoted in Geometric Mean $\mathrm{GM}(Y) = \prod_{i=1}^n Y_i^{1/n}$
$$J(\frac{\partial Y^*}{\partial Y}) = \prod_{i=1}^n Y_i^{\lambda-1} = \mathrm{GM}(Y)^{n(\lambda-1)} \tag{3.150}$$

MLE Estiamtor:

$$\begin{aligned}\hat{\beta}^* &= (X'X)^{-1}X'Y^* \\ \hat{\sigma}_n^2 &= \frac{1}{n}\text{SSE}^* \\ \text{SSE}^* &= \sum_{i=1}^{n}(Y_i^* - \hat{Y}_i^*)^2\end{aligned}$$

And when β, σ^2 take MLE estimator, $L(\beta, \sigma^2; \lambda)$ can be regarded a function of λ:

$$\ln L(\beta, \sigma^2; \lambda) = l(\lambda) = -\frac{n}{2}\ln\frac{\hat{\sigma}_n^2}{\text{GM}(Y)^{2(\lambda-1)}} + \text{const} \tag{3.151}$$

For simplification, denote $Z = Y * / J^{1/n}$ and get

$$\ell(\lambda) = -n\ln\sigma_{nZ}^2 + \text{const} \tag{3.152}$$

where

$$Z_i^* = \begin{cases} \dfrac{Y_i^\lambda - 1}{\lambda}\dfrac{1}{\prod_{k=1}^{n} Y_k^{\frac{\lambda-1}{n}}}, & \lambda \neq 0 \\ \ln Y_i \prod_{k=1}^{n} Y_k^{\frac{1}{n}}, & \lambda = 0 \end{cases} \tag{3.153}$$

Plot $l(\lambda)$-λ to determine a proper λ and transform $Y^* = \dfrac{Y^\lambda - 1}{\lambda}$:

– Selected λ should be closed to $\lambda_{\arg\max l}$, at least within CI[28]

$$\{\lambda | l(\lambda) \geq l(\lambda_{\arg\max l}) - \frac{1}{2}\chi^2_{1,1-\alpha}\} \tag{3.154}$$

– Should pick a λ which is **Interpretable**. e.g. If $\lambda = 1$ is within range $[0.94, 1.08]$, then take $\lambda = 1$ (does not transform).

▷ R. **Code**

```r
library(MASS)
bctrans <- boxcox(y~x,df,lambda = seq(-1.5, 1.5, length = 15))
bctrans$x[which.max(bctrans$y)]
```

Note: we can transform on X or Y or simultaneously to get better regression model.

3.5.2 Weighted Least Squares Regression

To deal with heterogeneous variance, use Weighted Least Squares (WLS) instead of OLS: Minimizing

$$\sum_{i=1}^{n} e_i^2 \longrightarrow \sum_{i=1}^{n} w_i e_i^2 \tag{3.155}$$

[28]Here CI can be derived using Wilk's Thm.

And e.g. take weight for each case as

$$w_i = \frac{1}{\sigma_i^2} \tag{3.156}$$

Solution:

$$\hat{\beta} = (X'WX)^{-1}X'WY \tag{3.157}$$

▷ R. **Code**

```
Wlmfit <- lm(y~x,weights=WEIGHT_VECTOR,data=df)
```

3.5.3 Remedies for Model Variable Selection & More Regression Model

Several Algorithm to search for best variable set:

- Exhaustive Search and Test: Used for $p \leq\sim 30$
- Greedy Search: Get a locally optimal solution.
  - Forward Selection: Start with $p = 0$, add one variable each times and conduct $t/F/p$-value test until a presupposed certain limit.
  - Backward Elimination: Start with p_{max}, eliminate one variable each times and conduct $t/F/p$-value test until a presupposed certain limit.
  - Stepwise Regression: Alternate forward selection & backward elimination until no add/elimination.
- Penalized Optimization:

  Recall: OLS regression model: Minimize SSE[29]

$$\hat{\beta} = \arg\min \|Y - X\beta\|_2^2 \tag{3.158}$$

  Idea: Add a penalty term in SSE, such that SSE increases with # of variables/value of variables.

  - LASSO (Least Absolute Shrinkage and Selection Operator)

    Penalty term: $\lambda\|\beta\|_1)$, where λ is a proper penalty parameter.

$$\hat{\beta} = \arg\min(\|Y - X\beta\|_2^2 + \lambda\,\|\beta\|_1) \tag{3.159}$$

    or equivlantly expressed as

$$\hat{\beta} = \arg\min \|Y - X\beta\|_2^2\,,\ \text{with}\ \|\beta\|_1 \leq s \tag{3.160}$$

    where s is a parameter correponding to λ. Select a proper value of λ(or equivlantly s) for expected model: Some $\hat{\beta}_i$ would be exactly 0.

  - Ridge Regression/Tikhonov Regularization:

    Penalty term: $\lambda\|\beta\|_2^2)$, where λ is penalty parameter.

$$\hat{\beta} = \arg\min(\|Y - X\beta\|_2^2 + \lambda\|\beta\|_2^2) \tag{3.161}$$

[29] Here expressed in ℓ_p norm, definition see sec.4.1.2, Norm

or equivlantly expressed as

$$\hat{\beta} = \arg\min \|Y - X\beta\|_2^2, \text{ s.t. } \|\beta\|_2^2 \leq s \tag{3.162}$$

Select a proper value of λ (or equivlantly s) for expected model. Generally Ridge regression **cannot** conduct variable selection, but usually used to avoid non-invertible $X'X$, or used to retain important but collinear variable.

Solution of Ridge regression:

$$\hat{\beta}_\lambda^{\text{Ridge}} = (X'X + \lambda I)^{-1} X'Y \tag{3.163}$$

[30]

– Mixed Model: Elastic Net

$$\hat{\beta} = \arg\min(\|Y - X\beta\|_2^2 + \lambda_1\|\beta\|_1 + \lambda_2\|\beta\|_2^2) \tag{3.164}$$

or equivalent form:

$$\begin{aligned} \hat{\beta} &= \arg\min_\beta \|Y - X\beta\|^2 \\ s.t. &\frac{\lambda_1}{\lambda_1+\lambda_2}\|\beta\|_1 + \frac{\lambda_2}{\lambda_1+\lambda_2}\|\beta\|_2^2 \leq s \end{aligned}$$

picking proper hyper-parameter $(s, \lambda = \dfrac{\lambda_2}{\lambda_1+\lambda_2})$

▷ R. **Code**

```
library('MASS')
Rfit <- lm.ridge(y~x,lambda=seq(0,0.1,0.001),data=df)
summary(Rfit)
whichLambda <- which.min(Rfit$GCV)
coef(fits)[whichLambda,]

library('lars')
Lfit <- lars(x,y,type='lasso')
summary(Lfit)
whichCp <- which.min(Lfit$Cp)
```

[30] Why Ridge regression can also fix the problem of olinearity, i.e. non-full rank XX':
Assume the SVD decomposition of X: $X = U\Sigma V'$, then

$$\begin{aligned} X'X + \lambda I =& V\Sigma U'U\Sigma V' + \lambda I \\ =& V \begin{bmatrix} \sigma_1^2+\lambda & 0 & \dots & 0 \\ 0 & \sigma_2^2+\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_{p+1}^2+\lambda \end{bmatrix} V' \end{aligned}$$

then for $\lambda > 0$, we can get a positive-definite matrix $X'X + \lambda I$

```
    Lfit$Cp[whichCp]
    Lfit$beta[whichCp,]
```

- Non-parametric Regression Model: Add smooth/penalty function.

  Example: `loess` (Locally Regression), `lowess` (Locally Weighted ScatterPlot Smoother), Regression Tree.

- Other Regression Model: 、

  – Standardized Regression Model For regression model $Y_i = \beta_0 + \sum_{j=1}^{p} X_{ij}\beta_j + \varepsilon_i$, $i = 1, 2, \ldots, n$, conduct Standardization (with an extra const $1/\sqrt{n-1}$) to Y and X.

$$Y_i^* = \frac{1}{\sqrt{n-1}}\frac{Y_i - \bar{Y}}{s_Y} \qquad X_{ij}^* = \frac{1}{\sqrt{n-1}}\frac{X_{ij} - \bar{X}_i}{s_{X_i}} \qquad \varepsilon_i^* = \frac{1}{\sqrt{n-1}}\frac{\varepsilon_i - \bar{\varepsilon}}{s_Y} \tag{3.165}$$

  And the regreeesion model for standardized data:

$$Y_i^* = 0 + \sum_{j=1}^{n} X_{ij}^* \beta_j^* + \varepsilon_i^* \tag{3.166}$$

  with

$$\beta_j^* = \frac{\beta_j s_{X_j}}{s_Y} \tag{3.167}$$

  Note: set the const as $\sqrt{n-1}$ so that

$$r_{X^*X^*} = X^{*T}X^* \qquad r_{Y^*X^*} = X^{*T}Y^* \tag{3.168}$$

  ▷ R. **Code**

```
scaledf <- data.frame(scale(df))
scalelmfit <- lm(~,scaledf)
summary(scalelmfit)
```

  – Polynomial Regression Model

  ▷ R. **Code**

```
polfit <- lm(y~x+I(x^2),df)
polfit <- lm(y~polym(x1,x2,degree=),df)
```

  – Interaction Model Example:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \varepsilon \tag{3.169}$$

  Re-write as

$$\begin{aligned} Y =& \beta_0 + (\beta_1 + \beta_3 X_2) X_1 + \beta_2 X_2 + \varepsilon \\ Y =& \beta_0 + \beta_1 X_2 + (\beta_2 + \beta_3 X_1) X_2 + \varepsilon \end{aligned}$$

  test the regression coefficient dependence on another variable.

Section 3.6 Factor Analysis of Variance

3.6.1 Single Factor Model

Single factor, or one-way analysis of variance focuses on continuous $Y \sim$ categorical X (numeric-factor). Regression goal is the mean response of each category π_i: whether & how much they are different.

Basic assumptions: Normal within each categories, Equal variance, independent

Model: See equation. 3.9 expression for single factor model

$$Y_{ij} = \mu + \tau_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \sim N(0, \sigma^2) \tag{3.170}$$

where τ_i for group effect, $\mu_i = \mu + \tau_i$ for factor effect. Originally only μ_i are estimatable.

▷ R. **Code**

`lm()` in `R.` uses cell means model, returns $\mu_i = \mu + \tau_i$ for each categories.

```
facfit <- lm(y~x,df) # where x should be as.factor() type
```

☐ **Statistical Inference to Individual μ, τ_i**

Note: rk$(X) = r <$ #variable $= r + 2 \Rightarrow$ estimator not unique. Usually use constraint

$$\sum_{i=1}^{r} c_i \tau_i = 0$$

usually take $c_i = 1$ or $c_i = n_i$

- Factor effect solution for $c_i = 1$, i.e. $\sum_{i=1}^{r} \tau_i = 0$

$$\begin{aligned} \hat{\mu} &= \frac{1}{r} \sum_{i=1}^{r} \bar{Y}_i = \frac{1}{r} \sum_{i=1}^{r} \sum_{j=1}^{n_i} \frac{Y_{ij}}{n_i} \\ \hat{\tau}_i &= \bar{Y}_i - \hat{\mu} \end{aligned}$$

- Factor effect solution for $c_i = n_i$, i.e. $\sum_{i=1}^{r} n_i \tau_i = 0$

$$\begin{aligned} \hat{\mu} &= \bar{Y} = \frac{1}{n_T} \sum_{i,j} Y_{ij} \\ \hat{\tau}_i &= \bar{Y}_i - \bar{Y} = \frac{1}{n_i} \sum_{j=1}^{n_i} Y_{ij} - \hat{\mu} \end{aligned}$$

☐ **One-Way ANOVA**

ANOVA table in the form of $r = p + 1$ multivariate ANOVA in page 60

Source	dof	SS	MS	F-Statistic
SSRegression	$r - 1$	$\sum_{i=1}^{r} (\hat{Y}_i - \bar{Y})^2$	SSR/dof_R	MSR/MSE
SSError	$n_T - r$	$\sum_{i=1}^{r} \sum_{j=1}^{n_i} (Y_{ij} - \hat{Y}_i)^2$	SSE/dof_E	
SSTotal	$n_T - 1$	$\sum_{i=1}^{r} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y})^2$	SST/dof_T	

Use MSE as estimator of σ^2:

$$\hat{\sigma^2} = \frac{1}{n_T - r}\sum_{i=1}^{r}\sum_{j=1}^{n_i}(Y_{ij} - \hat{Y}_i)^2 = \frac{1}{n_T - r}\left[\sum_{i=1}^{r}\sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^{r}\frac{\bar{Y}_i^2}{n_i}\right] \tag{3.171}$$

Also F-statistics for $H_0 : \tau_1 = \tau_2 = \ldots = \tau_r = 0$

$$F = \text{MSR}/\text{MSE} = \frac{\text{SSR}/(r-1)}{\text{SSE}/(n_T - r)} \sim F_{r-1, n_T - r}, \text{ under } H_0 \tag{3.172}$$

☐ **Statistical Inference to Difference**

We usually focus on 'difference' between factor effects, general form

$$\phi = \sum_{i=1}^{r}\xi_i\tau_i, \qquad \sum_{i=1}^{r}\xi_i = 0 \tag{3.173}$$

where ϕ with $\sum_{i=1}^{r}\xi_i = 0$ is called a contrast. Assume there are m estimator ϕ_k, $k = 1, 2, \ldots, m$, $m \leq \dfrac{r(r-1)}{2}$

$$\underset{m\times 1}{\phi} = \begin{bmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_m\end{bmatrix} = \underset{m\times r}{\xi}\underset{r\times 1}{\tau} = \begin{bmatrix}\xi_{11} & \xi_{12} & \ldots & \xi_{1r}\\ \xi_{21} & \xi_{22} & \ldots & \xi_{2r}\\ \vdots & \vdots & \ddots & \vdots\\ \xi_{m1} & \xi_{m2} & \ldots & \xi_{mr}\end{bmatrix}\begin{bmatrix}\tau_1\\ \tau_2\\ \vdots\\ \tau_r\end{bmatrix} \tag{3.174}$$

- Distribution of $\phi_k = \sum\limits_{i=1}^{r}\xi_{ki}\tau_i$, with $\sum\limits_{i=1}^{r}\xi_i = 0$:

$$\phi_k = \sum_{i=1}^{r}\xi_{ki}\tau_i \sim N(\sum_{i=1}^{r}\xi_{ki}\bar{Y}_i, \sigma^2\sum_{i=1}^{r}\frac{\xi_{ik}^2}{n_i}) \tag{3.175}$$

  Or use transform of multivariate normal in equation. 4.40

$$\phi \sim N_m(\xi\tau, \sigma^2\xi\xi') \tag{3.176}$$

- Sampling Distribution of $\hat{\phi}_k$:

$$\hat{\phi}_k \sim N(\sum_{i=1}^{r}\xi_{ki}\bar{Y}_i, \sigma^2\sum_{i=1}^{r}\frac{\xi_{ki}^2}{n_i}) \tag{3.177}$$

- Bonferroni's Confidence Region for $\underset{m\times 1}{\phi}$, using result in equation. 4.82

$$R(\phi) = \bigotimes_{k=1}^{m}\left(\sum_{i=1}^{r}\xi_{ki}\bar{Y}_i \pm \hat{\sigma}t_{n_T - r, \frac{\alpha}{2m}}\sqrt{\sum_{i=1}^{r}\frac{\xi_{ki}^2}{n_i}}\right) \tag{3.178}$$

- Scheffè's Confidence Region for $\underset{1\times 1}{\phi}$:

$$R(\phi) = \sum_{i=1}^{r}\xi_i\bar{Y}_i \pm \hat{\sigma}\sqrt{(r-1)F_{r-1, n_T - r, \alpha}}\sqrt{\sum_{i=1}^{r}\frac{\xi_{ki}^2}{n_i}} \tag{3.179}$$

- Tukey's Confidence Region for $\underset{1\times 1}{\phi}$, under condition $n_1 = \ldots = n_r = n$: focus on estimating $\tau_i - \tau_j$

- Def.: studentized range distribution: for $Z_1, \ldots, Z_n$ i.i.d. $\sim N(0,1)$, $mW^2 \sim \xi_m^2$, then

$$q = \frac{\max Z_i - \min Z_i}{W} \sim q_{n,m} \tag{3.180}$$

Then confidence interval for $\phi = \tau_i - \tau_j$

$$R(\phi) = \bar{Y}_i - \bar{Y}_j \pm q_{r,n_T-r,\alpha} \frac{\hat{\sigma}}{\sqrt{n}} \tag{3.181}$$

General case: $\phi = \sum_{i=1}^r \xi_i \tau_i$

$$R(\phi) = \sum_{i=1}^r \xi_i \bar{Y}_i \pm q_{r,n_T-r,\alpha} \frac{\hat{\sigma}}{2\sqrt{n}} \sum_{i=1}^r |\xi_i| \tag{3.182}$$

Comment: Scheffè is more conservative, i.e. shorter. If confidence interval does not include 0, we can say they are significantly different.

▷ R. **Code**

```
library('agricolae')
facaov <- aov(y~0+x,df)

LSD.test(facaov,trt='design',group=FALSE,console=TRUE)

scheffe.test(facaov,trt='design',group=FALSE,console=TRUE)

TukeyHSD(facaov,conf.level=0.95)
```

use `plot()` to view interval estimation

3.6.2 Double Factor Model

Double factor, or two-way analysis of variance, categories π_{ij}:

$$Y_{ijk} = \mu + \alpha_i + \beta_j + e_{ijk} \tag{3.183}$$

LS estimator with $\sum_{i=1}^a \alpha_i = 0$, $\sum_{j=1}^b \beta_j = 0$:

$$\begin{aligned} \hat{\mu} &= \frac{1}{ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \frac{Y_{ijk}}{n_{ij}} \\ \hat{\alpha}_i &= \frac{1}{b} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \frac{Y_{ijk}}{n_{ij}} - \hat{\mu} \\ \hat{\beta}_j & \frac{1}{a} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} \frac{Y_{ijk}}{n_{ij}} - \hat{\mu} \end{aligned}$$

MSE estimator of σ^2:

$$\hat{\sigma^2} = \frac{1}{n_T - ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (Y_{ijk} - \bar{Y}_{ij})^2 = \frac{1}{n_T - ab} \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} Y_{ijk}^2 - \sum_{i=1}^a \sum_{j=1}^b \frac{\bar{Y}_{ij}^2}{n_{ij}} \right] \tag{3.184}$$

Section 3.7 Generalized Linear Model

Recall: Linear model with normal assumption can be expressed as :

$$Y_i \sim N(\mu_i, \sigma_i^2) = N(x_i'\beta, \sigma_i^2) \tag{3.185}$$

Question: How to generalize the simple linear model?

- Generalize the distribution
- Generalize the dependent mode

☐ Distribution Generalize: Scaled Exponential Family

For different range and feature of Y we can use different distribution for regression. We usually use Exponential Family distribution $f(y;\vec{\theta},\vec{\phi})$ as in equation. 2.17, with some constraint on subfunctions for better distribution properties, written as linear scaled exponential family:

$$f(y;\vec{\theta},\vec{\phi}) = \exp\left\{\frac{y'\theta - b(\theta)}{a(\phi)} + c(y,\phi)\right\} \tag{3.186}$$

where $\vec{\theta}$ is the canonical parameter for location and $\vec{\phi}$ for scale(usually we take $a(\phi) \propto \phi$).

Properties of $f(y;\theta,\phi)$:

- Expectation

$$\mu \equiv \mathbb{E}(Y) = \int y f(y)\,\mathrm{d}y = \int \left(a(\phi)\frac{\partial}{\partial\theta} + \frac{\mathrm{d}b(\theta)}{\mathrm{d}\theta}\right) f(y)\,\mathrm{d}y = b'(\vec{\theta}) \tag{3.187}$$

- Variance

$$\sigma^2 \equiv var(Y) = \int yy^T f(y)\,\mathrm{d}y - \mathbb{E}(Y)\mathbb{E}(Y)^T \tag{3.188}$$

$$= \int \left(\frac{\partial^2}{\partial\theta\partial\theta^T} + (b'(\theta)y + yb'(\theta)) - b'(\theta)b'(\theta)^T + a(\phi)\frac{\mathrm{d}^2 b(\theta)}{\mathrm{d}\theta\mathrm{d}\theta^T}\right) f(y)\,\mathrm{d}y - \mathbb{E}(Y)\mathbb{E}(Y)^T \tag{3.189}$$

$$= a(\phi)\frac{\mathrm{d}^2 b(\vec{\theta})}{\mathrm{d}\theta\mathrm{d}\theta^T} = a(\phi)b''(\vec{\theta}) \tag{3.190}$$

- Examples: Normal, Binomial, Poisson
  - Normal $f(y) = \frac{1}{\sqrt{2\pi|\Sigma|}}\exp\left(-\frac{1}{2}(y-\mu)'\Sigma^{-1}(y-\mu)\right)$ with $\Sigma = \sigma^2 I$:

$$f(y) = \exp\left(\frac{y'\mu - \frac{1}{2}\mu'\mu}{\sigma^2} - \frac{y'y}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)\right) \tag{3.191}$$

    Compare with equation. 3.186, $\theta = \mu$: $b(\theta) = \frac{1}{2}\mu'\mu$, $a(\phi) = \sigma^2$

    * $\mathbb{E}(Y) = b'(\theta) = \mu$
    * $var(Y) = a(\phi)b''(\theta) = \sigma^2$

  - Binomial $\mathbb{P}(y) = \binom{n}{y}\pi^y(1-\pi)^{n-y} \sim B(n,\pi)$:

$$f(y) = \exp\left(y\ln(\frac{\pi}{1-\pi}) + n\ln(1-\pi) + \ln\binom{n}{y}\right) \tag{3.192}$$

    Compare with equation. 3.186, $\theta = \ln(\frac{\pi}{1-\pi}) \Leftrightarrow \pi = \frac{1}{1+e^{-\theta}}$: $b(\theta) = -n\ln(1-\pi) = -n\ln\frac{1}{1+e^{\theta}}$, $a(\phi) = 1$

* $\mathbb{E}(Y) = b'(\theta) = n \ln \frac{1}{1+e^{-\theta}} = n\pi$
* $var(Y) = a(\phi)b''(\theta) = n\pi(1-\pi)$

– Poisson $\mathbb{P}(y) = \frac{\lambda^y}{y!}e^{-\lambda} \sim P(\lambda)$:

$$f(y) = \exp\left(y \ln \lambda - \lambda - \ln y!\right) \tag{3.193}$$

Compare with equation. 3.186, $\theta = \ln \lambda \Leftrightarrow \lambda = e^{\theta}$: $v(\theta) = \lambda = e^{\theta}$, $a(\phi) = 1$

* $\mathbb{E}(Y) = b'(\theta) = \lambda$
* $var(Y) = a(\phi)b''(\theta) = \lambda$

□ **Dependent Mode Generalize: Link Function**

Note that $Y_i \sim N(\mu_i, \sigma_i^2) = N(x_i'\beta, \sigma_i^2)$ contains the dependency of μ_i on $x_i\beta$ thus we can further generalize the regression model as $\mu_i = x'\beta$, here μ_i stands for $\mathbb{E}(Y)$ as in equation. 3.187. However for different distributions, $\mu = \mathbb{E}(Y)$ have specific range, e.g. $\mu \in [0, n]$ for $B(n,p)$, while $x'\beta \in \mathbb{R}$, thus use a **link function**g: $I_\mu \to I_{x'\beta}$ to adjust the range:

$$x_i'\beta = g(\mu_i) \Leftrightarrow \mu_i = g^{-1}(x'\beta) \tag{3.194}$$

Note: Link function should be monodrome & differentiable such that g^{-1} exists. And here $x'\beta$ term still exist (because it's still generalized linear model), thus we denote $\eta := x'\beta$ as a linear predictor/classifier

$$\eta := x'\beta \tag{3.195}$$

Regression Model:

$$\eta_i = g(\mu_i) \Leftrightarrow \mu_i = g^{-1}(\eta_i) \tag{3.196}$$

□ **Useful Generalized Linear Model:**

Important Question: how to choose proper generalization 'pair' : Distribution & Link Function pair?

Idea: Use the expectation transform:

$$\text{Distribution: } \mu = \mathbb{E}(Y) = b'(\theta)$$
$$\text{Link Function: } \mu = g^{-1}(x'\beta)$$

Thus

$$g^{-1}(x'\beta) = b'(\theta) \Rightarrow \eta = x'\beta = g(b'(\theta)) \tag{3.197}$$

For model simplification, we can choose $g(\cdot), b(\cdot)$ such that

$$g(b'(\cdot)) = \mathrm{Id}(\cdot) \Leftrightarrow g^{-1}(\cdot) = b'(\cdot) \tag{3.198}$$

such condition is called **Canonical Link** of generalized linear model, such choise of link function makes $x'\beta$ the canonical parameter in model.

$$\theta = \eta = x'\beta = g(\mu) \rightsquigarrow g^{-1}(\theta) = g^{-1}(\eta) = g^{-1}(x'\beta) = \mu = \mathbb{E}(Y) \tag{3.199}$$

• Simle linear model: $N(\mu, \sigma^2)$, $g(\cdot) = \mathrm{Id}(\cdot)$

$$\mu_i = \eta_i \tag{3.200}$$

- Logistic Model: $B(n,\pi)$, $g(x) = \text{logit}(x) = \ln\dfrac{x}{1-x} \Leftarrow g^{-1}(y) = \text{logistic}(y) = \dfrac{1}{1+e^{-y}}$

$$n\pi_i = \mu_i = g^{-1}(\eta_i) \tag{3.201}$$

- Poisson Model: $P(\lambda)$, $g(\cdot) = \ln(\cdot) \Leftrightarrow g^{-1}(\cdot) = \exp(\cdot)$

$$\lambda_i = \mu_i = g^{-1}(\eta_i) \tag{3.202}$$

☐ **Solution of Generalized Linear Model**

Using the distribution of Y_i dependent on $x_i'\beta$, we can use MLE maximizing to solve β. Algorithm for such maximizing task is called Iteratice Re-weighted Least Squares, more specifically when using Newton-Raphson Method, this method is called Fisher's Scoring Method. Detail see section. 6.4.3.

Chapter. IV 多元统计分析部分

Instructor: Dong Li & Tianying Wang

Section 4.1 Multivariate Data

In this section, we consider a **Multivariate Statistic Model**. Sample comes from p dimension multivariate population $f(x_1, x_2, \ldots, x_p)$.

Notation : In this section, we still denote random variable in upper case and observed value in lower case, specially express random vector in bold font. **But** in this section we usually omit the vector symbol $\vec{\cdot}$. e.g. random vector with n **variable** is denoted as $\mathbf{X} = (X_{\cdot 1}, X_{\cdot 2}, \ldots, X_{\cdot p})$; sample of size n from the multivariate population is a $n \times p$ matrix $\{x_{ij}\}$, each sample item (a row in sample matrix) is denoted as x_i' or x_i^T.[31]

4.1.1 Matrix Representation

- Random Variable Representation
- Sample Representation
- Statistics Representation
- Sample Statistics Properties

☐ **Random Variable Representation:**

- Random Matrix: Definition and basic properties of r.v. see section. 1.3. Now extend the definition to matrix $X = \{X_{ij}\}$.

$$X = \{X_{ij}\} = \begin{bmatrix} X_{11} & X_{12} & \ldots & X_{1p} \\ X_{21} & X_{22} & \ldots & X_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ X_{1n} & X_{n2} & \ldots & X_{np} \end{bmatrix} \tag{4.1}$$

  And we can further define $\mathbb{E}(X) = \{\mathbb{E}(X_{ij})\}$. For any const matrix A, B we have

$$\mathbb{E}(AXB) = A\mathbb{E}(X)B \tag{4.2}$$

- Random Vector: For a $p \times 1$ random vector $\vec{X} = (X_1, X_2, \ldots, X_p)^T$, denote (Marginal) expectation and variance, and covariance, correlation coefficient between X_i, X_j as follows:

$$\begin{aligned} \mu_i &= \mathbb{E}(X_i) \\ \sigma_{ii} &= \sigma_i^2 = \mathbb{E}(X_i - \mu_i)^2 \\ \sigma_{ij} &= \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)] \\ \rho_{ij} &= \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}}\sqrt{\sigma_{jj}}} \end{aligned}$$

[31] Here sample item (or sample case) $x_i = [x_{i1}, x_{i2}, \ldots, x_{ip}]^T$ is a column vector.

and we have covariance matrix (as defined in section. 1.4.3, equation. 1.49)

$$\Sigma = \mathbb{E}[(X-\mu)(X-\mu)^T] = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \dots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{p2} & \dots & \sigma_{pp} \end{bmatrix} \tag{4.3}$$

and Standard Deviation Matrix

$$V^{1/2} = diag\{\sqrt{\sigma_{ii}}\} \tag{4.4}$$

Based on $\vec{X} = (X_1, X_2, \dots, X_p)$, consider the linear combination:$Y = c'X = c_1X_1 + c_2X_2 + \dots c_pX_p$

$$\mathbb{E}(y) = c'\mu \qquad var(Y) = c'\Sigma c$$

and $Z_i = \sum_{j=1}^{p} c_{ij}X_j$ (i.e. $Z = CX$):

$$\mu_Z = \mathbb{E}(Z) = C\mu_X \qquad \Sigma_Z = C\Sigma_X C^T \tag{4.5}$$

and Correlation Matrix

$$\rho = \begin{bmatrix} \rho_{11} & \rho_{12} & \dots & \rho_{1p} \\ \rho_{21} & \rho_{22} & \dots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1p} & \rho_{p2} & \dots & \rho_{pp} \end{bmatrix} = V^{-1/2}\Sigma V^{-1/2} \tag{4.6}$$

☐ **Sample Representation:**

Sample of n items from population characterized by p variables

$$\begin{array}{r|cccccc|} & \text{var } 1 & \text{var } 2 & \dots & \text{var } j & \dots & \text{var } p \\ \text{item } 1 & x_{11} & x_{12} & \dots & x_{1j} & \dots & x_{1p} \\ \text{item } 2 & x_{21} & x_{22} & \dots & x_{2j} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \text{item } i & x_{i1} & x_{i2} & \dots & x_{ij} & \dots & x_{ip} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \text{item } n & x_{n1} & x_{n2} & \dots & x_{nj} & \dots & x_{np} \end{array}$$

Or represented in condense notation:

$$X = \{x_{ij}\} = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} y_1 & y_2 & \dots & y_p \end{bmatrix} \tag{4.7}$$

☐ **Statistics Representation**

- Unit 1 vector:

$$\mathbf{1}_k = (\underbrace{1, 1, \ldots, 1}_{k \text{ 1 in total}})^T \tag{4.8}$$

Unit 1 matrix:

$$\mathcal{I}_n = \{1\}_{n\times n} = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ 1 & 1 & \ldots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \ldots & 1 \end{bmatrix}_{n\times n} \tag{4.9}$$

- Sample mean:

$$\bar{x}_i = \frac{x_{1i} + x_{2i} + \ldots + x_{ni}}{n} = \frac{y_i' \mathbf{1}_n}{n} \tag{4.10}$$

- Deviation of measurement of the i^{th} variable:

$$d_i = y_i - \bar{x}_i \mathbf{1}_n = \begin{bmatrix} x_{1i} - \bar{x}_i \\ x_{2i} - \bar{x}_i \\ \vdots \\ x_{ni} - \bar{x}_i \end{bmatrix} \tag{4.11}$$

- Covariance Matrix:
  - Variance of y_i:

$$s_i^2 = s_{ii} = \frac{1}{n} d_i' d_i = \frac{1}{n} \sum_{k=1}^{n} (x_{ki} - \bar{x}_i)^2, \quad i = 1, 2, \ldots p \tag{4.12}$$

  - Covariance between y_i and y_j:

$$s_{ij} = \frac{1}{n} d_i' d_j = \frac{1}{n} \sum_{k=1}^{n} (x_{ki} - \bar{x}_i)(x_{kj} - \bar{x}_j), \quad i, j = 1, 2, \ldots p \tag{4.13}$$

  - Correlation Coefficient:

$$r_{ij} = \frac{s_{ij}}{\sqrt{s_{ii}}\sqrt{s_{jj}}} = \frac{\sum_{k=1}^{n} (x_{ki} - \bar{x}_i)(x_{kj} - \bar{x}_j)}{\sqrt{\sum_{k=1}^{n} (x_{ki} - \bar{x}_i)^2} \sqrt{\sum_{k=1}^{n} (x_{kj} - \bar{x}_j)^2}}, \quad i, j = 1, 2, \ldots p \tag{4.14}$$

In condense notation, define Covariance Matrix from sample of size n:

$$S_n = \begin{bmatrix} s_{11} & s_{12} & \ldots & s_{1p} \\ s_{21} & s_{22} & \ldots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{1p} & s_{p2} & \ldots & s_{pp} \end{bmatrix} \tag{4.15}$$

and sample Correlation Coefficient Matrix:

$$R_n = \begin{bmatrix} r_{11} & r_{12} & \ldots & r_{1p} \\ r_{21} & r_{22} & \ldots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{1p} & r_{p2} & \ldots & r_{pp} \end{bmatrix} \tag{4.16}$$

- Generalized sample variance: $|S| = \lambda_1\lambda_2 \dots \lambda_p$, where λ_i are eigenvalues.
- 'Statistical Distance' between vectors: to measure the difference between two vectors $x = (x_1, x_2, \dots, x_p)$ and $y = (y_1, y_2, \dots, y_p)$.
  - Euclidean Distance:
  $$d_E(x, y) = \sqrt{(x-y)^T(x-y)} \tag{4.17}$$
  - **Mahalanobis Distance**: Scale invariant distance, and include information about relativity:
  $$d_M(x, y) = \sqrt{(x-y)'S^{-1}(x-y)} \tag{4.18}$$
  Note: P, Q are from the same distribution with covariance matrix S_p. When $S = I$, return to Euclidean distance.

    Remark: Mahalanobis distance is actually the normalized Euclidean distance in principal component space. So we can actually define the Mahalanobis distance for one sample case $\vec{x} = (x_1, x_2, \dots, x_p)$ from distribution of $(\vec{\mu}, \Sigma)$
  $$d_M(\vec{x}) = \sqrt{(\vec{x}-\vec{\mu})^T\Sigma^{-1}(\vec{x}-\vec{\mu})} \tag{4.19}$$
  Note: the hyper-sruface $d_M(\vec{x})$ forms a ellipsoid.

☐ **Sample Statistics Properties**

Consider take an n cases sample from r.v. population $\vec{X} = (X_1, X_2, \dots, X_p)$, population mean μ and covariance matrix Σ.

- $\mathbb{E}(\bar{\bar{X}}) = \mu$;
- $cov(\bar{X}) = \frac{1}{n}\Sigma$;
- $\mathbb{E}(S_n) = \frac{n-1}{n}\Sigma$

4.1.2 Review: Some Matrix Notation & Lemma

- Orthonormality: For square matrix P satisfies:
$$x_i^T x_j = \delta_{ij} \tag{4.20}$$
where x_i, x_j are columns of P.
- Eigenvalue and Eigenvector: For square matrix A, its eigenvalues λ_i and corresponding eigenvectors e_i satisfies:
$$Ae_i = \lambda_i e_i,\ \forall i = 1, 2, \dots p \tag{4.21}$$
Denote $P = [e_1, e_2, \dots, e_p]$, which is an orthonormal matrix. And denote $\Lambda = diag\{\lambda_1, \lambda_2, \dots, \lambda_p\}$.
$$A = \sum_{i=1}^{p} \lambda_i e_i e_i^T = P\Lambda P^T = P\Lambda P^{-1} \tag{4.22}$$
is called the Spectral Decomposition of A

- Square root matrix: Def. as
$$A^{1/2} = \sum_{i=1}^{p} \sqrt{\lambda_i} e_i e_i^T = P\Lambda^{1/2} P^T \tag{4.23}$$
Properties:
  - $A^{1/2}A^{1/2} = A$;
  - $A^{-1/2} = (A^{1/2})^{-1} = PL^{-1/2}P^T$;
  - $tr(A) = \sum_{i=1}^{n} \lambda_n$;
  - $|A| = \prod_{i=1}^{n} \lambda_n$.
- (Symmetric) Positive Definite Matrix: Say A a Positive Definite Matrix if
$$x^T Ax > 0,\ \forall x \in \mathbb{R}^p \tag{4.24}$$
where $x^T Ax$ is called a Quadric Form.

  Properties:
  - Use the Spectral Decomposition of A, we can write the Quadric Form as
$$x^T Ax = x^T P\Lambda P^T x = y^T \Lambda y = \sum_{i=1}^{p} \lambda_i y_i^2 = \sum_{i=1}^{p} (\sqrt{\lambda_i} y_i)^2 \tag{4.25}$$
  - Eigenvalues $\lambda_i > 0,\ \forall i = 1, 2, \dots, p$
  - A can be written as product of symmetric matrix: $A = Q^T Q$ (Q is symmetric);
- Trace of Matrix: For $p \times p$ square matrix A
$$tr(A) = \sum_{i=1}^{p} a_{ii} \tag{4.26}$$
Properties:
  - $tr(AB) = tr(BA)$;
  - $x'Ax = tr(x'Ax) = tr(Axx')$
- Matrix Partition: partition matrix $\underset{p\times p}{A}$ as
$$A = \begin{bmatrix} \underset{q_1\times q_1}{A_{11}} & \underset{q_1\times q_2}{A_{12}} \\ \underset{q_2\times q_1}{A_{21}} & \underset{q_2\times q_2}{A_{22}} \end{bmatrix} \tag{4.27}$$
where $p = q_1 + q_2$

  Property:
$$|A| = |A_{22}||A_{11} - A_{12}A_{22}^{-1}A_{21}| = |A_{11}||A_{22} - A_{21}A_{11}^{-1}A_{12}| \tag{4.28}$$
- Matrix Differentiation

  Calculus Notations: We want to take derivative of $y = (y_1, y_2, \dots, y_q)^T$ over $x = (x_1, x_2, \dots, x_p)^T$

We use 'Denominator-layout', which is

$$\frac{\partial y}{\partial x}=\frac{\partial y^T}{\partial x}=\begin{bmatrix}\frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \dots & \frac{\partial y_q}{\partial x_1}\\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_p}\\ \vdots & \vdots & \ddots & \vdots\\ \frac{\partial y_1}{\partial x_p} & \frac{\partial y_2}{\partial x_p} & \dots & \frac{\partial y_q}{\partial x_p}\end{bmatrix}\Leftrightarrow\left(\frac{\partial y}{\partial x}\right)_{ij}=\frac{\partial y_j}{\partial x_i} \tag{4.29}$$

Properties (under denominator-layout):[32]

- $\frac{\partial}{\partial x}Ax=A^T$;
- $\frac{\partial}{\partial x}x^TA=A$;
- $\frac{\partial}{\partial x}x^Tx=2x$;
- $\frac{\partial}{\partial x}x^TAx=Ax+A^Tx$;
- $\frac{\partial}{\partial x}\log(x^TAx)=\frac{2Ax}{x^TAx}$;
- $\frac{\partial|A|}{\partial A}=|A|A^{-1}$;
- $\frac{\partial tr(AB)}{\partial A}=B^T$;
- $\frac{\partial tr(A^{-1}B)}{\partial A}=-A^{-1}B^TA^{-1}$

• Kronecker Product: For matrix $\underset{m\times n}{A}=\{a_{ij}\}$, $\underset{p\times q}{B}=\{b_{ij}\}$. Their Kronecker product

$$A\otimes B=\begin{bmatrix}a_{11}B & a_{12}B & \dots & a_{1n}B\\ a_{21}B & a_{22}B & \dots & a_{2n}B\\ \vdots & \vdots & \ddots & \vdots\\ a_{1m}B & a_{m2}B & \dots & a_{mn}B\end{bmatrix} \tag{4.30}$$

• Norm:

- Vector Norm: for vector $x,y\in\mathbb{C}^m$, norm $\|\cdot\|$ is a function $\mathbb{C}^m\to\mathbb{R}$, with:

$$\begin{aligned}\text{Semi-definiteness: } & \|x\|\geq 0,= \text{ for } x=0\\ \text{Absolute homogeneity: } & \|kx\|=|k|\|x\|,\ k\in\mathbb{C}\\ \text{Triangle inequality: } & \|x\|+\|y\|\geq\|x+y\|\end{aligned}$$

[32] More matrix diffrenciation equation see book [9] P49. Or can be easily derivated using Einstein sumation notation.

the ℓ_p-norm of x is

$$\|x\|_p \equiv \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p} \tag{4.31}$$

Useful norm:

* ℓ_0-norm: # of none-0 elements in x;[33]
* ℓ_1-norm: $\|x\|_1 = \sum_{i=1}^{n} |x_i|$;
* ℓ_2-norm/Euclidean norm: $\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$;
* ℓ_∞-norm: $\max |x_i|$.

– Matrix Norm: for matrix $A, B \in \mathbb{C}^{m\times n}$, norm $\|\cdot\|$ is a function $\mathbb{C}^{m\times n} \to \mathbb{R}$, with:

$$\text{Semi-definiteness: } \|A\| \geq 0, = \text{ for } x = 0$$
$$\text{Absolute homogeneity: } \|kA\| = |k|\|A\|,\ k \in \mathbb{C}$$
$$\text{Triangle inequality: } \|A\| + \|B\| \geq \|A + B\|$$

further for $m = n$, i.e. $A, B \in \mathbb{C}^{m\times m}$, usually append

$$\text{Sub-multiplicative: } \|A\|\|B\| \geq \|AB\|$$
$$\text{Hermite: } \|A\| = \|A^*\|$$

Matrix norm induced by vector norm:

$$\|A\| = \max \frac{\|Ax\|}{\|x\|} \tag{4.32}$$

e.g. ℓ_p induced matrix norm:

* ℓ_1-norm: $\|A\|_1 = \max\limits_{1\leq j\leq n} \sum\limits_{i=1}^{m} |A_{ij}|$
* ℓ_2-norm/Euclidean norm: $\|A\|_2 = \sigma_{\max}(A)$;
* ℓ_∞-norm: $\|A\|_\infty = \max\limits_{1\leq i\leq m} \sum\limits_{j=1}^{n} |A_{ij}|$.

Non-induced matrix norm, e.g.

* Frobenius norm: $\|A\|_F = \left(\sum_{i=1}^{m}\sum_{j=1}^{n} |A_{ij}|^2\right)^{1/2} = \sqrt{tr(A^*A)}$
* Weighted Frobenius norm: $\|A\|_W = \|W^{-1/2}AW^{-1/2}\|_F$(or some textbooks uses $\|W^{1/2}AW^{1/2}\|_F$)
* Max norm: $\|A\|_{\max} = \max\limits_{i,j} |A_{ij}|$

• Sherman-Morrison Formula:

$$\left(A + u^T v\right)^{-1} = A^{-1} - \frac{A^{-1}u^T v A^{-1}}{1 + v^T A^{-1} u}$$

4.1.3 Useful Inequalities

• Cauchy-Schwartz Inequality:

Let b, d are any $p \times 1$ vectors.

$$(b'd)^2 \leq (b'b)(d'd) \tag{4.33}$$

[33]Note: actually triangle inequality is not satisfied for $\|\cdot\|_0$

- Extended Cauchy-Schwartz Inequality:

  Let B be a positive definite matrix.

$$(b'd)^2 \le (b'Bb)(d'B^{-1}d) \tag{4.34}$$

- Maximazation Lemma:

  d be a given vector, for any non-zero vector x,

$$\frac{(x'd)^2}{x'Bx} \le d'B^{-1}d \tag{4.35}$$

  Take Maximum when $x = cB^{-1}d$.

Section 4.2 Statistical Inference to Multivariate Population

Statistics model: a n cases sample $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$, where each $\mathbf{X}_i$ i.i.d. from a multivariate population (usually consider a multi-normal). i.e.

$$\mathbf{X} = \begin{bmatrix} X_{11} & X_{12} & \dots & X_{1p} \\ X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ X_{1n} & X_{n2} & \dots & X_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1' \\ \mathbf{X}_2' \\ \vdots \\ \mathbf{X}_n' \end{bmatrix} \tag{4.36}$$

4.2.1 Multivariate Normal Distribution

Univariate Noraml Distribution: $N(\mu, \sigma^2)$

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{(x-\mu)^2}{2\sigma^2} \tag{4.37}$$

Multivariate Normal Distribution: $X \sim N_p(\vec{\mu}, \Sigma)$[34]

$$f_{\mathbf{X}}(\vec{x}) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{(\vec{x}-\vec{\mu})'\Sigma^{-1}(\vec{x}-\vec{\mu})}{2}\right) \tag{4.38}$$

Note: Here in the exp, the $(\vec{x}-\vec{\mu})'\Sigma^{-1}(\vec{x}-\vec{\mu})$ is the Mahalanobis Distance d_M defined in equation. 4.19

Remark: A n-dimension multivariate normal has $\dfrac{p(p+1)}{2}$ free parameters. Thus for a very high dimension, contains too many free parameters to be determined!

Properties: Consider $X \sim N_p(\mu, \Sigma)$

- Linear Transform:

  - For a $p \times 1$ vector a:

$$X \sim N_p(\mu, \Sigma) \Leftrightarrow a'X \sim N(a'\mu, a'\Sigma a),\ \forall a \in \mathbb{R}^p \tag{4.39}$$

    (Proof: use characteristic function.)

[34] Detailed derivation see section. 1.8

– For a $q \times p$ const matrix A:

$$AX + a \sim N_q(A\mu + a, A\Sigma A') \tag{4.40}$$

– For a $p \times p$ square matrix A:

$$\mathbb{E}(X'AX) = \mu' A\mu + tr(A\Sigma) \tag{4.41}$$

• Conditional Distribution: Take partition of $\underset{p\times 1}{X} \sim N(\underset{p\times 1}{\mu}, \underset{p\times p}{\Sigma})$ into $\underset{q_1\times 1}{X_1}$ and $\underset{q_2\times 1}{X_2}$, where $q_1 + q_2 = p$. Write in matrix form:

$$\underset{p\times 1}{X} = \begin{bmatrix} \underset{q_1\times 1}{X_1} \\ \underset{q_2\times 2}{X_2} \end{bmatrix} \qquad \underset{p\times 1}{\mu} = \begin{bmatrix} \underset{q_1\times 1}{\mu_1} \\ \underset{q_2\times 2}{\mu_2} \end{bmatrix} \qquad \underset{p\times p}{\Sigma} = \begin{bmatrix} \underset{q_1\times q_1}{\Sigma_{11}} & \underset{q_1\times q_2}{\Sigma_{12}} \\ \underset{q_2\times q_1}{\Sigma_{21}} & \underset{q_2\times q_2}{\Sigma_{22}} \end{bmatrix} \tag{4.42}$$

i.e.

$$\underset{p\times 1}{X} = \begin{bmatrix} \underset{q_1\times 1}{X_1} \\ \underset{q_2\times 2}{X_2} \end{bmatrix} \sim N_{q_1+q_2}\left(\begin{bmatrix} \underset{q_1\times 1}{\mu_1} \\ \underset{q_2\times 2}{\mu_2} \end{bmatrix}, \begin{bmatrix} \underset{q_1\times q_1}{\Sigma_{11}} & \underset{q_1\times q_2}{\Sigma_{12}} \\ \underset{q_2\times q_1}{\Sigma_{21}} & \underset{q_2\times q_2}{\Sigma_{22}} \end{bmatrix} \right) \tag{4.43}$$

Independence: $X_1 \parallel X_2 \Leftrightarrow \Sigma_{21} = \Sigma_{12}^T = 0$

And the conditional dictribution $X_1|X_2 = x_2$ is given by [35]

$$X_1|_{X_2=x_2} \sim N_p(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2),\, \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}) \tag{4.45}$$

• Multivariate Normal & χ^2

Let $X \sim N_p(\mu, \Sigma)$, then

$$(X - \mu)^T \Sigma^{-1}(X - \mu) \sim \chi_p^2 \tag{4.46}$$

4.2.2 MLE of Multivariate Normal

Under the notation in equation. 4.36, i.e. each sample case $\mathbf{X}_i$ i.i.d. $\sim N_p(\mu, \Sigma)$, we can get the joint PDF of $\mathbf{X}$:

$$f_{\mathbf{X_1},\ldots,\mathbf{X_n};\mu,\Sigma}(x_1, \ldots, x_n) = \frac{1}{(2\pi)^{np/2}|\Sigma|^{n/2}} \exp\left(-\sum_{i=1}^{n} \frac{(x_i - \mu)'\Sigma^{-1}(x_i - \mu)}{2} \right) \tag{4.47}$$

and at the same time get likelihood function[36]:

$$L(\mu, \Sigma; x_1, \ldots, x_n) = \frac{1}{(2\pi)^{np/2}|\Sigma|^{n/2}} \exp\left[-\frac{1}{2} tr\left(\Sigma^{-1} \left(\sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})' + n(\bar{x} - \mu)(\bar{x} - \mu)' \right)\right)\right] \tag{4.49}$$

[35] In equation. 4.40, take

$$\underset{p\times p}{A} = \begin{bmatrix} \underset{q\times q}{I} & \underset{q\times(p-q)}{-\Sigma_{12}\Sigma_{22}^{-1}} \\ \underset{(p-q)\times q}{0} & \underset{(p-q)\times(p-q)}{I} \end{bmatrix} \tag{4.44}$$

[36] Here we need to use the property of trace

$$x'Ax = tr(x'Ax) = tr(Ax'x) \tag{4.48}$$

And we can get the MLE of μ and Σ as follows[37]:

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{x}$$
$$\hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})' = \frac{n-1}{n}S$$

Δ **Note:** In this section, S is used to denote $\hat{\Sigma}$, which is different from that in section. 2.1.1 (S^2 for $\hat{\Sigma}$)

And we can furthur construct MLE of function of μ, Σ (use invariance property of MLE), for example

$$\widehat{|\Sigma|} = |\hat{\Sigma}| \tag{4.50}$$

Note: $(\hat{\mu}, \hat{\Sigma})$ is sufficient statistic of multi-normal population.

4.2.3 Sampling distribution of $\bar{X}$ and S

$\hat{\mu} = \bar{X}$ and $\hat{\Sigma} = \dfrac{n-1}{n}S$ are statistics, with sampling distribution.

☐ **Sampling distribution of $\bar{X}$**

Similar to monovariate case:

$$\bar{X} \sim N_p(\mu, \frac{1}{n}\Sigma) \tag{4.51}$$

☐ **Sampling distribution of S^2**

- Monovariate case: Consider $(X_1, X_2, \dots, X_n)$ i.i.d. $\sim N(\mu, \sigma^2)$

  Then

$$\frac{(n-1)S}{\sigma^2} \sim \chi^2_{n-1} \tag{4.52}$$

- Multivariate case: Consider $(\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n)$ i.i.d. $\sim N_p(\mu, \Sigma)$

  Then

$$(n-1)S \sim W_p(n-1, \Sigma) \tag{4.53}$$

Where $W_p(n-1, \Sigma)$ is Wishart Distribution, details as follows:

For r.v. $Z_1, Z_2, \dots, Z_m$ i.i.d. $\sim N_p(0, \Sigma)$, def p dimensional **Wishart Distribution** with dof m as $W_p(m, \Sigma)$.[38]

$$W_p = \sum_{i=1}^{n} Z_i Z_i' \tag{4.54}$$

PDF of $W_p(m, \Sigma)$:

$$f_W(w; p, m, \Sigma) = \frac{|w|^{\frac{m-p-1}{2}} \exp\left(-\frac{1}{2}tr(\Sigma^{-1}w)\right)}{2^{\frac{mp}{2}}|\Sigma|^{-1/2}\pi^{\frac{p(p-1)}{4}}\prod_{i=1}^{p}\Gamma(\frac{m-i+1}{2})} \tag{4.55}$$

---

[37] Detailed proof see '*Applied Multivariate Statistical Analysis*' P130

[38] $W_p(m, \Sigma)$ is a distribution defined on $p \times p$ matrix space.

C.F.

$$\phi(T) = |I_p - 2i\Sigma T|^{-\frac{m}{2}} \tag{4.56}$$

Properties:

- For independent $A_1 \sim W_p(m_1, \Sigma)$ and $A_2 \sim W_p(m_2, \Sigma)$, then

$$A_1 + A_2 \sim W_p(m_1 + m_2, \Sigma) \tag{4.57}$$

- For $A \sim W_p(m, \Sigma)$, then

$$CAC' \sim W_p(m, C\Sigma C') \tag{4.58}$$

- Wishart distribution is the matrix generization of χ_n^2. When $p = 1, \Sigma = \sigma^2 = 1$, $W_p(m, \Sigma)$ naturally reduce to χ_m^2.

$$\chi_n^2 = W_1(n, 1) \tag{4.59}$$

▷ `R.` **Code**

Distribution functions are in package `MCMCpack`, or use `rWishart()` function.

☐ **Large sample $\bar{X}$ and S**

- $\sqrt{n}(\bar{X} - \mu) \xrightarrow{\mathscr{L}} N_p(0, \Sigma)$;
- $n(\bar{X} - \mu)' S^{-1} (\bar{X} - \mu) \xrightarrow{\mathscr{L}} \chi_p^2$

4.2.4 Hypothesis Testing for Normal Population

- **One-Population Hypothesis Testing**:

Conduct hypothesis testing to μ:

$$H_0 : \mu = \mu_0 \longleftrightarrow H_1 : \mu \neq \mu_0 \tag{4.60}$$

☐ **Hotelling's T^2 test**

- One-Dimensional case: t-test

$$T = \frac{\sqrt{n}(\bar{X} - \mu_0)}{S} \sim t_{n-1} \tag{4.61}$$

i.e.

$$T^2 = [\sqrt{n}(\bar{X} - \mu_0)] S^{-1} [\sqrt{n}(\bar{X} - \mu_0)] \sim t_{n-1}^2 = F_{1,n-1} \tag{4.62}$$

- Multi-Dimensional case: Hotelling's T^2

$$T^2 = [\sqrt{n}(\bar{X} - \mu_0)'] S^{-1} [\sqrt{n}(\bar{X} - \mu_0)] \sim N_p(0, \Sigma)' \frac{W_p(n-1, \Sigma)}{n-1} N_p(0, \Sigma) = \frac{p}{n-p}(n-1) F_{p,n-p} \tag{4.63}$$

And we can get the distribution of **Hotelling's** T^2:

$$\frac{n-p}{p} \frac{T^2}{n-1} \sim F_{p,n-p} \tag{4.64}$$

Rejection Rule:

$$T^2 > \frac{p(n-1)}{n-p} F_{p,n-p,\alpha} \tag{4.65}$$

Property:

Invariant for X transform: For $Y = CX + d$, then

$$T_Y^2 = n(\bar{X} - \mu_0)' S^{-1} (\bar{X} - \mu_0) = T_X^2 \tag{4.66}$$

☐ **LRT of $\hat{\mu}$**

Monovariate case see section. 2.4.3.

LRT uses the statistic:

$$\Lambda = \frac{\max_{H_0} L(\mu_0, \Sigma)}{\max_{H_0 \cup H_1} L(\mu, \Sigma)} = (1 + \frac{T^2}{n-1})^{-n/2} \tag{4.67}$$

where $T^2 = n(\bar{x} - \mu_0)' S^{-1} (\bar{x} - \mu_0)$

- **Two-Population Hypothesis Testing**:

Conduct hypothesis testing to $\delta = \mu_1 - \mu_2$:

$$H_0 : \delta = \delta_0 \longleftrightarrow H_1 : \delta \neq \delta_0 \tag{4.68}$$

Notation: The two sample of size n_1, n_2, each denoted as

$$X_{1,ij} \qquad X_{2,ij} \tag{4.69}$$

with mean μ_1, μ_2 and covariance matrix Σ_1, Σ_2

  – Paired Samples: $n_1 = n_2$

  For two paires samples $\{X_{1,ij}\}$, $X_{2,ij}$, take subtraction as

$$D_{ij} = X_{1,ij} - X_{2,ij} \tag{4.70}$$

  denote $\bar{D} = \frac{1}{n}\sum_{j=1}^n D_j$, $S_D^2 = \frac{1}{n-1}\sum_{j=1}^n (D_j - \bar{D}'(D_j - \bar{D}))$
  and conduct test to

$$H_0 : \bar{D} = \delta_0 \longleftrightarrow H_1 : \bar{D} \neq \delta_0 \tag{4.71}$$

  And the folloeing steps are as in One-population testing, test

$$T^2 = n(\bar{D} - \delta)'(S_D^2)^{-1}(\bar{D} - \delta) \sim \frac{(n-1)p}{n-p} F_{p,n-p} \tag{4.72}$$

  – Under Equal Unknown Variance: $\Sigma_1 = \Sigma_2$

$$\bar{X}_1 = \frac{1}{n_1}\sum_{j=1}^{n_1} X_{1,j} \qquad \bar{X}_2 = \frac{1}{n_2}\sum_{j=1}^{n_2} X_{1,j} \tag{4.73}$$

$$S_1 = \frac{1}{n_1 - 1}\sum_{j=1}^{n_1}(X_{1,j} - \bar{X}_1)(X_{1,j} - \bar{X}_1)' \qquad S_2 = \frac{1}{n_2 - 1}\sum_{j=1}^{n_2}(X_{2,j} - \bar{X}_2)(X_{2,j} - \bar{X}_2)' \tag{4.74}$$

  And denote pooled variance

$$S_{\text{pooled}} = \frac{1}{n_1 + n_2 - 2}((n_1 - 1)S_1 + (n_2 - 1)S_2) \sim \frac{W_p(n_1 + n_2 - 2, \Sigma)}{n_1 + n_2 - 2} \tag{4.75}$$

  Under H_0, we have

$$T^2 = \frac{1}{\frac{1}{n_1} + \frac{1}{n_2}}(\bar{X}_1 - \bar{X}_2 - \delta_0)' S_{\text{pooled}}^{-1}(\bar{X}_1 - \bar{X}_2 - \delta_0) \sim \frac{p(n_1 + n_2 - 2)}{n_1 + n_2 - p - 1} F_{p, n_1 + n_2 - p - 1} \tag{4.76}$$

4.2.5 Confidence Region

Estimate the confidence region for μ of $X \sim N_p(\mu, \Sigma)$, Monovariate case see section. 2.3.3

- Confidence Region:

  Also use Hotelling's T^2

$$\frac{n-p}{p}\frac{T^2}{n-1} \sim F_{p,n-p} \tag{4.77}$$

  And take $100(1-\alpha)\%$ confidence region of μ as

$$R(x) = \{x|T^2 \le c^2\} \qquad c^2 = \frac{p}{n-p}(n-1)F_{p,n-p,\frac{\alpha}{2}} \tag{4.78}$$

  The shape of $R(x)$ is an ellipsoid.

- Individual Converage Interval

  Use the decomposition of S^2 as a positive finite matrix $S^2 = A^T A$, where A is some $p \times p$ matrix, then

$$T^2 = [\sqrt{n}(\bar{X}-\mu_0)']S^{-1}[\sqrt{n}(\bar{X}-\mu_0)] = [A^{-1\prime}\sqrt{n}(\bar{X}-\mu_0)]'[A^{-1\prime}\sqrt{n}(\bar{X}-\mu_0)] \tag{4.79}$$

  Thus denote $Z = A^{-1\prime}(X-\mu_0) \sim N_p(0, A^{-1\prime}\Sigma A^{-1})$, the T^2 estimator of Z would be

$$T_Z^2 = [\sqrt{n}\bar{Z}]'S_Z^{-1}[\sqrt{n}\bar{Z}] = n\bar{Z}'\bar{Z} = \frac{1}{n}\sum_{i=1}^{n}\bar{Z}_i^2 \sim F_{p,n-p} \tag{4.80}$$

  As a simplified case, we can take the **Individual Converage Interval** of Z_i, which is

$$\frac{\sqrt{n}Z_i}{s_{Z_i}} \sim t_{n-1} \tag{4.81}$$

  And we can take the Confidence Region[39] as

$$R(z) = \bigotimes_{i=1}^{n}(\bar{Z}_i \pm s_{Z_i}t_{n-1,\frac{\beta}{2}}) \tag{4.82}$$

  where β take

$$1 - p\beta = 1 - \alpha \tag{4.83}$$

  Note: Consider that

$$P(\text{all } Z_i \text{ in CI}_i) \ge 1 - m\beta = 1 - \alpha \tag{4.84}$$

  So the real CR for μ should be larger.

  The shape of $R(x)$ is an oblique cubold.

[39] The confidence region of Z can be transformed to that of X using $\hat{Z} = A^{-1\prime}(\hat{X} - \bar{X})$.

4.2.6 Large Sample Multivariate Inference

Basic point:

$$\bar{X} \xrightarrow{\mathscr{L}} \mu \qquad S \xrightarrow{\mathscr{L}} \Sigma \tag{4.85}$$

- One-sample Mean:

$$n(\bar{X}-\mu)S^{-1}(\bar{X}-\mu) \xrightarrow{\mathscr{L}} \chi_p^2 \tag{4.86}$$

- Unequal Variance Two-sample Mean:

$$\bar{X}_1 - \bar{X}_2 \xrightarrow{\mathscr{L}} N\left(\mu_1-\mu_2, \frac{1}{n_1}\Sigma_1 + \frac{1}{n_2}\Sigma_2\right) \qquad \frac{1}{n_1}S_1 + \frac{1}{n_2}S_2 \xrightarrow{\mathscr{L}} \frac{1}{n_1}\Sigma_1 + \frac{1}{n_2}\Sigma_2 \tag{4.87}$$

Test:

$$T^2 = \left[(\bar{X}_1-\bar{X}_2)-(\mu_1-\mu_2)\right]'(\frac{1}{n_1}S_1+\frac{1}{n_2}S_2)^{-1}\left[(\bar{X}_1-\bar{X}_2)-(\mu_1-\mu_2)\right] \xrightarrow{\mathscr{L}} \chi_p^2 \tag{4.88}$$

Section 4.3 Principal Component Analysis

PCA and next subsection FA focus on data dimension reduction. Why?

☐ **'Curse of Dimensionality'**

- Difficulty in computation complexity: Many algorithms has complexity $O(n^2)$ or more, high dimension n cause high complexity.
- Hughes Phenomenon: As the number of feature dimension increases, the classifier's performance increases as well until an optimal dimension. Adding more features based on the same size as the training set will then degrade the classifier's performance. [a]

[a] Example: Volumn of unit sphere in n-dim space

$$V_n = \pi^{n/2}\frac{1}{\Gamma(1+n/2)} \to \left(\frac{2\pi e}{n}\right)^{n/2} \to 0 \tag{4.89}$$

i.e. data will naturally become 'sparse' in high dimension data → difficult to extract information.

Key Idea of PCA: Find the components most powerful in explaining variance. (Similar to the idea of ANOVA)

4.3.1 Population Principal Component

For population $\vec{X} = (X_1, X_2, \dots, X_p) \sim (\mu, \Sigma)_p$, conduct spectrum decomposition to Σ such that

$$\Sigma P = P\Lambda \qquad P = \left[e_1, e_2, \dots, e_p\right] \qquad \Lambda = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_p\},\ \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \tag{4.90}$$

where (λ_i, e_i) is the i^{th} eigenvalue-eigenvector pair of Σ, large λ_i suggests X is more 'extended' in e_i direction(large variance).

Then the **Principal Components** $Y = \{Y_i\}$

$$Y = P'X \sim (P'\mu, P'\Sigma P)_p = (P'\mu, \Lambda) \tag{4.91}$$

$$\begin{cases} Y_1 = e_1'X \sim (e_1'\mu, \lambda_1) \\ \vdots \\ Y_p = e_p'X \sim (e_p'\mu, \lambda_p) \end{cases} \tag{4.92}$$

Properties & Definitions:

- Trace of cov. matrix:

$$\sum_{i=1}^{p} \sigma_{ii} = \sum_{i=1}^{p} var(X_i) = \sum_{i=1}^{p} var(Y_i) = \sum_{i=1}^{p} \lambda_i \tag{4.93}$$

- $corr$ between Y_i, X_j:

$$\rho_{Y_i, X_j} = \frac{cov(Y_i, X_j)}{\sqrt{\lambda_i}\sqrt{\sigma_{jj}}} = \frac{(e_i)_j\sqrt{\lambda_i}}{\sqrt{\sigma_{jj}}} \tag{4.94}$$

- Factor Loading:

$$\text{FL}_{ij} = (e_i)_j\sqrt{\lambda_i} \tag{4.95}$$

- PC Score:

$$\text{PC Score}_i = Y_i = e_i'X \text{ or } Y_i = e_i'(X - \mu) \tag{4.96}$$

In practice, we pick the first several m PC such that

$$\sum_{i=1}^{m} \frac{\lambda_i}{\sum_{k=1}^{p} \lambda_k} \text{ large enough} \tag{4.97}$$

Note: Another important point for PCA is the **interpretability** of principal components.

☐ **Standardized Principal Component**

To cancel out the influence due to scale, we can also obtain standardized PC from $Z = (V)^{-1/2}(X_\mu)$, where V is standard deviation matrix as def. in equation. 4.4.

And we have $\vec{Z} = (Z_1, Z_2, \ldots, Z_p) \sim N_p(0, V^{-1/2}\Sigma V^{-1/2\prime}) = N_p(0, \rho)$. Then obtain (λ_i, e_i) pairs[40] from ρ to form PC.

$$\rho P = P\Lambda \qquad P = \left[e_1, e_2, \ldots, e_p\right] \qquad \Lambda = diag\{\lambda_1, \lambda_2, \ldots, \lambda_p\},\ \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \tag{4.98}$$

Then the Principal Components $W = \{W_i\}$

$$W = P'Z \sim (0, P'\rho P)_p = (0, \Lambda) \tag{4.99}$$

$$\begin{cases} W_1 = e_1'Z \sim (0, \lambda_1) \\ \vdots \\ W_p = e_p'Z \sim (0, \lambda_p) \end{cases} \tag{4.100}$$

Properties:

[40] The eigenvalue-eigenvector pairs obtained from ρ is generally **different** from Σ.

- Trace of cov. matrix:

$$\sum_{i=1}^{p} var(Z_i) = \sum_{i=1}^{p} var(W_i) = \sum_{i=1}^{p} \lambda_i = p \tag{4.101}$$

- $corr$ between Y_i, X_j:

$$\rho_{W_i,Z_j} = (e_i)_j \sqrt{\lambda_i} \tag{4.102}$$

4.3.2 Sample Principal Component

For sample matrix X denoted in equation. 4.36, with cov. matrix S in equation. 4.15. Then conduct the above spectrum decomposition to S to get sample PCs.

$$\hat{Y} = \hat{P}\hat{\Lambda}\hat{P}' \qquad \hat{P} = \left[\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_p\right] \quad \hat{\Lambda} = diag\{\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_p\}, \, \hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \ldots \geq \hat{\lambda}_p \tag{4.103}$$

Properties and Definitions

- Trace of cov. matrix:

$$\sum_{i=1}^{p} s_{ii} = \sum_{i=1}^{p} \hat{\lambda}_i \tag{4.104}$$

- Sample corr & factor load:

$$\rho(\hat{y}_i, x_j) = \frac{(\hat{e}_i)_j \sqrt{\hat{\lambda}_j}}{\sqrt{s_{jj}}} \tag{4.105}$$

☐ **Large Sample & Normal PCA**

Under normal assumption or large sample case, i.e.

$$X \sim N_p(\mu, \Sigma) \text{ or } X \xrightarrow{\mathscr{L}} N_p(\mu, \Sigma) \tag{4.106}$$

We can examine the (asymptotic) distribution of $(\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_p)$ and $(\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_p)$:

- $\hat{\lambda}$:

$$\sqrt{n}(\hat{\lambda} - \lambda) \sim N_p(0, 2\Lambda^2) \tag{4.107}$$

- $\hat{e}_i$:

$$\sqrt{n}(\hat{e}_i - e_i) \sim N_p(0, E_i), \quad E_i = \lambda_i \sum_{k \neq i} \frac{\lambda_k}{(\lambda_k - \lambda_i)^2} e_k e_k' \tag{4.108}$$

- Independence:

$$\hat{\lambda}_i \perp\!\!\!\perp \hat{e}_i \tag{4.109}$$

Section 4.4 Factor Analysis

Key idea of FA: For a model with p variable $X = (X_1, X_2, \ldots, X_p) \sim (\mu, \Sigma)_p$ (especially when p large and X_i interrelated), there would be some internal, latent **factors** F behind X determining the model structure.[41]

[41] As the most simplified case, here only consider X linear dependent on F.

4.4.1 Orthogonal Factor Model

$$\underset{p\times 1}{X-\mu} = \underset{p\times m}{L}\,\underset{m\times 1}{F} + \underset{p\times 1}{\varepsilon},\ m<p \tag{4.110}$$

where L is the const **loading matrix** ; F is r.v. **factor**; and ε is r.v. error.

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{bmatrix} \quad L = \begin{bmatrix} \ell_{11} & \ell_{12} & \dots & \ell_{1m} \\ \ell_{21} & \ell_{22} & \dots & \ell_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \ell_{p1} & \ell_{p2} & \dots & \ell_{pm} \end{bmatrix} \quad F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_m \end{bmatrix} \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_p \end{bmatrix}$$

Note: Intuitively, we cannot estimate $(m+p)$（unobserable) r.v. from p r.v., so we need the following assumptions on F and ε

$$\begin{aligned} &\mathbb{E}(F) = 0 && cov(F) = I_n \\ &\mathbb{E}(\varepsilon) = 0 && cov(\varepsilon) = \Psi = diag\{\psi_1, \psi_2, \dots, \psi_p\} \\ &\varepsilon \perp\!\!\!\perp F \Leftrightarrow cov(F, \varepsilon) = 0 \end{aligned} \tag{4.111}$$

Derived Conclusions:

- Representation of Σ:

$$cov(X) = \Sigma = LL' + \Psi \tag{4.112}$$

  - Diagonal Elements:

$$var(X_i) = \sum_{k=1}^{m} \ell_{ik}^2 + \psi_i = h_i^2 + \psi_i \tag{4.113}$$

    where h_i^2 is Communality, ψ_i is Specific variance.

  - NonDiagonal Elements:

$$cov(X_i, X_j) = \sum_{k=1}^{m} \ell_{im}\ell_{jm} \tag{4.114}$$

- relation bet. X and F:

$$cov(X, F) = L \tag{4.115}$$

□ **Factor Rotation** For any orthonormal rotation/reflection matrix $\underset{m\times m}{T}$, $\tilde{L} = LT$ satisfies the same factor model (with a different $\tilde{F}$):

$$\begin{aligned} X &= LF + \varepsilon = LTT'F + \varepsilon = \tilde{L}\tilde{F} + \varepsilon \qquad \tilde{L} = LT,\ \tilde{F} = T'F \\ \Sigma &= LL' + \Psi = \tilde{L}\tilde{L}' + \Psi \end{aligned}$$

Comment: Factor rotation reflects the arbitrariness of selection of L, allowing us to choose an **interpretable** L for FA model.

4.4.2 Principal Component Approach

Origin: when $m = p$, factor decomposition reduces to spectrum(PC) decomposition.(At the same time Ψ can be taken 0.)

$$\begin{aligned} X &= LF + \varepsilon = PY && \Rightarrow \Psi = 0 \\ \Sigma &= LL' + \Psi = P\Lambda P' && \Rightarrow L = P\Lambda^{1/2} \end{aligned} \tag{4.116}$$

Then take the first m eigenvectors to form L, and use $\psi_i = \sigma_{ii} - \sum_{k=1}^{m} \ell_{ik}^2$ as an approximation.

$$\Sigma = LL' + \Psi \qquad L = \left[\sqrt{\lambda_1}e_1, \sqrt{\lambda_2}e_2, \ldots, \sqrt{\lambda_m}e_m\right] \qquad \Psi = diag\{\psi_i\} \tag{4.117}$$

☐ **Sample Factor Decomposition**

From sample cov. matrix S and eigenvalue-eigenvector pairs $(\hat{\lambda}_i, e_i)$, pick the first m paris to form $L = \{\ell_{ij}\}$:

$$\hat{L} = \{\hat{\ell}_{ij}\} = \left[\sqrt{\hat{\lambda}_1}\hat{e}_1, \sqrt{\hat{\lambda}_2}\hat{e}_2, \ldots, \sqrt{\hat{\lambda}_m}\hat{e}_m\right] \qquad \hat{\Psi} = diag\{s_{ii} - \sum_{k=1}^{m} \hat{\ell}_{ik}^2\} \tag{4.118}$$

- Selection of m: Construct Residual Matrix

$$\hat{E} = S - (\hat{L}\hat{L}' + \hat{\Psi}) \tag{4.119}$$

Residual matrix is trace 0, pick m such that

$$\text{Sum of All Elements in } \hat{E} < \sum_{k=m+1}^{p} \hat{\lambda}_k^2 \text{ small enough} \tag{4.120}$$

4.4.3 MLE Method

Assumption: Factor F and error ε are normal.(Then also $X \sim N_p(\mu, \Sigma)$ is normal)

$$F \sim N_m(0, I_m) \quad \varepsilon \sim N_p(0, \Psi) \quad X \sim N_p(\mu, \Sigma) \tag{4.121}$$

Likelihood Function:

$$L(\mu, \Sigma) = (2\pi)^{-np/2}|\Sigma|^{-n/2} \exp\left(-\frac{1}{2}tr\left[\Sigma^{-1}\left(\sum_{k=1}^{n}(x_k - \bar{x})(x_k - \bar{x})' + n(\bar{x} - \mu)(\bar{x} - \mu)'\right)\right]\right) \tag{4.122}$$

Maximize L to get $\hat{L}$ and $\hat{\Psi}$, usually for convenient (and to counteract the arbitrariness of factor rotation) we further assume

$$L'\Psi^{-1}L = \Xi \text{ (diagonal matrix)} \tag{4.123}$$

- Estimtor of communality variance h_i^2:

$$\hat{h}_i^2 = \sum_{k=1}^{m} \hat{l}_{ik}^2 \tag{4.124}$$

Section 4.5 Canonical Correction Analysis

Key idea of CCA: For a model with two multivariate population $X^{(1)} = (X_1^{(1)}, X_2^{(1)}, \ldots, X_p^{(1)})$, $X^{(2)} = (X_1^{(2)}, X_2^{(2)}, \ldots, X_q^{(2)})$ with covariance

$$\underset{(p+q)\times(p+q)}{\Sigma} = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \tag{4.125}$$

find a few condensed variable to measure their similarity.

4.5.1 Canonical Variate Pair

By using the linear combination, we can construct a pair of vector $\underset{p\times 1}{a}$ and $\underset{q\times 1}{b}$ such that $corr(a'X^{(1)}, b'X^{(2)})$ large, i.e.

$$\{a, b\} = \arg\max_{a,b\neq 0} \frac{a'\Sigma_{12}b}{\sqrt{a'\Sigma_{11}a}\sqrt{b'\Sigma_{22}b}} \tag{4.126}$$

where $U_1 = a'X^{(1)}$, $V_1 = b'X^{(2)}$ with $var(U_1) = var(V_1) = 1$ are the **(first) canonical variate pair**, and $\rho_1^* = corr(U_1, V_1)$ is the **(first) canonical correlation**.

Similarly, the k^{th} canonical pair (U_k, V_k) satisfy the same criterion as equation. 4.126 but with $a_k \in \text{span}\{a_1, \ldots, a_{k-1}\}^{\perp}$, $b_k \in \text{span}\{b_1, \ldots, b_{k-1}\}^{\perp}$, $k \leq \min\{p, q\}$.

Result: U_k, V_k can be expressed as

$$U_k = a_k'X^{(1)} = e_k'\Sigma_{11}^{-1/2}X^{(1)} \qquad V_k = b_k'X^{(2)} = f_k'\Sigma_{22}^{-1/2}X^{(2)} \tag{4.127}$$

where e_k is the k^{th} eigen vector of $\Sigma_{11}^{-1/2}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11}^{-1/2}$, f_k is the k^{th} eigenvector of $\Sigma_{22}^{-1/2}\Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1/2}$. e_k and f_k satisfies:

$$f_k = \frac{1}{\rho_k^*}\Sigma_{22}^{-1/2}\Sigma_{21}\Sigma_{11}^{-1/2}e_k \quad e_k = \frac{1}{\rho_k^*}\Sigma_{11}^{-1/2}\Sigma_{12}\Sigma_{22}^{-1/2}f_k \tag{4.128}$$

4.5.2 Canonical Correlation based on Standardized Variables

Using standardized variable of X:

$$Z_k^{(\nu)} = \frac{X_k^{(\nu)} - \mu_k^{(\nu)}}{\sqrt{\sigma_{kk}^{(\nu)}}}, \ k = 1, 2, \ldots p \text{ or } q, \ \nu = 1, 2 \tag{4.129}$$

with covariance

$$\underset{(p+q)\times(p+q)}{\rho} = V^{-1/2}\Sigma V^{-1/2} = \begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix} \tag{4.130}$$

And similarly, the CCA pair is

$$U_k = a_k'Z^{(1)} = e_k'\rho_{11}^{-1/2}Z^{(1)} \qquad V_k = b_k'Z^{(2)} = f_k'\rho_{22}^{-1/2}Z^{(2)} \tag{4.131}$$

with e_k is the k^{th} eigenvector of $\rho_1 1^{-1/2}\rho_{12}\rho_{22}^{-1}\rho_{21}\rho_{11}^{-1/2}$, $f_[k]$ is the k^{th} eigenvector of $\rho_{22}^{-1/2}\rho_{21}\rho_{11}^{-1}\rho_{12}\rho_{22}^{-1/2}$, and

$$f_k = \frac{1}{\rho_k^*}\rho_{22}^{-1/2}\rho_{21}\rho_{11}^{-1/2}e_k \quad e_k = \frac{1}{\rho_k^*}\rho_{11}^{-1/2}\rho_{12}\rho_{22}^{-1/2}f_k \tag{4.132}$$

4.5.3 Sample Canonical Correlation

Replacement:

$$\Sigma \longrightarrow S \qquad \rho \longrightarrow R \tag{4.133}$$

to get

$$\hat{U} = \hat{A}x^{(1)} \qquad \hat{V} = \hat{B}x^{(2)} \tag{4.134}$$

and we can use $\hat{U}, \hat{V}$, $\hat{A}, \hat{B}$ to express S_{12} as

$$S_{12} = \hat{A}^{-1} \begin{bmatrix} \hat{\rho}_1^* & 0 & \dots & 0 \\ 0 & \hat{\rho}_2^* & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \hat{\rho}_p^* \end{bmatrix} (\hat{B}^{-1})' \tag{4.135}$$

When applying CCA, we pick the first r canonical variable, thus some infomation is lost. But we hope the first r canonical variables can contain enough information of $X^{(1)}$ and $X^{(2)}$.

Determine of r: consider the error if approximation by expressing

$$\hat{A}^{-1} = [\alpha_1, \alpha_2, \dots, \alpha_p] \qquad \hat{B}^{-1} = [\beta_1, \beta_2, \dots, \beta_p] \tag{4.136}$$

and

$$\begin{aligned} S_{12} =& \sum_{i=1}^{p} \hat{\rho}_i^* \alpha_i \beta_i' \\ S_{11} =& \hat{A}^{-1}(\hat{A}^{-1})' = \sum_{i=1}^{p} \alpha_i \alpha_i' \\ S_{22} =& \hat{B}^{-1}(\hat{B}^{-1})' = \sum_{i=1}^{p} \beta_i \beta_i' \end{aligned}$$

Total sample variance explained by the first r canonical variables:

$$\frac{\sum_{i=1}^{r} \alpha_i' \alpha_i}{tr(S_{11})} \qquad \frac{\sum_{i=1}^{r} \beta_i' \beta_i}{tr(S_{22})} \tag{4.137}$$

Section 4.6 Discriminant Analysis

Key idea of DA: for $\underset{n\times p}{X}$ with an extra column labeling the classification, we want to determine a rule to assign new objects. More specifically, determine the classification region R_i for each class π_i.

4.6.1 Classification Criterion

- Two-category classification case:Each row of X is labeled in π_1 or π_2, for two-category, only one of R_1, R_2 is needed.

  Some basic concept in classification model:

  - Prior Possibility $p_i, i = 1, 2$;
  - Penalty for misclassification $c(i|j), i, j = 1, 2$: cost if a π_j object is classified in R_i.
  - Conditional Probability $\mathbb{P}(i|j), i, j = 1, 2$: probability that a π_j object falls in region R_i

  □ **Determination Criterion:**

  - Expected Cost of Misclassification (ECM) Criterion: Minimizing ECM,

$$\text{ECM} = c(2|1)\mathbb{P}(2|1)p_1 + c(1|2)\mathbb{P}(1|2)p_2 \tag{4.138}$$

For two-category problem, R_1, R_2 can be determined as

$$
\begin{aligned}
R_1 =& \frac{f_{\pi_1}(x)}{f_{\pi_2}(x)} \geq \frac{c(1|2)}{c(2|1)} \frac{p_2}{p_1} \\
R_2 =& \complement_{R_x}^{R_1} = \arg_{x\in R} \frac{f_{\pi_1}(x)}{f_{\pi_2}(x)} < \frac{c(1|2)}{c(2|1)} \frac{p_2}{p_1}
\end{aligned}
$$

– Total Probability of Misclassification (TPM) Criterion: Minimizing TPM,

$$
\text{TPM} = \mathbb{P}(\text{misclass}) = \mathbb{P}(2|1)p_1 + \mathbb{P}(1|2)p_2 \tag{4.139}
$$

actually $\arg\min \text{TPM} = \underset{c(1|2)=c(2|1)}{\arg\min} \text{ECM}$

– Posterior Probability Criterion: Maximize posterior probability $P(\pi_i|x_0)$,

$$
\mathbb{P}(X \in \pi_i|X = x_0) = \frac{p_i f_{\pi_i(x_0)}}{p_1 f_{\pi_1}(x_0) + p_2 f_{\pi_2}(x_0)}, \; i = 1, 2 \tag{4.140}
$$

Also equivalent to ECM for $c(1|2) = c(2|1)$

- Here only introduce ECM: $\{R_i\} = \arg\min \text{ECM}$

$$
\begin{aligned}
\text{ECM}(i) =& \sum_{j\neq i} c(j|i)\mathbb{P}(j|i) \\
\text{ECM} =& \sum_{i=1}^{g} p_i \text{ECM}_i = \sum_{i=1}^{g} \sum_{j\neq i} c(j|i)p(j|i)p_i
\end{aligned}
$$

4.6.2 Linear & Quadratic Discriminant Analysis

Now take two-category ECM criterion as example. An estimation to $\mathbb{P}(1|2)$, $\mathbb{P}(2|1)$, i.e. to f_{π_1}, f_{π_2} is needed.

Assumption: for $\pi_1 : X \sim N(\mu_1, \Sigma_1)$,$\pi_2 : X \sim N(\mu_2, \Sigma_2)$, further for

- $\Sigma_1 = \Sigma_2 = \Sigma$: Linear Discriminant Analysis (LDA).

$$
f_{\pi_i}(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_i)'\Sigma^{-1}(x-\mu_i)\right), \; i = 1, 2 \tag{4.141}
$$

then

$$
\begin{aligned}
R_1 = \arg_{x\in R} (\mu_1 - \mu_2)'\Sigma^{-1}x - \frac{1}{2}(\mu_1 - \mu_2)'\Sigma^{-1}(\mu_1 - \mu_2) \geq \ln\left(\frac{c(1|2)}{c(2|1)} \frac{p_2}{p_1}\right) \\
R_2 = \arg_{x\in R} (\mu_1 - \mu_2)'\Sigma^{-1}x - \frac{1}{2}(\mu_1 - \mu_2)'\Sigma^{-1}(\mu_1 - \mu_2) < \ln\left(\frac{c(1|2)}{c(2|1)} \frac{p_2}{p_1}\right)
\end{aligned}
$$

Note that L.H.S. is a linear combination of x, thus called LinearDA.

Sample estimation to Σ: use pooled variance in equation. 4.75.

- $\Sigma_1 \neq \Sigma_2$: Quadratic Discriminant Analysis (QDA).

$$
f_{\pi_i}(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_i)'\Sigma_i^{-1}(x-\mu_i)\right), \; i = 1, 2 \tag{4.142}
$$

then

$$R_1 = -\frac{1}{2}x'(\Sigma_1^{-1} - \Sigma_2^{-1})x + (\mu_1'\Sigma_1^{-1} - \mu_2'\Sigma_2^{-1})x - \frac{1}{2}\ln\left(\frac{|\Sigma_1|}{|\Sigma_2|}\right) + \frac{1}{2}(\mu_1'\Sigma_1^{-1}\mu_1 - \mu_2'\Sigma_2^{-1}\mu_2) \geq \ln\left(\frac{c(1|2)}{c(2|1)}\frac{p_2}{p_1}\right)$$
$$R_2 = -\frac{1}{2}x'(\Sigma_1^{-1} - \Sigma_2^{-1})x + (\mu_1'\Sigma_1^{-1} - \mu_2'\Sigma_2^{-1})x - \frac{1}{2}\ln\left(\frac{|\Sigma_1|}{|\Sigma_2|}\right) + \frac{1}{2}(\mu_1'\Sigma_1^{-1}\mu_1 - \mu_2'\Sigma_2^{-1}\mu_2) < \ln\left(\frac{c(1|2)}{c(2|1)}\frac{p_2}{p_1}\right)$$

Note that L.H.S. is a quadric form of x, thus called QuadraticDA.

- Two extension: allow more flexible estimation to variance:
  - $\hat{\Sigma}_i(\alpha) = \alpha\hat{\Sigma}_i + (1-\alpha)\hat{\Sigma}$, shrink between QDA and LDA;
  - $\hat{\Sigma}_i(\gamma) = \gamma\hat{\Sigma} + (1-\gamma)\hat{\sigma}^2 I$, shrink toward scalar cov.

4.6.3 Fisher's Discriminant Analysis

Project X onto some hyperplane and conduct low-dimensional classification.

Project x onto some hyperplane by $y = a'x$, then we maximize $\psi = \frac{\text{mean of treatment}^2}{\text{variance}}$[42]. i.e.

$$\psi = \frac{\sum_{i=1}^{g}(\mu_{iY} - \mu_Y)^2}{\sigma_Y^2} = \frac{a'\left(\sum_{i=1}^{g}(\mu_i - \mu)(\mu_i - \mu)'\right)a}{a'\Sigma a} = \frac{a'B_\mu a}{a'\Sigma a}$$

Result: a is the largest eigen vector of $W^{-1}B$.

Relation between FDA and LDA: in FDA, take the first ξ eigenvectors to conduct classification, thus loses more information. But when $\xi = g-1$, FDA $\equiv$ LDA.[43]

4.6.4 Evaluation of Discriminant Model

☐ **Judging Index:**

- Total Probability of Misclassification (TPM):

$$\text{TPM} = p_1\mathbb{P}(2|1) + p_2\mathbb{P}(1|2) = p_1\int_{R_2} f_{\pi_1}(x)\,\mathrm{d}x + p_2\int_{R_1} f_{\pi_2}(x)\,\mathrm{d}x \tag{4.143}$$

- APparent Error Rate (APER): used with cross validation (CV). The fraction of misclassification in training set.

Section 4.7 Clustering Analysis

Key idea of CA: Group a collection of data according to similarity and relation of objects.

[42] MANOVA Model: For g groups with same Σ, consider an MANOVA model: $X_{ij} = \mu + \tau_i + e_{ij}$. Then MANOVA table gives Sum of Squares and cross Products (SSP):

$$\text{Treatment:}B = \sum_{i=1}^{g} n_i(\bar{x}_i - \bar{x})(\bar{x}_i - \bar{x})'$$
$$\text{Residual:}W = \sum_{i=1}^{g}\sum_{j=1}^{n_i}(x_{ij} - \bar{x}_i)(x_{ij} - \bar{x}_i)'$$
$$\text{Total:}T = B + W = \sum_{i=1}^{g}\sum_{j=1}^{n_i}(x_{ij} - \bar{x})(x_{ij} - \bar{x})'$$

use B and W to measure the variance of sample.

[43] Because a is eigenvector of $W^{-1}B$, while $\text{rk}(B) = g-1$, thus there are $g-1$ non-zero eigenvalues at most.

4.7.1 Agglomerative Clustering Algorithm

☐ **Clustring Algorithm**

Hierarchical clustering: start with individual points and combine them to form groups.

Algorithm *Hierarchical Clustering*

---

1. All $k = n$ points are individual clusters;
2. In each iteration step k:
   (a) Use a distance/dissimilarity matrix $\underset{k\times k}{D}$ to express distances between clusters; the 'distance' between clusters is diversified, choice of which see the following part;
   (b) merge the closest pair of clusters(or points) to form a larger cluster, and now number of clusters
   (c) $k = k - 1$;
3. Only $k = 1$ cluster is left
4. Choose a proper threshold of distance to determine K

☐ **Choice of between-cluster distance: To express distance between two clusters A and B,**

- Choice of distance functional $D(\cdot,\cdot)$:
  - Euclidean Distance D_{E};
  - Mahalanobis Distance D_{M};
  - Jaccard Distance $D_{\mathrm{J}} = 1 - \dfrac{|A\cap B|}{|A\cup B|}$;
  - etc.
- Location choice of cluster:
  - Complete link: $\max D(a\in A, b\in B)$;
  - Single link: $\min D(a\in A, b\in B)$;
  - Centroid distance: $D(A\,\text{centroid}, B\,\text{centroid})$;
  - Group average: $\langle D(a\in A, b\in B)\rangle$
- Note: pros-and-cons of agglomerative clustering algorithm
  - No assumptions for final k needed;
  - Intuitive display of relations;
  - Large computational requirement: $\sim O(n^3)$;
  - Sensitive to noise and outliers.

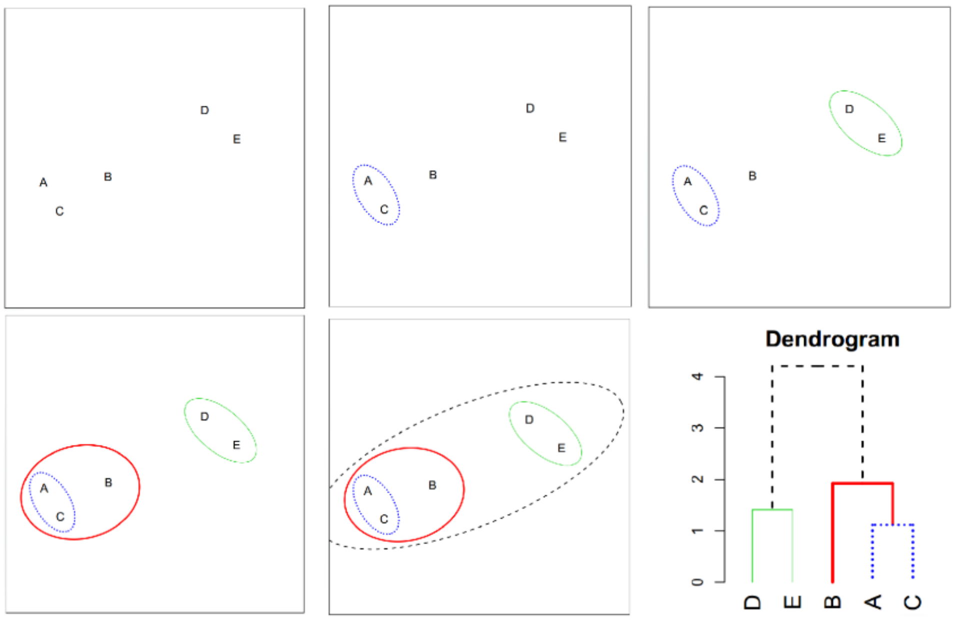


图 3: Illustration of Hierarchical Clustering

4.7.2 K-Means Clustering Algorithm

Assume we have a preset number K of clusters , we can use K-means clustering.

Algorithm *K-Means Clustering*

---

1. Choose/Preset number of clusters K;
2. Select K points as initial centroids, useful methods:
   - Randomly select;
   - Use Centroid of agglomerative algorithm;
   - Successively pick the farthest point from others.
3. In each iteration of centroids:
   (a) For all points i, calculate its distance from the l^{th} centroid $D(i, l)$
   (b) Classify each i point to the nearest centroid cluster;
   (c) Re-calculate the centroid of new K clusters;
4. Repeat until convergence.(Convergence criterion can be e.g. $< \sum_i D(i \in g_l, l) > \to$ const)

Note: prosandcons of K-Means clustering algorithm

- Efficient:$\sim O(n)$;
- Sensitive to outliers;
- Ineffective for non-convex shapes.

4.7.3 Expectation Maximization Algorithm for Gaussian Mixture Model

The Gaussian Mixture Model (GMM) for clustering assumes X is generated from a mixed distribution of K normal, i.e. X has probability π_l to be generated from corresponding normal $N(\mu_l, \Sigma_l)$:

$$X \sim \sum_{l=1}^{K} \pi_l N(\mu_l, \Sigma_l) = \sum_{l=1}^{K} \pi_l N(\theta_l), \quad \sum_{l=1}^{K} \pi_l = 1,\ \pi_l \geq 0. \tag{4.144}$$

Use its likelihood function $L(\theta; x)$ and maximize posterior probability by $\dfrac{\partial \ell}{\partial \theta}$:

$$L(\{\pi_l\}, \{\theta_l\}; x) = \prod_{i=1}^{N} \sum_{l=1}^{K} \pi_l \frac{1}{(2\pi)^{p/2} |\Sigma_l|^{1/2}} \exp\left(-\frac{1}{2}(x_i - \mu_l)' \Sigma_l^{-1} (x_i - \mu_l) \right) \tag{4.145}$$

E-M Algorithm uses the ELBO maximizing method, detail see section. 6.5. For simplification express $\theta \equiv \{\cup \pi_l, \cup \mu_l, \cup \Sigma_l\}$. The maximizing function $Q(\theta|\theta^{(t)})$ for GMM model and corresponding iteration:

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)}) = \arg\max_{\theta} \sum_{i=1}^{N} \sum_{l=1}^{K} \gamma_{il}^{(t)} \log \pi_l \phi(x_i|\mu_l, \Sigma_l), \quad \gamma_{il}^{(t)} \equiv \frac{\pi_l^{(t)} \phi(x_i|\mu_l^{(t)}, \Sigma_l^{(t)})}{\sum\limits_{j=1}^{K} \pi_j^{(t)} \phi(x_i|\mu_j^{(t)}, \Sigma_j^{(t)})}$$

Lagrange Multiplier: Extreme value $\arg\max\limits_{\theta} Q(\theta|\theta^{(t)})$ with constraint $\sum_{l=1}^{K} \pi_l = 1$ requires

$$\frac{\partial Q(\theta|\theta^{(t)})}{\partial \mu_l} = 0 \quad \frac{\partial Q(\theta|\theta^{(t)})}{\partial \Sigma_l^{-1}} = 0 \quad \frac{\partial Q(\theta|\theta^{(t)}) + \lambda(\sum_{j=1}^{K} \pi_l - 1)}{\partial \pi_j} = 0, \quad \forall l = 1, 2, \ldots, K \tag{4.146}$$

Result:

$$\begin{cases} \mu_l^{(t+1)} = \dfrac{\sum\limits_{i=1}^{N} \gamma_{il}^{(t)} x_i}{\sum\limits_{i=1}^{N} \gamma_{il}^{(t)}} \\ \Sigma_l^{(t+1)} = \dfrac{\sum\limits_{i=1}^{N} \gamma_{il}^{(t)} (x_i - \mu_l)(x_i - \mu_l)'}{\sum\limits_{i=1}^{N} \gamma_{il}^{(t)}} \\ \pi_l^{(t+1)} = \dfrac{1}{N} \sum_{i=1}^{N} \gamma_{il}^{(t)} \end{cases} \tag{4.147}$$

$$\gamma_{il}^{(t)} \equiv \frac{\pi_l^{(t)} \phi(x_i|\mu_l^{(t)}, \Sigma_l^{(t)})}{\sum\limits_{j=1}^{K} \pi_j^{(t)} \phi(x_i|\mu_j^{(t)}, \Sigma_j^{(t)})} \tag{4.148}$$

where γ_{il} is the posterior probability that the i^{th} object belongs to the l^{th} group.

The above constraint equations are difficult to solve, use iteration algorithm:

Algorithm *EM-Algorithm for Gaussian Mixture Model*

1. Use e.g. K-means method to set an initial estimation as $(\hat{\mu}_l^{(0)}, \hat{\Sigma}_l^{(0)})$, $\hat{\pi}_l^{(0)} = 1/K$;
2. Repeat Expectation & Maximization:

(a) E$_{\text{xpectation}}$-Step: Compute posterior of latent variable on each point;

$$\hat{\gamma}_{il}^{(t)} = \frac{\pi_l^{(t)}\phi(x_i|\mu_l^{(t)},\Sigma_l^{(t)})}{\sum\limits_{j=1}^{K}\pi_j^{(t)}\phi(x_i|\mu_j^{(t)},\Sigma_j^{(t)})}, \quad 1\leq i\leq N,\ 1\leq l\leq K \tag{4.149}$$

(b) M$_{\text{aximize}}$-Step: Re-calculate parameters $\{\mu_l,\Sigma_l,\pi_l\}$ by equation. 4.147.

3. Repeat until convergence.

Note: EM method for Gaussion Mixture Model is a greedy algorithm $\longrightarrow$ local maximum.

4.7.4 DBSCAN & OPTICS Density Clustering Algorithm

DBSCAN algorithm (Density-Based Spatial Clustering of Application with Noise) is a kind of density clustering algorithm. OPTICS algorithm (Ordering Point To Indentify the Cluster Structure) is its improved version.

☐ **DBSCAN Algorithm**

Key (preset) index in DBSCAN:

- Eps ε: Radius of neighbourhood of a point;
- MinPts M: Minimum number of points to be indentified as cluster core point, usually choose $M\geq \mathrm{dim}+1$;
- (Also, a distance norm is needed, e.g. Euclidean D).

Notation:

- ε neighbourhood of point x_i:

$$\mathcal{N}_\varepsilon(x_i)\equiv\{y\in\mathbb{R}^n:0<D(y,x)<\varepsilon\} \tag{4.150}$$

- 'Density' (is actually an integer):

$$\rho_\varepsilon(x_i)\equiv\#x_j\in\mathcal{N}_\varepsilon(x_i) \tag{4.151}$$

- Three types of Points: X_c, X_{bd}, X_{noi}.
  - Core Point: label an x_i as core point if

$$\rho_\varepsilon(x_i)\geq M \tag{4.152}$$

    Denote the set of core point as X_c, and set of non-core point as X_{nc}

  - Border Point: label an $x_j\in X_{nc}$ as border point if

$$\exists(x_i\in X_c)\in\mathcal{N}_\varepsilon(x_j)\&x_j\in X_{nc} \tag{4.153}$$

    Denote the set of border point as X_{bd}

  - Noise Point: the set of noise point is

$$X_{noi}\equiv\complement_X^{X_c\cup X_{bd}} \tag{4.154}$$

- Point Relations: DDR, DR, DC
  - Directly Density Reachable: For $x_i,x_j\in X$, if $x_i\in X_c$, $x_j\in\mathcal{N}_\varepsilon(x_i)$, then say x_j is DDR from x_i;

  - Density Reachable: For point chain $x_{i_1}, x_{i_2}, \ldots, x_{i_m}$, $m \geq 2$. If $x_{i_{\kappa+1}}$ is DDR from x_{i_κ}, $\forall 1 \leq \kappa \leq m-1$, then say x_{i_m} is DR from x_{i_1}.
  - Density Connected: For point $x_{i_1}, x_{i_2}, x_{i_3}$, if x_{i_2} and x_{i_3} are both DR from x_{i_1}, then say x_{i_2} and x_{i_3} are DC.

Note: DR is not symmetric for x_{i_1} and x_{i_m}; while DC is.

DBSCAN algorithm classify all points that are Density Connected to each other into a cluster $C \subset X$, i.e.

$$\text{Maximality:} x \in C \&\& y \text{ DR from } x \Rightarrow y \in C$$

$$\text{Connectivity:} x, y \in C \Rightarrow x, y \text{ DC}.$$

Pros and cons of DBSCAN:

- Insensitive to noise;
- Based on density, with no constraint on the shape of cluster;
- Suitable for clusters with uniformly densed data, otherwise difficult to choose proper Eps ε;
- Complexity $\sim O(n^2)$, at least $O(n \log n)$.

☐ **OPTICS Algorithm**

OPTICS is based on DBSCAN and shares most of the basic concepts and ideas. Further define the following distance (preset ε and M):

- Core Distance: For $x_i \in X_c$, the smallest distance allowing x_i to become core point.

$$\text{CD}(x_i) = D(x_i, N_\varepsilon^M(x_i)),\ \rho_\varepsilon(x_i) \geq M \tag{4.155}$$

  where $N_\varepsilon^M(x_i)$ is the M^{th} closest point from x_i;

- Reachablity Distance: For $y \in X,\ x_i \in X_c \subset X$,

$$\text{RD}(y, x_i) = \max\{CD(x_i, D(y, x_i))\} \tag{4.156}$$

  Or equivlantly

$$\text{RD}(y, x_i) = \underset{\rho_d(x_i) \geq M, y \in \mathcal{N}_d(x_i)}{\arg\min} d \tag{4.157}$$

Algorithm flow:

Algorithm *OPTICS*

---

1. Construct X_c based on preset M, ε;
2. Pick an 'unprocessed' point $x_{n_i} \in X_c$ and calculate $\text{RD}(x_j, x_{n_i})$, $\forall$'unprocessed'$x_j \in \mathcal{N}_\varepsilon(x_{n_i}) \cap X_c$. Pick the $x_j \in X_c$ with smallest RD and label as $x_{n_{i+1}}$ processed;
3. Repeat step 2 until all points are processed. Output $\{x_{n_i}\} = (x_{n_1}, x_{n_2}, \ldots, x_{n_{|X_c|}})$. Each x_{n_i} is attached with a $\text{CD}(x_{n_i})$ and a $r(x_{n_i}) := \text{RD}(x_{n_{i-1}}, x_{n_i})$[44].

Then break the ordering sequence n_i according to $r(x_{n_i})$, .e.g. break n_i if $r(x_{n_i}) \geq \tilde{\varepsilon}$

Comment: OPTICS is more stable than DBSCAN, capable of dealing with multi-density clustering.

[44] For $i = 1$, just define as 0

Chapter. V 数据科学导论部分

Instructor: Sheng Yu

This section contains basic data acquisition, data cleaning, data processing, date visualization methods. Details for data analysis are not covered.

☐ Road to Data Scientist

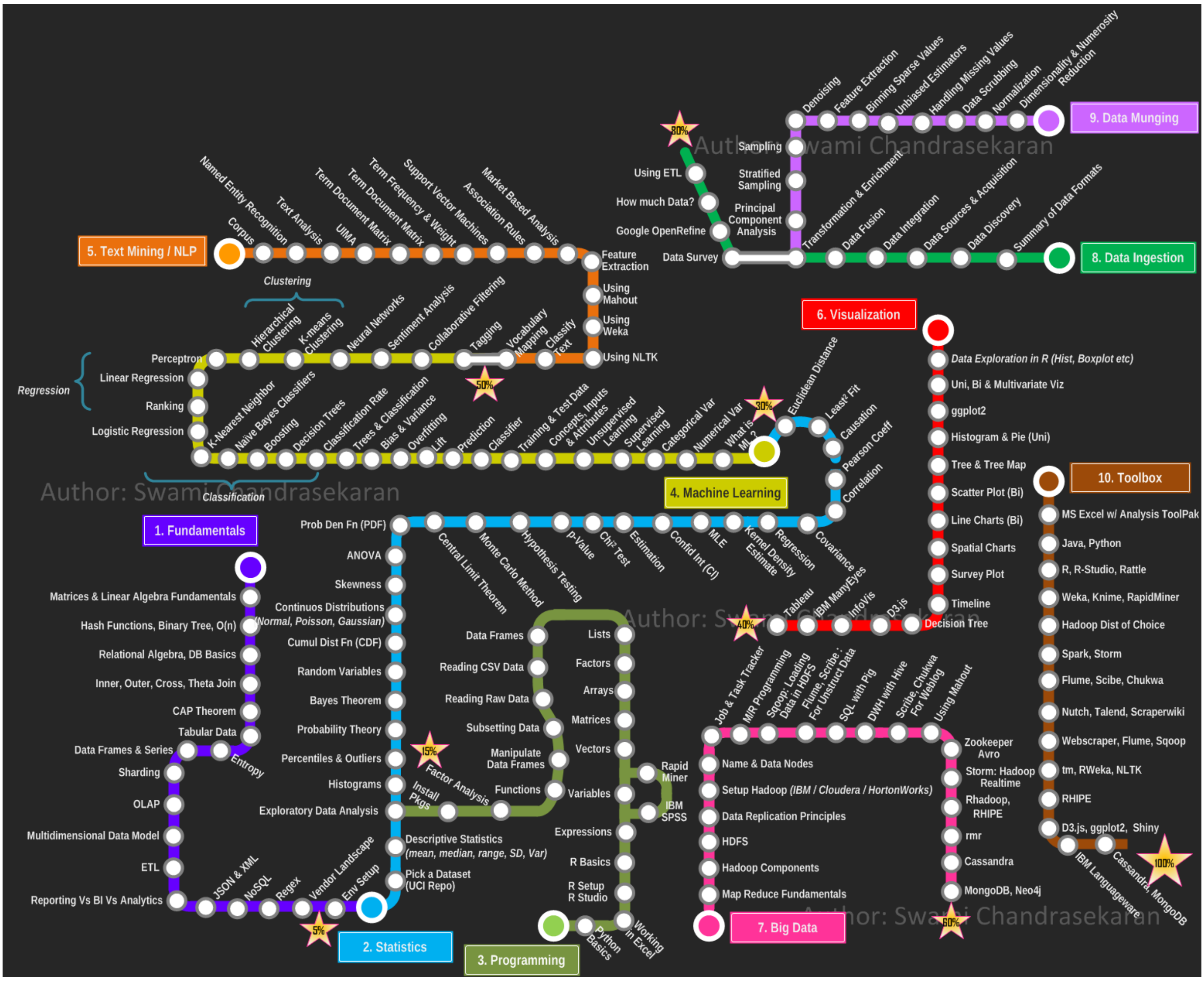


图 4: Road to Data Scientist

Comparison of `R`, `python`:focus on different aspects of 'Statistics':

- Differnece in programming philosophy: `R` for data analysis and `python` for data processing
- Difference in operating domain: `R` for statistical programming while `python` for general programming.

Section 5.1 Basic R. Manipulation

5.1.1 Installation and Maintenance of R.

☐ **Installing and Updating**

`R.`: update by delete old version and install new version.

- In CRAN (The Comprehensive `R` Archive Network): `https://cran.r-project.org`
- In Mirror@TUNA: `https://mirrors.tuna.tsinghua.edu.cn/CRAN`

RStudio: `https://www.rstudio.com`

☐ **Running `R.` command :**

- In `R.` GUI;
- In `R.` command line terminal;
- `R. CMD BATCH`;
- `Rscript`;
  - Use > to redirect output(overwrite);
  - Use >> to append output.

☐ **`R.` package library: packages are collection of `R.` functions (as well as test data and sample code).**

- `.libPaths()` show package library location[45] ;
- `library('PACKAGE_NAME1','PACKAGE_NAME2',...)` load packages.
- `install.packages('PACKAGE_NAME1','PACKAGE_NAME2',...)` install package from CRAN/mirrors;
- `installed.packages()` show all installed packages;
- `updata.packages(checkBuilt = TRUE, ask = FALSE)` update installed packages;

☐ **Working directory manipulation:**

- `getwd()` get current working directory;
- `setwd('TARGET_PATH')` set working directory (as an existing path).
- `dir()` show current directory.

☐ **Recommended `R.` Project Organization : working directory organized like**

- `data/` folder for structured original dataset;
- `result/` folder for output result;
- `presentation/` folder for result representing slides/reports/etc.;
- `.r` project file $\times n$.

☐ **Looking for Help/Example of function:**

[45] Unlike in `C` or `python` where `.` is an operator, `.` in `R.` is just a common character, without special meaning. This feature can be used in naming self-defined functions: use `.FUN_NAME1` for within-project function while `FUN_NAME2` for external interface.

- `?FUN_NAME();`
- `help('FUN_NAME');`

5.1.2 Data Structure and Basic Manipulation in R.

☐ **Atomic Classes**

- `'abc'` Character;
- `3L` Integer;
- `2.4` Numeric;
- `TRUE`,`FALSE`,`T`,`F` Logical;
- Special types: `NA`, `NaN`, `NULL`, `Inf`

☐ **Operators**

- Numerical Operators: `+`, `-`, `*`(multiply by column), `/`, `%*%`(matrix multiply), `^`, `%%`(remainder operate);
- Logical Operators: ==,etc.; `&` and `|` for common operator, `&&` and `||` for comparing the first element;
- Round a numeric:
  - `as.integer()`, round towards 0
  - `trunc()`
  - `ceiling()`
  - `floor()`
  - `round(NUMBER_TO_ROUND,digits = DIGITS)`

☐ **Type Conversion**

- First need to meet the need of

Key Criterion: when converting mixed type in to the same type, use the type with more compatibility.

- Logical → Numeric:

☐ **Data Structure**

- **Atomic Vector** : Column vector is the **basic** data structure in `R`. (scalar is length=1 vector).

  Only data of the same class can be held in one vector.

  Initialization:

  - Ordinary way:
    * `c(1,2,3)`, `c(T,FALSE,TRUE)`, `c('a',NA,'b')`
    * `vector(mode = MODE,length = LENGTH)`
    * `logical(LENGTH)` return `FALSE` vector

  where `c()` for 'combine';

  `c()` combines all things into one vector, e.g. `c(c(1,2,3),c(1,2))=(1,2,3,4,5)`.

  - Sequence vector:
    * `1:3.5=c(1,2,3)`, `3:1=c(3,2,1)`
    * `seq(from, to ,by, length.out)`, `length.out` for total vector length;
    * `rep(SEQ_TO_REP, times, lenght.out ,each)`, used in k-fold cross validation labelling.

  Operations:

  - between vectors of different length `SHORT` and `LONG`: First `SHORT <-rep(SHORT, length.out=length(LONG))`. Then operate `SHORT` and `LONG`.
  - Element access: `a[i]`

  Vectorized Operation: All operation in `R.` are based on vector, and vectorized operation is Parallel Arithmetic, which is **much faster** than loop such as `for` ⟶ Consider using vectorized opertion when writing code for **Speed**! Detail see section. 5.1.4.

- **Factor** : A special kind of 'vector' in `R.`, used to label discrete categorical data.[46]

  Initialization:

  `factor(FACTOR_SEQ, levels = FACTOR_LEVEL, labels = ...)`, `FACTOR_LEVEL` is the 'rank' of each factor, `labels` is the 'tag' of levels.

  A quick way to factorize a numeric vector `x` by interval division:

  `cut_number(x, NUM_OF_LEVELS)`

- **Matrix** : Only data of the same class can be held in one matrix.

  Initilaization:

  `matrix(DATA_SEQ, nrow, ncol, byrow = FALSE, dimnames = NULL)`

  If `length(DATA_SEQ)< nrow*ncol`, then `DATA_SEQ` is repeated with `length.out=nrow*ncol`.

  Default: fill by column (because matrix is stored by column).

  Operation:

  - Common operators `+-*/^` etc. operate in column-by-column mode (vectorized operation).
  - Binding matrix: `cbind` for `[A,B]` and `rbind` for `[A;B]`
  - Transpose: `t()`
  - Matrix multiplication: `%*%`
  - Inverse matrix: `solve()` (The essence of inversion is solving linear equations)
  - Diagonal matrix:
    * `diag(VECTOR)` returns a matrix diag{`VECTOR`}
    * `diag(MATRIX)` returns the diagonal element vector
  - Element access: `a[i,j]`, `a$OBJECT_NAME`
  - Dimension: `dim()`, `nrow()`, `ncol()`
  - Rank: `qr(MATRIX)$rank`

[46] Factor vector is stored as integer vector.

- **List** : A pack containing various datatype, generally also a kind of vector(but not atomic vector)

  Initialization: `list(OBJECT1,OBJECT2,...)`

  Element access: `a[[i]]`

- `data.frame`: 'Mixture' of matrix and list. `data.frame` is actually a kind of list(with some constraint), organized in the shape of matrix (but allowing different datatype for different columns, each column is a list object).

  Each column of `data.frame` has name: `names(DATA_FRAME)`, `colnames(DATA_FRAME)`

  Element access: `a[i,j]`, `a[[i]]`, `a$COL_NAME`

☐ **Data Read & Write**

- Common R&W: `read.`/`write.`
  - `read.table(FILE_NAME,header = FALSE,sep,colClasses,stringAsFactors = FALSE)`
  - ⋆ `read.csv()` basically the same as `read.table`
  - ⋆ `write.table(DF,FILE_NAME,sep,row.names=FALSE)`
  - `readxl::read_xlsx(FILE_NAME,sheet = SHEET_NUM,range = 'RANGE')`

  Some relative arguments:

  - `quote="'"`, use `'` to quote/identify string, set `quote=''` to avoid misread strings such as 'Levene's Test'
  - `encoding='UTF-8'`, char encoding system, used especially for dataset containing CJK char.
  - `nrows=LINE_NUM` read first `LINE_NUM` lines

- Large Data Read & Write:
  - preset `colClasses`

```
temp.dat <- read.table(FILE_NAME, nrows = 100)
classes <- sapply(temp.dat, class)
dat <- read.table(FILE_NAME, colClasses = classes)
```

  - `readr::read_delim(FILE_NAME,delim=SEP)` can speed up

- Text Write: `sink(FILE_NAME,append=FALSE)`, write output into a file, the same as > in terminal.
- `.RData` Binary Format Read & Write: RW in `.RData` format, fast to load.
  - `save(DF,file = FILENAME)`
  - `load(FILE_NAME)`

5.1.3 Functions and Control Flow

☐ **Program Speed:**

`system.time({COMMAND})`

☐ **Function Call**

- `FUN_NAME(ARGUs)`

- `do.call('FUN_NAME',LIST_OF_ARGUs)`, look for a function naming `FUN_NAME` in `R.` and call.
- `a % NEW_OPRTR % b` to call self-defined binary operator.
- `'*'` etc. used in `apply(FUN = '*')`
- `R.` allows auto-completion to `ARGUs`, e.g. `rep(0,length.out=10)` = `rep(0,length=0)`

☐ **Function Definition**

▷ `R.` **Code**

Basic function definition in `R.`

```
FUNC_NAME <- function(ARG1 = ARG1_DEF_VALUE , ARG2, ...) {
    FUNCTION_BODY
}
```

More key elements in `funtion{}`

- `return(RETURN_OBJ)` at the end of function, without `return()`, output the last line
- `stopifnot(COND1,COND2,...)` at the beginning of function, used to test `ARG` class
- `stop(ERROR_MESG)` output error message
- `...` as a special argument
  - Pass `...` to another func in this function
  - Handle arbitrary number of input
- Function can be defined within function
- Function is a kind of variable ⟶ used in `apply`, `sapply` etc. for vectorized programming.
- Anonymous function: used in `sapply(X,FUN=function(){STATs})` for quick definition
- `FUNC_NAME` can be used for new-defined binary operator as `'%NEW_OPRTR%'<-function()`

☐ **Flow Control**

- `if` and `else if`, example:

```
if(COND1) {
    STATEMENT
} else if(COND2) {
    STATEMENT
} else {
    STATEMENT
}
```

- `ifelse(COND,IF_YES_STAT,IF_NO_STAT)` a vectorized version of `for+if else`.
- `for`: Loop in `R.` is **Extremely Slow**, avoid loop, use **vectorized operation**.

```
for(VAR in SEQ) {
    STATEMENT
}
```

- `switch(TEST_EXPR,CASE1 = RETN1,CASE2 = RETN2,...)`

5.1.4 Vectorized Operation

- `apply()` function series:
  - `apply(MAT,MARGIN,FUN)` for matrix apply, `MARGIN=1` for each row, 2 for each column
  - `lapply(LIST,FUN)` for list/`data.frame`, apply `FUN` on each list elements,`list` returned
  - ⋆ `sapply(X,FUN)` for list/`data.frame` apply+simplify, `vector/matrix/list` returned
  - `tapply(X,INDEX,FUN)`: for each index, use `FUN` respectively.
  - `mapply(FUN,ARGU_OF_FUN)`, use argument name to label `ARGU_OF_FUN`, or causes bad readability.

    Example:

    ```
    mapply(function(x,y,z,k){(x+k)^(y+z)} , x = ,y = ,z = ,k = )
    ```

- `Vfunc <-Vectorize(FUNC_NAME)`: define vectorize version of function.
- `with()` and `within()`:
  - `with(DF,aggregate(PART,by,FUN))`
  - `with(DF,STATE),within(DF,STATE)`, `within` allows new column append
- `outer(VEC1,VEC2,FUN)`: A Two-variate extension of `mapply()`, output wedge of two vectors.
- `ifelse(COND,YES_STAT,NO_STAT)`, vectorization supported.

5.1.5 Subsetting

- By position: `x[RANGE]`
  - `x[4]`
  - `x[-4]`: without the 4th item (different from `python`, where selects reciprocal 4th element).
  - `x[2:4]`
  - `x[c(1,2,5)]`
- By name: `x[,'COL_NAMEs']`, `x[,'COL_NAME1':'COL_NAME2']`
- By condition: basically, `x[LOGI_VEC]`
  - `x[x==10]`
  - `x[x %in% c(1,3,4)]`, linear search, not based on hash algorithm[47].

[47] If really needed, use `env()` to reset environment.

Usually used for conditional selection of `data.frame`

- Subsetting for `data.frame` and list: `x[[RANGE]]`

  Simplified/Preserved subsetting: whether preserved datatype, e.g. df → df (preserved) v.s. df → vector (simplified).

DataType	Simplified	Preserved
vector	`x[[1]]]` / `x[1]`	
list	`x[[1]]`	`x[1]`
factor	`x[1:4,drop=T]`	`x[1:4]`
matrix	`x[,1]`	`x[,1,drop=F]`
`data.frame`	`x[,1]`,`x[[1]]`	`x[,1,drop=F]`,`x[1]`

表 2: Simplified/Preserved subsetting

- Other subsetting:
  - `%in%`
  - `unique()`, return with each element appears only one times
  - `duplicated()`, `TRUE` when appear the $n > 1$ times
  - `which(x==4)`, return position of matched element
  - `which.min()`, `which.max`, `min()`, `max()`
  - `grep(REGEX,X,value)`, search for elements with `REGEX` pattern: `value=F` returns position, `value=T` returns elements, `grepl(REGEX,X)` returns logical vector
  - `match(TO_BE_MATCHED,TARGET)`, returns the index of elements of `TO_BE_MATCHED` in `TARGET`

    ▷ `R.` **Code**

    Example:

```
vec1 <- c('a','a','b','b','d','d','b')
vec2 <- c('d','a','b')
match(vec1,vec2)
> [1] 2 2 3 3 1 1 3
```

  - `subset(X,...)`, `...` a series of select criterion. **not** allowed: `subset(X,...)<-`

- Use subsetting to sample: `DATA[sample(1:nrow(DATA),NUM_OF_SAMPLE,replace),]`, `replace=T` for with replacement

5.1.6 Data Manipulation With dplyr. And tidyr.

`dplyr` and `tidyr` are two useful package for data cleaning & manipulation. Use package `tidyverse` include both of them.

`tidyverse` for `tidyuniverse`, includes `dplyr`, `tidyr`, `readr`, `ggplot2`, `stringr`, etc.

☐ **%>% pipe in `tidyverse`: functions in `tidyverse` use `FUNC(DF,...)`, where `DF` can be passed on by %>%.**

☐ `dplyr` **Package.**

- Cheet Sheet: https://nyu-cdsc.github.io/learningr/assets/data-transformation.pdf
- `select(DF,...)`, where `...` can use column index/name range as in subsetting, or some helper function for advanced subsetting:
  - matching position:
    - `everything()`
    - `last_col()`
  - matching column name:
    - `start_with('PATTERN')`, `end_with('PATTERN')`, `contains('PATTERN')`
    - `match('REGEX')`, column name with `REGEX` pattern
    - `num_range('x',1:4)` delect column name `c('x1','x2','x3','x4')`
    - `any_of(CHR_VEC)` select column from `CHR_VEC`
  - `where(FUN)`, select those `FUN(COL_NAME)` returns `TRUE`
- `filter(DATA,CONDs)`, select elements with `CONDs` conditions
- `arrange(DATA,COL)`, sort by `COL`, `arrange(DATA,desc(COL))` for descending order
- `mutate(DATA,...)`, append new columns according to `...` definition; `transmute()` drops original columns.

  `...` definition can use advanced window function:
  - `lead(COL)`,`lag(COL)`, e.g. `lead(COL)[i]=COL[i+1]`, can use `...=COL-lead(COL)` for differnetial
  - `dense_rank(COL)`, `percent_rank(COL)` rank number
  - `ntile(COL,N)` break into `N` groups labeling `1:N`
  - `cume_dist(COL)`, `cummean(COL)`, `cumsum(COL)`, `cummax(COL)`, `cummin(COL)`, etc. cumulative value
- `summarise(data,...)`, `...` for summarise function.
- Row selection:
  - `slice(DF,ROW_RANGE)`
  - `distinct(DF)` remove duplicated rows
  - `sample_frac(DF,FRAC,replace)`, sample `FRAC` fraction from `DF`
  - `sample_n(DF,N,replace)`, sample `N` cases from `DF`
  - `top_n(DF,AMOUNT,RANK_COL)` select `AMOUNT` top ranking by `RANK_COL` cases
- Data combining see slides.

☐ `tidyr` **Package**

- Cheet Sheet: https://leadousset.github.io/intro-to-R/cheatsheet_tidy.pdf
- `gather(DF,key='KEY_NAME',value='VALUE_NAME',...,na.rm)`, melt a `data.frame`.

e.g. `gather(df,'KEY','VALUE',c('COL1','COL2','COL3'))` transfers ... as:

ID	COL1	COL2	COL3
1	a_1	b_1	c_1
2	a_2	b_2	c_2
⋮	⋮	⋮	⋮

$\rightarrow$

ID	KEY	VALUE
1	COL1	a_1
2	COL1	a_2
⋮	⋮	⋮
1	COL2	b_1
2	COL2	b_2
⋮	⋮	
1	COL3	c_1
2	COL3	c_2
⋮	⋮	

- `spread(DF,key='KEY_NAME',value='VALUE_NAME')`, inverse of `gather()`
- `separate(DF,COL,into=SET_VEC,sep='REGEX')`, separate `COL` into columns with name in `SET_VEC`, sep according to `sep`
- `unite(DF,COL,SET_VEC,sep='')` inverse of `separate()`

Section 5.2 Text Processing & Text Mining

- Data cleaning
- Data manipulation
- Information extraction: mode identifying/relation extraction
- Text mining: anaylzing token distribution, ignore word order
- NLP: concept identifying based on sentence; untimate goal: 'understand' sentence meaning.

Tools for Text processing:

- `R.`: suitable for easy task
- `python.`: best
- `java`: strong, but not suitable for deep learning
- `c++`: fast, inadequate package
- `Notepad++/Vim`

5.2.1 Basic Text Manipulation With stringr.

☐ **`R. base` & `stringr` package:**

The prior one is used more often

- Cheet Sheet: http://edrub.in/CheatSheets/cheatSheetStringr.pdf
- `str_length(STRING)`, `nchar(STRING)`

- `paste(...,collapse=NULL)`,`str_c(...)`, both are vectorized operation

  Argument:

  – `sep`: sep between each ... corresponding elements, with `collapse=NULL`, return a char vector

  – `collapse`: sep when combining `collapse=NULL` vector elements, `NULL` for not combining

  – Special character: `\t` tab, `\r` & `\n` & `\r\n` new line, `\xad` '-' at end on line for word-connecting

- `str_split(STRING,pattern='REGEX')/strsplit()`, split string at `REGEX` pattern fitted, list returned

- `str_sub(STRING,start,end)`, `substr()`. The `start` char to `end` char of string, use negative index as in `python`.

  Can be used to replace: `str_sub(...)<-REP_STR`

- `str_locate_all('STRING',pattern='REGEX')/str_match_all('STRING',pattern='REGEX')`

  `grep(pattern='REGEX',x='STRING',value=T)`, search for elements with `REGEX` pattern: `str_locate_all()` or `value=F` returns position, `str_match_all()` or `value=T` returns elements.

- `str_replace_all('STRING',pattern='REGEX',replacement='REP')` `grepl(REGEX,X)` returns logical vector, include or not. `str_extract_all('STRING',pattern='REGEX')`

- `gsub(pattern='REGEX',replacement='REP',x='STRING')`, replace `REGEX` field with `REP`

- `str_trim(...,side = )`, trim extra white space at `side='both'/'left'/'right'`

5.2.2 Regular Expression

Regular expression is a text pattern/mode. abbr. regex/regexp. Regex is supported in most common language, same syntax used.

Tutorial: https://www.runoob.com/regexp/regexp-tutorial.html

☐ **Key Elements**

- Literal: common char, e.g. `a`. Include most char on keyboard. Upper/Lower case sensitive.

- Metacharacters: `\^$.|?*+()[]{}`, use e.g. `\.` to escape meaning.

  Note: when typing regex in programming language, sometimes use `\\.`: `\\.` $\xrightarrow{\text{language interpreter}}$ `\.` $\xrightarrow{\text{regex interpreter}}$ identifying `.`

- Character Class: `[]`, identify one of elements in `[]`. `^` within `[]` for C.

  – e.g. `gr[ae]y` identifies `grey` and `gray`.

  – e.g. `[0-9]` numbers, `[a-zA-z]` letter

  – e.g. `q[^x]` matches `question`, not matchs `qxestion`, not matches `Iraq`

  character class shorthand

ShortHand	Meaning	Equivalant REGEX
`\d`	numeric digit	`[0-9]`
`\D`	Not numeric digit	`[^\d]`
`\w`	a word character	`[a-zA_Z0-9_]`
`\s`	white space	`[\t\r\n\f]`

- Wildcard（通配符）: `.` matches any single character except line break `\r`,`\n`
- Anchor（词边界/定位符）: match 'word boundary' (not the space at the start/end of string).

  `^` string start, `$` string end, `\b` word boundary, `\B` not-a-word-boundary position
- Repetition/Quantifier: here `X` for some regex pattern like `CHAR`, `[]` etc.

Greedy	⋆ Reluctant	Possessive	Freq of Occurrence
`X?`	`X??`	`X?+`	$0, 1$
`X+`	`X+?`	`X++`	≥ 1
`X*`	`X*?`	`X*+`	$0, > 1$
`X{n}`	`X{n}?`	`X{n}+`	n
`X{n,}`	`X{n,}?`	`X{n,}+`	$\geq n$
`X{n,m}`	`X{n,m}?`	`X{n,m}+`	$[n, m]$

  Example: Search 'foo' in 'xfooxxxxxxfoo':

  – Greedy: 'xfooxxxxxxfoo' found at index 0-13

  ⋆ Reluctant: 'xfoo' found at index 1-4, 'xxxxxxfoo' found at index 4-13

  – Possessive: no match found (not usually used)

  Example: regex match 'aaaa'

  –

- Alternation & Grouping & Back Reference: `XA|XB` identify `XA` or `XB`, use grouping `()` to set boundary of XA,XB.

  Use `\n` for back reference the n^{th} group. ▷ `R.` **Code**

  Example: search for immediate repeat word in a sentence

```
(\b[a-zA-Z]+\b) \1
```

- Lookaround:

  – LookAhead: `(?<=X)q`

  – LookBehind: `q(?=X)`

5.2.3 Web Scraping

Basic elements of web page:

- HTML (HyperText Markup Language): structure and content of page
- CSS (Cascading Style Sheet): page style.
- JavaScript: functionality, interaction

Basic `html` document format: ▷ `R.` **Code**

```
<!DOCTYPE html> # an html document
<html> # html page begin
<head> # head elements declare
<meta charset="utf-8">
<title> TITLE OF WEB PAGE </title>
</head>
<body> # html body begin

<h1> HEADING 1 </h1>
<p class='TEST_TEXT'> PARAGRAPH 1 </p>

</body>
</html>
```

We can use elements like <p> or `class` to extract page information.

☐ **Web Scraping with** `rvest`.

- `pge <-read_html('URL')`: page read

  Proxy set: `Sys.setenv(https_proxy='http://127.0.0.1:7890')`
- `pge %>% html_elements(css='.CSS_CLASS_NAME')%>% html_text()`: basic scraping. use SelectGadget tool for help finding proper css label.

Section 5.3 Graphic in R.

5.3.1 R::base Plotting

Plot function in `R::base`:

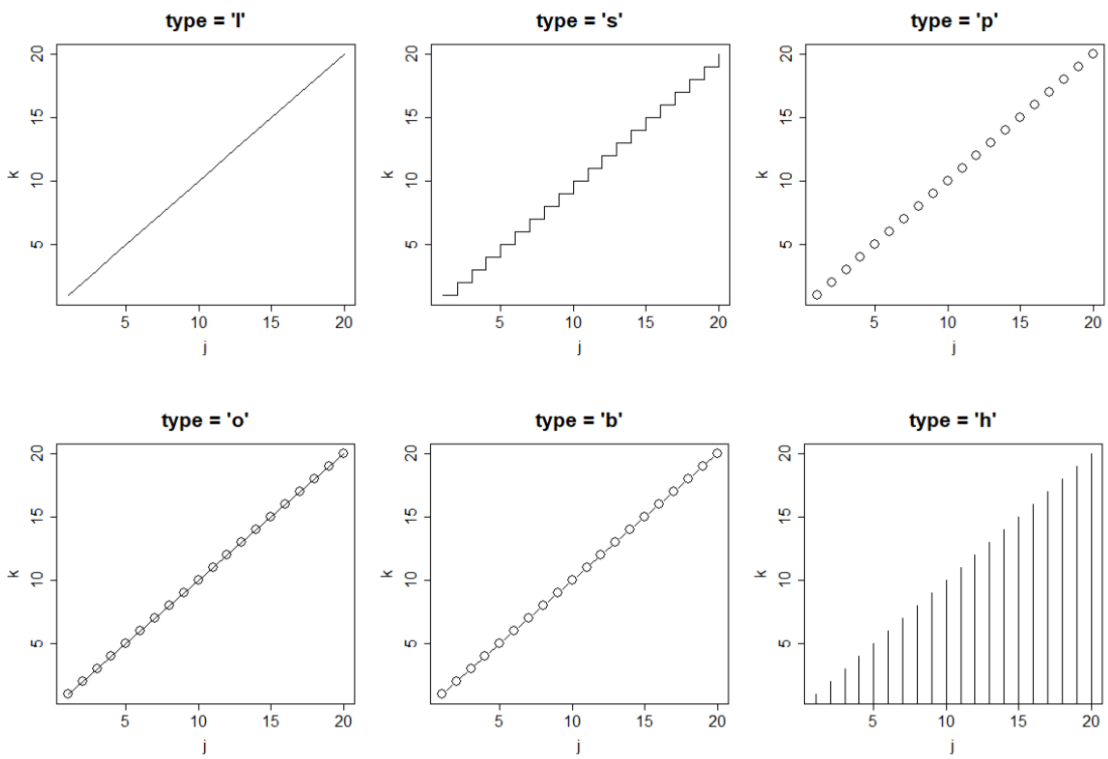
```
plot(X,Y) # scatter/line plot of Y-X
plot(FUNC_OBJ, from = , to = ) # function plot ranging in c(from, to)
plot(FACTOR) # barplot of factors
plot(FACTOR, Y) # boxplot of numeric v.s. levels of factor
plot(DATA.FRAME) # correlation plot
```

```
plot(ANY_PLOTTABLE_OBJ) # plot any plottable object
```

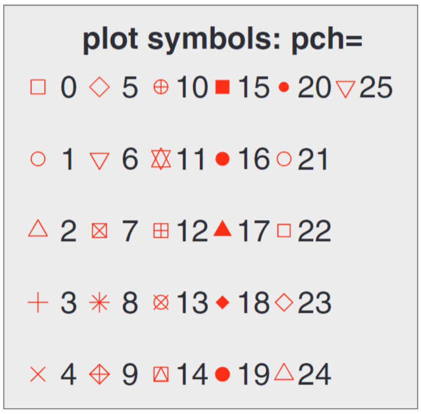
- Plot saving: first open a plotting device, then make plot and close the device

```
pdf("PLOT_FILE_NAME.pdf", FIG_HEIGHT, FIG_WIDTH)
plot(PLOT_PARAM)
dev.off()
```

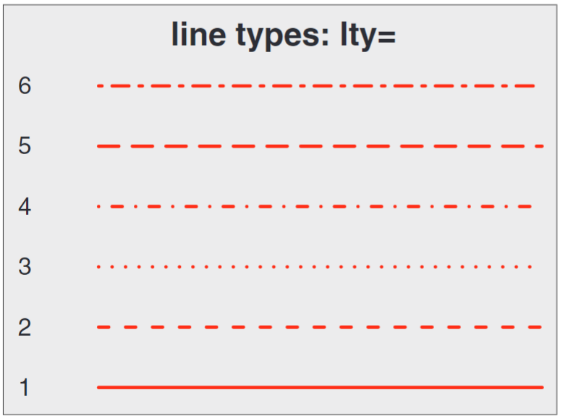
- `plot()` plotting parameters:
  - `main =` string for title; or use `title('TITLE')` as the next command
  - `sub =` string for subtitle;
  - `xlab =` , `ylab =` string axis labels;
  - adding LaTeXexpression as text: use `main = expression(PLOTMATH_EXPRESSION)`, use `?plotmath` to look for possible symbols
  - `xlim =` , `ylim =` axis range, e.g. use `xlim = c(0,100)`
  - `type =` value taken in `c('p', 'l', 'b', 'o', 's', 'h')` for plot **type**



  - `pch =` **point ch** aracter, value taken in `0:25` for defulat point charaters listed below, or use (vector of) charater to specify, e.g. `pch = c(' ')`



– `lty =` **l**ine **ty**pe, value taken in `1:6` (0 for not shown)



– `cex =` **c**haracter **ex**pansion, relative size with 1 as baseline and default.

Some derivative function to control size of other plotting elements:

∗ `cex.axis =` relative size of axis node text
∗ `cex.lab =` relative size of labels
∗ `cex.main =` relative size of title
∗ `cex.sub =` relative size of subtitle

– `lwd =` **l**ine **wid**th, relative width of line with 1 as baseline and default

– `col =` **col**or of elements in plot, value examples for color white:

∗ Index: `col = 1` predefined color in `R`.
∗ Color name: `col = 'white'`, use `colors()` to see all available color names
∗ Hexadecimal code: `col = '#FFFFFF'`
∗ RGB code: `col = rgb(1,1,1)`, `col = rgb(255,255,255, maxColorValue = 255)`
∗ HSV code: `col = hsv(0,0,1)`

`col =` can accept vector for various colors, or acccept some function for continuous colors:

∗ Discrete color: `col = c('red','blue')`, or use `col = df$GROUP` to color different groups
∗ Continuous color function: `rainbow(NUM_OF_COLORS)`, `heat_colors()`, `terrain.colors()`, `topo.colors()`, `cm.colors()`

Some derivative function to control color of other plotting elements:

    * `col.axis =` color of axis node text
    * `col.lab =` color of labels
    * `col.main =` color of title
    * `col.sub =` color of subtitle
    * `bg =` color of background

  - `font =` **font** used in plot, with 1 = plain, 2 = bold, 3 = italic, 4 = bold italic

    Some derivative function to control font of other plotting elements:

    * `font.axis =` font of axis node text
    * `font.lab =` font of labels
    * `font.main =` font of title
    * `font.sub =` font of subtitle
    * `ps =` baseline font **p**oint **s**ize, i.e. text size = `ps*cex`
    * `family =` extra text type, value taken in `c('serif', 'sans', 'mono')`m etc. use `names(pdfFonts())` to see possible font families

  - `bty =` **b**ox **ty**pe of the box surrounding the figure. Value taken in `c('o', '7', 'L', 'U', 'C', 'n')`

- `axis()` parameters for axis settings: after using `xaxt = 'n'` or `yaxt = 'n'` to remove correponding axis when executing `plot()`, other variation of axis could be made by using `axis()`
  - `axis(1)` for creating x aixs, `axis(2)` for creating y aixs. Here we would use x axis in the following parts.
  - `aixs(1, at = )` to specify ticks.
  - `plot(las = )` to specify rotation of ticks, value taken in `c('Parallel', 'Horizontal', 'Perpendicular', 'Vertical')`
  - `plot(xlim = c( , ), ylim = c( , ))` for axis limits
  - `plot(log = )` for log transfrom on axis, value taken in `c('x', 'y', 'xy')`.

- `legend()` parameters:
  - `x =` position of legend, value taken in `c("top", "bottom", "topleft", "topright", "bottomleft", "bottomright")`
  - `inset =`
  - other parameters are set following the setting in `plot`. An example:

```
legend("bottomright", legend = c("red", "green"), lty = c(2,4),
   lwd = 3, col = c("red", "green"))
```

- `text(X_COOR, Y_COOR, labels = TEXT)` parameters for adding text in figure. An application is `text(df$X, df$Y, labels = df$Z)` to label each point.
  - `pos =` **pos**ition of text around the coordinate point, value taken in `c(1,2,3,4)`

- `lines()` to put an extra line on existing figure (device). Parameters are similarly set as `plot()`

- `par()` to set global **par**ameters. An example to put 3 different figure in the same device:

```r
opar <- par(no.readonly = TRUE) # copy original setting
par(mfrow = c(1,3))
plot()
plot()
plot()
par(opar)
```

☐ **More Charts**

- `barplot(counts, horiz, besides, ...)` for bar plot. Data should be first prepared by `counts <-table(Y_TO_COUNT)`.
- `hist(x, breaks, freq, ...)` for histogram.
- `plot(density(df, kernel = ), ...)` for density plot.
- `boxplot(x, ...)` for box plot. use `boxplot(x ~GROUP, data = , ...)` to plot grouped boxplot
- `dotchart(x, labels, groups, ...)` to compare x value for categories

5.3.2 R::ggplot2 Plotting

`ggplot2`: **G**rammar of **G**raphics **plot** (2nd edi). It provides a convenient way to produce fancy plots. Reference see https://ggplot2.tidyverse.org/reference/

Basic steps for `ggplot2`:

1. Specify data and arsthetic mapping
2. Adding 'layers' with `geom_`
3. Adding labels

An example:

```r
ggplot(data=mtcars, aes(x=wt, y=mpg)) +
    geom_point(pch=17, color="blue", size=2) +
    geom_smooth(method="lm", color="red", linetype=2) +
    labs(title="Automobile Data", x="Weight", y="Miles Per Gallon")
```

Elements in `ggplot2`:

- `aes()` to specify **aes**thetic mapping, e.g. `aes(x = , y = , col = , ...)`. Used in `ggplot()` as global setting, in `geom_()` as local override (different `geom_()` may need different local settings). Examples:

```r
aes(x = mpg ^ 2, y = wt / cyl, col = am)
#> Aesthetic mapping:
#> * x -> mpg^2
#> * y -> wt/cyl
```

```
#> * color -> am
```

- `geom_` layer to specify statistical figure you want. Some useful plot:

`geom_()` Function	Charts	Options
`geom_bar()`	bar plot	`color, fill, alpha`
`geom_boxplot()`	box plot	`color, fill, alpha, notch, width`
`geom_density`	density plot	`color, fill, alpha, linetype`
`geom_histogram()`	histogram	`color, fill, alpha, linetype, binwidth`
`geom_hline()`	horizontal line	`color, alpha, linetype, size`
`geom_vline()`	vertical line	`color, alpha, linetype, size`
`geom_line()`	line gragh	`color, alpha, linetypem size`
`geom_point()`	scatter plot	`color, alpha, shape, size`
`geom_smooth()`	fitted line	`method, formula, color, fill, linetype, size`
`geom_violin()`	violin plot	`color, fill, alpha, linetype`
`geom_text()`	text annotation	see functon help

- `labs(title, x, y)` to specify labels and title
- `facet_grid()` and `facet_wrap()` to plot multiple plot, with factor levels as categories, parameters:
  - `facets =` facet variable. For `facet_wrap()` use `~VAR1` (one variable); `facet_grid()` use `.~VAR1` or `VAR1~.` or `VAR1~VAR2` (allow two variable)
  - `nrow = , ncol =` grid shape
  - `shrink =` whether adjust ticks, set `TRUE` or `FALSE`
  - `drop =` whether drop levels with censored data, set `TRUE` or `FALSE`
- `theme()` to set fonts, backgrouds, gridlines, etc.

  There are some pre-defined theme: `theme_grey()`, `theme_bw()`, `theme_linedraw()`, `theme_light()`, `theme_dark()`, `theme_minimal()`, `theme_classic()`, `theme_void()`, `theme_test()`.

  Detailed elements in a plot is adjust by passing `element_()`:
  - `element_line()` set some line element
  - `element_rect()` set some rectangular element
  - `element_text()` set some text element

  Some useful command:
  - `plot.title = element_text(hjust = 0.5)` adjust position of title to mid. Other similar parameters: `plot.background, plot.title.position, plot.subtitle, plot.caption, plot.caption.position, plot.tag, plot.tag.position, plot.margin`

  - `panel.background = element_rect(fill = 'white', color = 'blue')` adjust figure background and border. Other similar parameters: `panel.grid.major/minor.x/y`
  - `aspect.ratio =` height:width
  - `legend.position = 'none'` to remove automatic legend

- `ggsave('FILE_NAME', PLOT, WID, HEI)`, or use `ggsave('FILE_NAME')` to save the active device.

Chapter. VI 统计计算与软件部分

Instructor: Zaiying Zhou

Section 6.1 Algorithm Theory Introduction

6.1.1 Finite Precision Computation

An arbitrary real number $r \in \mathbb{R}$ is represented as (the nearest adjacent) float number v_r. A float is basically stored as (example take 32-bit float): 1 bit **S**ign + 8 bit **E**xponent + 23 bit **M**antissa.

$$v = (-1)^S \times 2^{E-127} \times \left(1 + \sum_{i=1}^{23}(M_i \times 2^{-i})\right) \tag{6.1}$$

Further, extreme value of (M, E) is used for some 'special value': denormalized number, NaN, inf, etc.

- Denormalized number: to fill the gap $[0, \pm 2^{-126}](E = 1)$, for $E = 0$ extremely small number, definition use

$$v_{\text{denormalized}} = (-1)^S \times 2^{1-127} \times \left(0 + \sum_{i=1}^{23}(M_i \times 2^{-i})\right) \tag{6.2}$$

  i.e. for $E = 0$, range $[2^{-127}, 2^{-126})_{\text{nor}} \to [0, 2^{-126})_{\text{denor}}$.

- NaN: $(E = 255, M \neq 0)$
- inf: $(E = 255, M = 0)$

	$E = 0$	$0 < E < E_{\max}$	$E = E_{\max}$
$M = 0$	± 0	$v_{\text{normalized}}$	$\pm\infty$
$M \neq 0$	$v_{\text{denormalized}}$		NaN

表 3: Normalized Number

Use v_r to represent r: approximation $r \sim v_r$, the round-off error of r:

- Absolute rounding error:

$$\varepsilon = |r - v_r| \tag{6.3}$$

- Relative rounding error:

$$\varepsilon_{\text{machine}} = \frac{|r - v_r|}{|r|} = \text{const} \tag{6.4}$$

Note that for large $|r|$, the adjacency between floats $|r - v_r| = |r|\varepsilon_{\text{machine}}$ might be large, even cause some integer missing.

☐ **Representation and arithmetic of floating-point number follows IEEE-754 standard**

- For 32-bit float (single precision float): 1 bit **S**ign + 8 bit **E**xponent + 23 bit **M**antissa. $\varepsilon_{\text{machine}} = 0.5 \times 2^{-23} = 2^{-24}$

$$v = (-1)^S \times 2^{E-127} \times \left(1 + \sum_{i=1}^{23}(M_i \times 2^{-i})\right) \in [-3.4 \times 10^{38}, 3.4 \times 10^{38}] \tag{6.5}$$

- For 64-bit float (double precision float): 1 bit **S**ign + 11 bit **E**xponent + 52 bit **M**antissa. $\varepsilon_{\text{machine}} = 0.5 \times 2^{-52} = 2^{-53}$

$$v = (-1)^S \times 2^{E-1023} \times \left(1 + \sum_{i=1}^{52} (M_i \times 2^{-i})\right) \in [-1.79 \times 10^{308}, 1.79 \times 10^{308}] \tag{6.6}$$

Key point for algorithm design: aviod plus/minus of numbers of significantly large magnitude difference.

6.1.2 Stability & Accuracy

- Forward/Backward Error:

  For a algorithm design $\tilde{f}$ of a problem f, with input x. Denote:

  – Expected output: $y \equiv f(x)$
  – Algorithm output: $\tilde{y} \equiv \tilde{f}(x)$
  – Forward Error: $\Delta_F = \tilde{f}(x) - f(x)$
  – Backward Error: $\Delta_B = \underset{f(\tilde{x})=\tilde{f}(x)}{\arg\min} |\tilde{x} - x|$

- (Forward) Stability: An algorithm $\tilde{f}$ is stable if

$$\frac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(\tilde{x})\|} = O(\varepsilon_{\text{machine}}), \forall \frac{\|\tilde{x} - x\|}{\|x\|} = O(\varepsilon_{\text{machine}}) \tag{6.7}$$

- Condition Number of problem f:

  – Absolute condition number:

$$\hat{\kappa}(x) = \lim_{\varepsilon \to 0} \sup_{\|\delta x\| < \varepsilon} \frac{\|\delta f(x)\|}{\|\delta x\|} = \left\| \frac{\partial f}{\partial x} \right\| \tag{6.8}$$

  – Relative condition number:

$$\kappa(x) = \lim_{\varepsilon \to 0} \sup_{\|\delta x\| < \varepsilon} \frac{\|\delta f\| / \|f\|}{\|\delta x\| / \|x\|} \tag{6.9}$$

  Condition Number of Matrix $\underset{m\times m}{A}$:

  – $f(x) \equiv Ax$:

$$\kappa = \|A\| \frac{\|x\|}{\|Ax\|} \leq \|A\| \|A^{-1}\| \tag{6.10}$$

  – $f(b) \equiv$ solving $Ax = b$

$$\kappa = \|A^{-1}\| \frac{\|b\|}{\|x\|} \leq \|A^{-1}\| \|A\| \tag{6.11}$$

  Thus for matrix A, denote

$$\kappa(A) \equiv \|A\| \|A^{-1}\| \tag{6.12}$$

  – For ℓ_2 norm $\|\cdot\|_2$: $\kappa(A) = \frac{\sigma_1}{\sigma_m}$[48]

[48] Knowledge about matrix norm see section. 4.1.2

6.1.3 Iteration Algorithm

Iteration methods are used especially for problems without analytical solution, to obtain a numerical solution.

Iteration method: for problem f with solution x^* design an iteration function g: $X \to X$ so that

$$\lim_{n\to\infty} g^{\{n\}}(x) = \lim_{n\to\infty} \underbrace{g(g(g(\ldots g(g}_{n}(x))\ldots))) = x^* \tag{6.13}$$

then get solution by setting initial input value $x^{(0)}$ and calculate $x^{(t+1)} = g(x^{(t)})$ repeatedly until convergence as approximate solution.

☐ **Three Steps for Iteration:**

Algorithm *General Steps for Iteration*

---

1. Starting: set $x^{(0)}$, more trials to initial value is recommended
2. Updating: $x^{(t+1)} = g(x^{(t)})$, $\forall t = 0, 1, 2, \ldots$
3. Stopping: when to stop, can choose various stopping criterion, e.g.
   - Absolute convergence criterion

$$|x^{(t+1)} - x^{(t)}| < \varepsilon \tag{6.14}$$

   - Relative convergence criterion

$$\frac{|x^{(t+1)} - x^{(t)}|}{|x^{(t)}|} < \phi \tag{6.15}$$

   - Relative convergence criterion (2), avoid $x^{(t)} = 0$

$$\frac{|x^{(t+1)} - x^{(t)}|}{|x^{(t)}| + \xi} < \phi \tag{6.16}$$

☐ **Convergence Order and Convergence Rate**

For each iteration value $x^{(t)}$, define iteration error as $\varepsilon^{(t)} \equiv x^{(t)} - x^*$. Then an iteration method $\lim_{t\to\infty} \varepsilon^{(t)} = 0$ has convergence order α and convergence rate c as:

$$\lim_{t\to\infty} \frac{|\varepsilon^{(t+1)}|}{|\varepsilon^{(t)}|^\alpha} = c \tag{6.17}$$

A large α and small c declare a quick convergence.(Large α is needed more)

Comment: Actually convergence rate and order are generally dependent on specific problem, so we usually estimate α, c using some approximation/scaling to represent a generally case.

6.1.4 Constrained Optimize Theory

☐ **Primal Problem**

For optimize problem in convex set $\mathcal{X}$

$$\begin{aligned} \arg\min_{x\in\mathcal{X}} \quad & f(x) && \text{(P)} \\ s.t. \quad & g_i(x) \leq 0, \quad i = 1, 2, \ldots, k && (6.18) \\ & h_j(x) = 0, \quad j = 1, 2, \ldots, l && (6.19) \end{aligned}$$

which is called the **primal problem** for optimization.

The **generalized Lagrange function** for primal problem defined as

$$\begin{aligned} \mathcal{L}(x, \kappa, \lambda) \equiv & f(x) + \sum_{i=1}^{k} \kappa_i g_i(x) + \sum_{j=1}^{l} \lambda_j h_j(x) \\ w.r.t. \quad & \kappa_i \geq 0, \quad i = 1, 2, \ldots, k \end{aligned} \tag{6.20}$$

and we could further define a function of x:

$$\theta_P(x) \equiv \max_{\kappa,\lambda:\kappa_i\geq 0} \mathcal{L}(x, \kappa, \lambda) = \begin{cases} f(x) & \text{constraint } g,\ h \text{ satisfied} \\ +\infty & \text{contraint unsatisfied} \end{cases} \tag{6.21}$$

which means we can give the solution value of primal problem (P) simply by minimizing $\theta_P(x)$, minimum denoted p^*

$$p^* \equiv \min_x \theta_P(x) = \min_x \max_{\kappa,\lambda:\kappa_i\geq 0} \mathcal{L}(x, \kappa, \lambda) \tag{6.22}$$

☐ **Dual Problem**

Similar to primal problem, we can define a function of κ, λ:

$$\theta_D(\kappa, \lambda) \equiv \min_x \mathcal{L}(x, \kappa, \lambda) \tag{6.23}$$

and similarly get the **dual problem** of primal, value denoted d^*

$$d^* \equiv \max_{\kappa,\lambda:\kappa\geq 0} \theta_D(\kappa, \lambda) = \max_{\kappa,\lambda:\kappa\geq 0} \min_x \mathcal{L}(x, \kappa, \lambda) \tag{6.24}$$

it is obvious that

$$d^* = \max_{\kappa,\lambda:\kappa\geq 0} \min_x \mathcal{L}(x, \kappa, \lambda) \leq \min_x \max_{\kappa,\lambda:\kappa_i\geq 0} \mathcal{L}(x, \kappa, \lambda) = p^* \tag{6.25}$$

☐ **Karush-Kuhn-Tucker Condition (KKT Condition)**

KKT condition to allow $d^* = p^*$ at $(x^*, \kappa^*, \lambda^*)$: in the case that

- $f(x)$ and $g_i(x)$ are convex
- $h_j(x)$ in the form of affine function $A_j x + b$
- $g_i(x)$ are feasible constraints

then KKT $\Leftrightarrow$ $p^* = d^* = \mathcal{L}(x^*, \kappa^*, \lambda^*)$.

the KKT conditions are:

$$\begin{aligned}
&\nabla_x \mathcal{L}(x^*, \kappa^*, \lambda^*) = 0 \\
&\kappa_i^* g_i(x^*) = 0 && i = 1, 2, \ldots, k \\
&g_i(x^*) \leq 0 && i = 1, 2, \ldots, k \\
&\kappa_i \geq 0 && i = 1, 2, \ldots, k \\
&\lambda_j(x^*) = 0 && j = 1, 2, \ldots, l
\end{aligned} \tag{6.26}$$

Section 6.2 Algebratic Problem in Statistics

Considering the data structure and algorithm implement, many fundamental problems in statistics are basically algebratic problem, e.g.

- Matrix multiplication:

$$y = Ax, \text{ solve } y \tag{6.27}$$

- Linear equation solution:

$$b = Ax = \sum_{i=1}^{n} x_i a_i, \text{ solve } x \tag{6.28}$$

- OLS solution:

$$\hat{\beta} = (X'X)^{-1}XY \tag{6.29}$$

Generally speaking matrix A can be constructed in an arbitrary form, so an algorithm implementation needs **matrix composition** so that we have a better form to handle.

6.2.1 Matrix Operation

- Inverse Matrix: Inverse matrix of $A = [a_1, \ldots, a_m]$ satisfies

$$A^{-1}A = AA^{-1} = I \tag{6.30}$$

  then $Ax = b \Leftrightarrow x = A^{-1}b$

  Or generally speaking, solve inverse matrix $A^{-1} = [\alpha_1, \ldots, \alpha_m]$ is solving linear equations

$$A\alpha_i = e_i \tag{6.31}$$

  In the view of column space transfrom, A and A^{-1} are mappings between space span$\{e_1, \ldots, e_m\}$ and span$\{a_1, \ldots, a_m\}$, i.e.

$$\text{span}\{e_1, \ldots, e_m\} \underset{A^{-1}b}{\overset{Ax}{\rightleftharpoons}} \text{span}\{a_1, \ldots, a_m\} \tag{6.32}$$

- Unitary Matrix: Furthur for unitary A, denoted as Q with $QQ^* = I$, is an orthonormal transformation.

  - $|Q| = 1$ for rotation, $|Q| = -1$ for reflection.
  - $\lambda_Q = \pm 1$
  - Geometric structure preserved, e.g. inner product and norm.

- Projection:
  - Basic definition of projector P_X: idempotent matrix, project onto hyperplane X

$$P_X^2 = P_X \tag{6.33}$$

  - Complementary projector $I - P_X$: onto the complementary space of X

$$(I - P)^2 = I - P \tag{6.34}$$

  - Orthogonal Projection: Projector such that $Pv \perp (I - P)v$. Thm.: $Pv \perp (I - P)v \Leftrightarrow P^* = P$

    Derivation: Projection of vector v on hyperplane X satisties (denoted as Xp)

$$0 = \langle Xp, Xp - v\rangle = p^* X^*(Xp - v) \Rightarrow p = (X^* X)^{-1} X v \Rightarrow Xp = X(X^* X)^{-1} X v = P_X v \tag{6.35}$$

    More Properties of orthogonal projector see section. 3.3.2.

  - Orthogonal projector onto vector q:

$$P_q = q(q^* q)^{-1} q^* = \frac{qq^*}{\|q\|_2^2} \tag{6.36}$$

6.2.2 Projection and Least Square Problem

Recall: Linear model $Y = X\beta + \varepsilon$, basically solving linear equation $Y = X\beta$, however generally $Y \notin \text{span}(X)$, then we use OLS method to reach an estimation of β :

$$\hat{\beta} = \arg\min_{\beta} \|Y - X\beta\|^2 \tag{6.37}$$

where for $\|\cdot\| = \ell_2$-norm, $X\hat{\beta}$ is the projection of $X\beta$ onto hyperplane X:

$$X\hat{\beta} = X(X^* X)^{-1} X^* Y \equiv HY = P_X Y \tag{6.38}$$

For non-full rank $A = X^* X$: use pseudoinverse $A^+ = (A^* A)^{-1} A^*$

☐ **Task of OLS: Solve $\hat{\beta} = (X^* X)^{-1} X^* Y$, or equivalently solve $X^* X\hat{\beta} = X^* Y$**

- Cholesky decomposition algorithm: computation complexity $\sim mn^2 + \dfrac{n^3}{3}$
  1. Use Cholesky decomposition for $X^* X$:

$$A^* A = R^* R \Rightarrow R^* R\hat{\beta} = X^* Y \tag{6.39}$$

  2. Solve $\xi = \arg\{R^* \xi = X^* Y\}$:

$$R^* R\hat{\beta} = X^* Y = R^* \xi \Rightarrow R\hat{\beta} = \xi \tag{6.40}$$

3. Solve $R\hat{\beta} = \xi$ to get $\hat{\beta}$

- QR decomposition algorithm: computation complexity $\sim 2mn^2 - \dfrac{2}{3}n^3$
  1. Use e.g. Householder Reflection algorithm to compute $X = QR$
  2. use the orthonormal property of Q:

$$X^*X\hat{\beta} = X^*Y \Rightarrow R^*Q^*QR\hat{\beta} = R^*R\hat{\beta} = R^*Q^*Y \Rightarrow R\hat{\beta} = Q^*Y \tag{6.41}$$

  3. Solve $R\hat{\beta} = Q^*Y$ to get $\hat{\beta}$

- SVD algorithm: computation complexity $\sim 2mn^2 + 11n^3$
  1. Compute SVD of X: $X = U\Sigma V^*$

$$X^*X\hat{\beta} = X^*Y \Rightarrow V\Sigma^2V^*\hat{\beta} = V\Sigma U^*Y \Rightarrow \Sigma V^*\hat{\beta} = U^*Y \tag{6.42}$$

  2. Solve $\hat{\beta} = V\Sigma^{-1}U^*Y$ to get $\hat{\beta}$

Algorithm comparison: faster $\leftrightsquigarrow$ less stable.

6.2.3 Gaussian LU Decomposition & Cholesky Decomposition

□ Gaussian Elimination Algorithm

Gaussian Elimination decomposes matrix A as lower triangular matrix $\times$ upper triangular matrix

$$\underset{m\times m}{A} = \underset{m\times m}{L}\,\underset{m\times m}{U} = \begin{bmatrix} * & & & \\ * & * & & \\ \vdots & \vdots & \ddots & \\ * & * & \dots & * \end{bmatrix} \begin{bmatrix} * & * & \dots & * \\ & * & \dots & * \\ & & \ddots & \vdots \\ & & & * \end{bmatrix} \tag{6.43}$$

Conducted by continuously row transformation of A:

$$L_{m-1}\dots L_2L_1A = L^{-1}A = U \tag{6.44}$$

where each L_i corresponds to a gauss elimination operation such that $[L_i(L_{i-1}\dots L_2L_1A)]_{i+1:m,i} = 0$, with $[L_i(L_{i-1}\dots L_2L_1A)]_{1:i,:}$ fixed. L_i has the form as

$$L_i = I - l_ie_i^*, \qquad l_i = [0,\dots,l_{i+1,i},\dots,l_{m,i}]^T \quad l_{j,i} = A_{ji}/A_{ii} \tag{6.45}$$

Then we have $L = L_1^{-1}L_2^{-1}\dots L_{m-1}^{-1}U$, with $U = L_{m-1}\dots L_2L_1A$

If some pivot element $(L_{i-1}\dots L_1A)_{ii} = 0$, use a row transformation P_i such that $(P_iL_{i-1}\dots L_1A)_{ii} \neq 0$, thus LU decomposition is expanded as

$$L_{m-1}P_{m-1}\dots L_2P_2L_1P_1A = U \tag{6.46}$$

Good properties of $L_i = I - l_ie_i^*$: enable a quick algorithm implement of LU decomposition:

- Inverse of L_i:

$$L_i^{-1} = (I - l_ie_i^*)^{-1} = I + l_ie_i^* \tag{6.47}$$

- Multiplication of L_i^{-1}:

$$L_i^{-1}L_{i+1}^{-1} = (I + l_i e_i^*)(I + l_{i+1}e_{i+1}^*) = I + l_i e_i^* + l_{i+1}e_{i+1}^* \tag{6.48}$$

- Interchangeability of P_i and L_j :

$$L_{m-1}P_{m-1}\dots L_2P_2L_1P_1 = (\tilde{L}_{m-1}\dots\tilde{L}_2\tilde{L}_1)(P_{m-1}\dots P_2P_1), \qquad \tilde{L}_i = P_{m-1}\dots P_{i+1}L_iP_{i+1}^{-1}\dots P_{m-1}^{-1} \tag{6.49}$$

where note that P_k only exchange row/column k and $\kappa > k$, thus $\tilde{L}_i$ is still left triangular.

Thus get expression of LU decomposition $PA = LU$:

$$PA = LU \quad \begin{cases} P = P_{m-1}\dots P_2P_1 \\ L = (\tilde{L}_{m-1}\dots\tilde{L}_2\tilde{L}_1)^{-1} \\ \tilde{L}_i = P_{m-1}\dots P_{i+1}L_iP_{i+1}\dots P_{m-1} \\ U = L_{m-1}P_m\dots L_2P_2L_1P_1A \end{cases} \tag{6.50}$$

Complexity of Gaussian Elimination:

$$\text{flops}_{\text{GE}} = \sum_{i=1}^{m-1}\sum_{k=i+1}^{m} 2(m-i+1) \sim \frac{2}{3}m^3 \tag{6.51}$$

□ **Cholesky Decomposition**

Hermitian positive-definite matrix A can LU decompose as

$$A = LU = R^*R \tag{6.52}$$

Algorithm: write A in partitioned matrix then conduct symmetric row/column transformation

$$A = \begin{bmatrix} 1 & w_1^* \\ w_1 & K \end{bmatrix} \tag{6.53}$$

$$= \begin{bmatrix} 1 & 0 \\ w_1 & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & K - w_1w_1^* \end{bmatrix} \begin{bmatrix} 1 & w_1^* \\ 0 & I \end{bmatrix} \tag{6.54}$$

$$= R_1^*K_1R_1 \tag{6.55}$$

Note that K_1 is still hermite positive-definite, we can repeat the above process

$$K_1 = \begin{bmatrix} 1 & 0 \\ 0 & K - w_1w_1^* \end{bmatrix} \tag{6.56}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & w_2 & I \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & K - w_1w_1^* - w_2w_2^* \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & w_2^* \\ 0 & 0 & I \end{bmatrix} \tag{6.57}$$

$$= R_2^*K_2R_2 \tag{6.58}$$

repeat untill $K_m = I$: $A = (R_m R_{m-1} \dots R_1)^* I (R_m R_{m-1} \dots R_1) = R^* R$

Complexity of Cholesky Decomposition:

$$\text{flops}_{\text{CD}} = \sum_{i=1}^{m} \sum_{k=i}^{m} 2(m-k+1)+1 \sim \frac{1}{3} m^3 \tag{6.59}$$

6.2.4 QR Decomposition: Gram-Schmidt/Householder/Givens Method

QR Decomposition: Orthogonal Triangularization of matrix A

$$\underset{m\times n}{A} = \underset{m\times n}{Q} \underset{n\times n}{R} \tag{6.60}$$

$$A = \begin{bmatrix} a_1 & \dots & a_n \end{bmatrix} = QR = \begin{bmatrix} q_1 & \dots & q_n \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & \dots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix} \tag{6.61}$$

Every $\underset{m\times n}{A} \in \mathbb{C}^{m\times n}$ $(m \geq n)$ has QR decomposition, specially:

- Full decomposition exists
- Reduced decomposition with $r_{ii} > 0$ is unique.

Here introduce 3 kinds of algorithm:

- Gram-Schmidt Orthogonalization: $\sim O(2mn^2)$, sequentially orthogonalizes the columns of A, traditional way
- ⋆ Householder Reflection: $\sim O(2mn^2 - \frac{2}{3}n^3)$, most commonly used, stable for ill & dense matrix
- Givens Rotation: $\sim O(3mn^2 - n^3)$, used for sparse matrix, e.g. Hessenberg matrix

☐ **(Classical) Gram-Schmidt Orthogonalization**

Key idea: project a_i onto $\text{span}\{q_1, \dots, q_{i-1}\}^\perp$ as q_i, with q_1 initialized as $\hat{a}_1$, projection coefficient r_{ij} forms R.

For each projection, the projector matrix is

$$P_i = I - \sum_{k=1}^{i-1} q_k q_k^* \tag{6.62}$$

expression of q_i and r_{ij}:

$$r_{ij} = \begin{cases} q_i^* a_j & i \neq j \\ \|a_i - \sum_{k=1}^{i-1} r_{ki} q_k\| & i = j \end{cases} \qquad q_i = \frac{a_i - \sum_{k=1}^{i-1} r_{ki} q_k}{r_{ii}} = \frac{a_i - \sum_{k=1}^{i-1} q_k q_k^* a_i}{\|a_i - \sum_{k=1}^{i-1} q_k q_k^* a_i\|} \tag{6.63}$$

Note: Algorithm implementation of q_i is $(q_{<i}) \to r_{k<i,i} \to q_i \& r_{ii} \to (q_{>i})$

☐ **Modified Gram-Schmidt Orthogonalization Algorithm**

In equation. 6.62, projection of G-S orthogonalization for each a_i is conducted 'simultaneously', while modified G-S decomposition is conducted step by step.

$$P_i = I - \sum_{k=1}^{i-1} q_k q_k^* = \prod_{k=1}^{i-1}(I - q_k q_k^*) \tag{6.64}$$

Decomsition result are the same, but modified algorithm is more stable for numerical computation, avoid problem of recursive q_i.

▷ R. **Code**

Algorithm of CGS/MGS

```
GS <- function(A,MGS=FALSE){
    stopifnot(is.matrix(A))
    m <- dim(A)[[1]]
    n <- dim(A)[[2]]
    v=matrix(0,nrow = m,ncol=m)
    r=matrix(0,nrow = m,ncol=n)
    q=matrix(0,nrow = m,ncol=m)
    for(j in 1:n){
        v[,j] <- A[,j]
        if(j>1){
        for(i in 1:(j-1)){
          r[i,j]=sum(q[,i]*ifelse(MGS,v[,j],A[,j]))#对MGS取v, CGS取a
          v[,j] <- v[,j]-r[i,j]*q[,i]
        }}
        r[j,j] <- sqrt(sum(v[,j]^2))
        q[,j] <- v[,j]/r[j,j]
    }
  return(list(q,r))
}
```

☐ **Householder Reflection**

Key idea: Reflect $A_{i:m,i}$ onto $e_1 \in \mathbb{C}^{m-i+1}$ as a vector of the same length $\|A_{i:m,i}\|e_1 \in \mathbb{C}^{m-i+1}$ (later we denote the l^{th} unit vector $e_l \in \mathbb{C}^{m-i+1} \equiv e_{m-i+1,l}$), reflector F_i in $\mathbb{C}^{(m-i+1)\times(m-i+1)}$ and auxiliary vector v_i:[49]

$$\mathbb{C}^{(m-i+1)\times(m-i+1)} \ni F_i = I_{m-i+1} - 2\frac{vv^*}{\|v\|_2^2} \qquad v = \operatorname{sgn}(A_{i,i})\|A_{i:m,i}\|e_{m-i+1,1} + A_{i:m,i} \tag{6.65}$$

where $\operatorname{sgn}(\cdot)$ corresponds to reflection onto $\hat{e}$ or $-\hat{e}$. Reflector on $A \in \mathbb{C}^{m\times n}$:

$$Q_i = \begin{bmatrix} I_{i-1} & 0 \\ 0 & F_i \end{bmatrix} \tag{6.66}$$

and QR calculated by (note that $F^2 = I_{m-i+1}$)

$$R = Q_n \dots Q_2 Q_1 A \qquad Q = Q_1 Q_2 \dots Q_n \tag{6.67}$$

[49] Here sgn() for reflecting toward $-e_1/e_1$.

Householder Reflection is more stable than Gram-Schmidt Orthogonalization

Error of Householder Reflection $A = \tilde{Q}\tilde{R} + E$, residual is controlled by $\|E\| \le \|A\| O(\varepsilon_{\text{machine}})$

Mainly caused by stability and accuracy of orthogonal matrix $\tilde{Q}$.

▷ `R.` **Code**

`R.` uses Householder Reflection to conduct QR decomposition.

```r
A.qr <- qr(A)
Q <- qr.Q(A.qr)
R <- qr.R(A.qr)
```

☐ **Givens Rotation**

Key idea: use rotation

$$Rx = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} = \begin{bmatrix} \sqrt{x_i^2 + x_j^2} \\ 0 \end{bmatrix} \Leftrightarrow \begin{cases} \cos\theta = \dfrac{x_i}{\sqrt{x_i^2 + x_j^2}} \\ \sin\theta = \dfrac{x_j}{\sqrt{x_i^2 + x_j^2}} \end{cases} \tag{6.68}$$

act on $A_{i-1:i,j:n}$ so that $A_{i,j} = 0$, each time use two rows to create 1 zero. Slow, used for special sparse matrix.

6.2.5 Eigenvalue Decomposition

For square matrix $A \in \mathbb{C}^{m\times m}$, its eigenvector is the vector x_i whose direction (subspace) is invariant under transform operator A.

$$Ax_i = \lambda_i x_i \tag{6.69}$$

Properties:

- Determinant and trace of A:

$$\det(A) = \prod_{i=1}^{m} \lambda_i \qquad tr(A) = \sum_{i=1}^{m} \lambda_i \tag{6.70}$$

- x_i for special kinds of A: if $\text{span}\{q_i\} = \mathbb{C}^m$, then (generally X is **not** orthogonal)

$$AX = X\Lambda \Rightarrow A = X\Lambda X^{-1} \tag{6.71}$$

Further for $AA^* = A^*A$ (Normal Matrix 规范矩阵. Include: hermitian $A = A^*$, skew hermitian $A = -A^*$, unitary $A^{-1} = A^*$, circulant matrix[50], and such $A + kI$), orthonormality of $x_i \to q_i$:

$$\langle q_i, q_j \rangle = \delta_{ij} \tag{6.73}$$

[50] Circulant Matrix, or similarly Latin Square.

$$C = \begin{bmatrix} c_0 & c_1 & c_2 & c_3 \\ c_3 & c_0 & c_1 & c_2 \\ c_2 & c_3 & c_0 & c_1 \\ c_1 & c_2 & c_3 & c_0 \end{bmatrix} \tag{6.72}$$

Eigenvalue Decomposition/Spectrum Decomposition, $X \to Q$:

$$AQ = Q\Lambda \Rightarrow A = Q\Lambda Q^{-1} = Q\Lambda Q^* \tag{6.74}$$

- Eigenvalue decomposition and positive definite matrix (Gershgorin circle thm.), λ_i falls in neighbourhood of a_{ii}:

$$D(\lambda_i, a_{ii}) < \sum_{j=1, j\neq i}^{m} |a_{ij}| \tag{6.75}$$

- Rayleigh quotient:

$$\max R(A, q) \equiv \max \frac{q^* A q}{q^* q} = \lambda_1 \tag{6.76}$$

Eigenvactor Algorithm: Power method to find leading eigen pair.

for independent eigenvectors x_i and an arbitrary vector $\xi = \sum_{i=1}^{m} c_i x_i$:

$$A^k \xi = A^k \sum_{i=1}^{m} c_i x_i = \sum_{i=1}^{m} c_i \lambda_i^k x_i = c_1 \lambda_1^k \left[x_1 + \sum_{i=2}^{n} \frac{c_i}{c_1} \left(\frac{\lambda_i}{\lambda_1} \right)^k x_i \right] \to c_1 \lambda_1^k x_1 \tag{6.77}$$

- pick a random q_0
- compute normalized $\dfrac{Aq_i}{\|Aq_i\|} = q_{i+1}$
- repeat until $\|q_{i-1} - q_{i-2}\| < \varepsilon_{\text{preset}}$
- q_i as the eigenvector, $q_i^T A q_i \approx q_i^T \lambda_1 q_i = \lambda_1$

This algorithm requires $|\lambda_1| > |\lambda_2| \geq \ldots$ for quick convergence.

6.2.6 SVD Decomposition

□ SVD (Singular Value Decomposition) Form:

- Reduced Form:

$$\underset{m\times n}{A} = \underset{m\times n}{U} \underset{n\times n}{\Sigma} \underset{n\times n}{V^*} \tag{6.78}$$

$$A = \begin{bmatrix} a_1 & \ldots & a_n \end{bmatrix} = U\Sigma V^* = \begin{bmatrix} u_1 & \ldots & u_n \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} \begin{bmatrix} v_1^* \\ v_2^* \\ \vdots \\ v_n^* \end{bmatrix} \tag{6.79}$$

- Full Form:

$$\underset{m\times n}{A} = \underset{m\times m}{U} \underset{m\times n}{\Sigma} \underset{n\times n}{V^*} \tag{6.80}$$

$$A = \begin{bmatrix} a_1 & \dots & a_n \end{bmatrix} = U\Sigma V^* = \begin{bmatrix} u_1 & u_2 & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \\ 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} v_1^* \\ v_2^* \\ \vdots \\ v_n^* \end{bmatrix} \tag{6.81}$$

Existence and uniqueness of SVD:

- Every $A \in \mathbb{C}^{m\times n}$ has SVD with $\{\sigma_i\}$ unique

$$A = U\Sigma V^* = \sum_{i=1}^{n} \sigma_i u_i v_i^* \tag{6.82}$$

- if A is squared, then U, V determined
- if $A \in \mathbb{R}^{m\times n}$, then $U, V \in \mathbb{R}$

☐ **SVD Expression**

U, V are eigenvectors of AA^*, A^*A respectively

$$A^*A = V\Sigma^2 V^* \qquad AA^* = U\Sigma^2 U^* \qquad u_j = \frac{Av_j}{\sigma_j} \quad \sigma_j = \sqrt{\lambda_{A^*A}} = \sqrt{\lambda_{AA^*}} \tag{6.83}$$

☐ **Properties of SVD:**

- rank of A: $r = \text{rk}(\underset{m\times n}{A}) = \#$ non-zero σ_i
- Space of A:
  - $\mathcal{R}(A) = \text{span}\{u_1, \dots, u_r\}$
  - $\mathcal{C}(A) = \text{span}\{v_1, \dots, v_r\}$
  - $\mathcal{N}(A) = \text{span}\{v_{r+1}, \dots, v_n\}$
- Norm:
  - Euclidean Norm: $\|A\|_2 = \sigma_1$
  - Frobenius Norm: $\|A\|_F = \sqrt{\sum_{i=1}^r \sigma_i^2}$
  - Nuclear Norm: $\|A\|_* = \sum_{i=1}^r \sigma_i$
- Square matrix:
  - if $A = A^*$, then $\sigma_j = |\lambda_A|_j$
  - $\det(A) = \prod_{i=1}^m \sigma_i$
- Low-rank Approximation of A using SVD:

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^* = A - \sum_{j=k+1}^{r} \sigma_j u_j v_j^* \tag{6.84}$$

is the 'nearest' rank k matrix from A

$$\min_{\text{rk}(\Xi)=k} \|A-\Xi\|_2 = \|A-A_k\|_2 = \sigma_{k+1} \tag{6.85}$$

☐ **When A is positive definite, SVD and ED get the same result.**

$$A = Q\Lambda Q^* \Rightarrow A = Q\text{sgn}(\Lambda)|\Lambda|Q^* = U\Sigma Q^* = U\Sigma V^* \tag{6.86}$$

6.2.7 Schur Decomposition

Unitary Triangularization of matrix A (always exists in $\mathbb{C}^{m\times m}$):

$$A = QTQ^*,\ Q \text{ unitary, } T \text{ upper-triangular} \tag{6.87}$$

for $A \in \mathbb{R}^{m\times m}$: T is quasi-triangular, diag of T is $Re(\lambda_i)$

Section 6.3 Numeric Optimization Algorithm I

Algorithm Optimization in Statistics: e.g.

- MLE Maximazation
- Linear/Logistics Regression: Minimizing error
- Clustering: minimizing within-cluster distance & maximizing between-cluster distance
- Box-Cox λ determining
- Machine Learning Model training, minimizing loss function

☐ **Duality of Optimization and Rooting:**

- Optimization: e.g. minimizing function $g(x)$:

$$\arg\min g(x) \leftrightharpoons \arg\{\nabla g(x) = 0\} \tag{6.88}$$

- Rooting: extract root $f(x) = 0$:

$$\arg\{f(x) = 0\} \leftrightharpoons \arg\min f(x)^T f(x) \tag{6.89}$$

More specific example: expand function to 2^{nd} as $g(x) \approx \frac{1}{2}x^T Ax - bx + c$ (differnetiation of quadric $x^T Ax$ see section. 4.1.2)

$$\arg\min \frac{1}{2}x^T Ax - bx + c \leftrightharpoons \arg\{\frac{A+A^T}{2}x = b\} \tag{6.90}$$

Δ i.e. for optmizing task $\arg\min g(x)$, we can either minimizing $g(x)$, or rooting $f(x) \equiv \nabla g(x)$

☐ **Algorithm Design Aim:**

- Robustness: can be applied on various problems

- Accuracy: reach solution with great precision, at the same time insensitive to machine error
- Efficiency: computer time/storage not required

□ Iteration in Optimization Problem

Usually iteration is used in optmizing problem, by approximate solution x^* step by step.

- Bracketing method means the solution x^* is always within some iteration interval $I^{(t)} = [x_{\text{left}}, x^*, x_{\text{right}}]$, use convergence condition $m(I^{(t)}) < \varepsilon$ to obtain solution.
- Open method: Not necessarily $x^* \in I^{(t)}$, but convergence using $d(x^{(t)}, x^{(t-1)}) < \varepsilon$. Usually faster than bracketing, but less stable, and sensitive to initial value.
- Hybird Method: Mixture of bracketing and open according to iteration step feature

□ Content

- Golden Section & Fibonacci Section Search: Bracketing method direct search for minimizer;
- Bisection Search: Bracketing method direct search for root
- Interpolation Method: Include either bracketing/open method, approximate function to obtain root/minimizer
  - Regula Falsi: Bracketing linear interpolation for rooting
  - Secant Interpolation: Open linear interpolation for rooting
  - Parabolic Interpolation: Open parabolic interpolation for minimizing
  - Inverse Parabolic Interpolation (IQI): Open interpoation for rooting
- Hybrid Method: Combination of bracketing method and open interpolation method for rooting. Include Dekker's and Brent's, most used method
  - Dekker's Method: Hybrid of bisection and secant interpolation method for rooting
  - ⋆ Brent's Method: Hybrid of bisection, secant interpolation and IQI for rooting
- Fixed Point Iteration Method: Open method for rooting, including univariate and multivariate linear case.
  - Univariate Fixed Point Iteration
  - Jacobi Method
  - Gauss Seidel Method
  - Successive Over-Relaxation Method
- ⋆ Nelder-Mead Method/Simplex Method: Open method for minimizer based on simplex iteration

□ Default Methods in `R`.

- `optim(VEC_OF_INI_VAR,FUN)`: Nelder-Mead Simplex search method, use `method=c('Nelder-Mead', 'BFGS','L-BFGS-B','CG','SANN','Brent')` to choose different methods
- `uniroot(FUN,INTERVAL)`: Brent's Method;
- `optimize(FUN,INTERVAL)`: Golden Section+Parabolic Interpolation.

6.3.1 Golden Section/Fibonacci Section Search

Problem: minimizing univariate function $g(x)$, within a pre-estimated interval $[x_1^{(0)}, x_4^{(0)}]$. For f that is undifferenetiable/complicated to compute, this method is often used.

Basic idea: within a unimodal interval $I^{(0)} = [x_1^{(0)}, x_4^{(0)}]$ of $f(x)$, pick two symmetric points $x_2^{(0)}, x_3^{(0)}$ in I_0 so that

$$x_2^{(0)} - x_1^{(1)} = x_4^{(0)} - x_3^{(0)} = (1 - r^{(0)})(x_4^{(0)} - x_1^{(0)}) \quad r^{(t)} > 1/2 \tag{6.91}$$

then extreme point should falls in one of $[x_1^{(t)}, x_3^{(t)}]$ or $[x_2^{(t)}, x_4^{(t)}]$, iteration the interval by comparing $g(x_2)$ and $g(x_3)$: use one of them as the next interval. And for less computation, we hope that one of $g(x_2^{(t)})$ of $g(x_3^{(t)})$ can be used in step $t+1$ as $g(x_3^{(t+1)})$ or $g(x_2^{(t+1)})$, i.e.

$$\text{if } g(x_2^{(t)}) > g(x_3^{(t)}) : [x_1^{(t+1)}, x_2^{(t+1)}, x_4^{(t+1)}] := [x_2^{(t)}, x_3^{(t)}, x_4^{(t)}] \tag{6.92}$$

$$\text{if } g(x_2^{(t)}) \le g(x_3^{(t)}) : [x_1^{(t+1)}, x_3^{(t+1)}, x_3^{(t+1)}] := [x_1^{(t)}, x_2^{(t)}, x_3^{(t)}] \tag{6.93}$$

also use equation. 6.91, we have (here use $g(x_2^{(t)}) > g(x_3^{(t)})$ case for derivation)

$$r^{(t+1)} = \frac{x_4^{(t)} - x_2^{(t)}}{x_4^{(t)} - x_1^{(t)}} = \frac{x_4^{(t+1)} - x_2^{(t+1)}}{x_4^{(t+1)} - x_1^{(t+1)}} = \frac{x_4^{(t)} - x_3^{(t)}}{x_4^{(t)} - x_2^{(t)}} = \frac{1 - r^{(t)}}{r^{(t)}} \tag{6.94}$$

Algorithm *Golden Section/Fibonacci Section Search*

1. Initialize $I^{(0)} = [x_1^{(0)}, x_4^{(0)}]$ with $x^* \in I^0$
2. For each step $x^{(t)}$:
   (a) Calculate $r^{(t)}$, and then $g(x_2^{(t)})$, $g(x_3^{(t)})$
   (b) compare $g(x_2^{(t)})$ and $g(x_3^{(t)})$, and update interval

$$\text{if } g(x_2^{(t)}) > g(x_3^{(t)}) : [x_1^{(t+1)}, x_2^{(t+1)}, x_4^{(t+1)}] \equiv [x_2^{(t)}, x_3^{(t)}, x_4^{(t)}] \tag{6.95}$$

$$\text{if } g(x_2^{(t)}) \le g(x_3^{(t)}) : [x_1^{(t+1)}, x_3^{(t+1)}, x_4^{(t+1)}] \equiv [x_1^{(t)}, x_2^{(t)}, x_3^{(t)}] \tag{6.96}$$

3. Repeat until convergence $m(I^{(t)}) < \varepsilon$

Choice of $r^{(t)}$: for algorithm robustness and avoid ill sequence, we will usually use some special $r^{(t)}$:

- Golden Section Search: use $r^{(t)} = r = \text{const}$, such r should satisfies

$$r = \frac{1-r}{r} \Rightarrow r = \frac{\sqrt{5}-1}{2} = \frac{1}{\phi} \approx 0.618 \tag{6.97}$$

  Convergence at

$$m(I^{(t)}) = r^t m(I^{(0)}) < \varepsilon \tag{6.98}$$

- Fibonacci Section Search: choose for $t=0$ as $r^{(0)}=\dfrac{F_{n-1}}{F_n}$, where $\{F_n\}$ is Fibonacci sequence, then

$$r^{(0)} =\frac{F_{n-1}}{F_n} \tag{6.99}$$
$$r^{(1)} =\frac{1-r^{(0)}}{r^{(0)}}=\frac{F_{n-2}}{F_{n-1}} \tag{6.100}$$
$$r^{(2)} =\frac{1-r^{(1)}}{r^{(1)}}=\frac{F_{n-3}}{F_{n-2}} \tag{6.101}$$
$$\vdots \tag{6.102}$$
$$r^{(t)} =\frac{F_{n-t-1}}{F_{n-t}} \tag{6.103}$$
$$\vdots \tag{6.104}$$
$$r^{(n-3)} =\frac{F_2}{F_3}=\frac{1}{2}\text{(the last step of iteration)} \tag{6.105}$$

To determine the preset n, first use convergence condition

$$m(I^{(n-2)})=\prod_{i=0}^{n-3}r^{(i)}m(I^{(0)})=\frac{F_2}{F_n}m(I^{(0)})<\varepsilon\Rightarrow\begin{cases}F_n>\dfrac{m(I^{(0)})}{\varepsilon}\\ F_{n-1}<\dfrac{m(I^{(0)})}{\varepsilon}\end{cases} \tag{6.106}$$

then conduct iteration, using $r^{(t)}=\dfrac{F_{n-t-1}}{F_{n-t}}$.

Basically the two methods have similar background, noticing that the eigen equation of Fibonacci sequence is $x^2=x+1$, and $\lim_{n\to\infty}\dfrac{F_{n-1}}{F_n}=\dfrac{\sqrt{5}-1}{2}=\dfrac{1}{\phi}$[51]

Can be proven: Golden section need one more iteration call than Fibonacci section:

$$n_{\text{GS}}=n_{\text{Fib}}+1 \tag{6.108}$$

Convergence order $\alpha=1$, rate $c=\dfrac{1}{\phi}$

6.3.2 Bisection Search Method

Problem: rooting univariate function $f(x)$, with a pre-estimated interval $I^{(0)}=[x_1^{(0)},x_2^{(0)}]$, with $f(x_1^{(0)})f(x_2^{(0)})<0$

Idea: Intermediate value thm.: for continuous $f:[a,b]\to\mathbb{R}$, $f(a)f(b)<0\Rightarrow\exists x^*, s.t. f(x^*)=0$.

Algorithm *Bisection Search*

---

1. Initialize $I^{(0)}=[x_1^{(0)},x_2^{(0)}]$ satisfying $f(x_1^{(0)})f(x_2^{(0)})<0$
2. In each iteration $x^{(t)}$:

[51] General Formula of Fibonacci sequence:

$$F_n=\frac{1}{\sqrt{5}}\left((\phi)^n-(-\frac{1}{\phi})^n\right) \tag{6.107}$$

(a) compute midpoint function value

$$x_m^{(t)} = \frac{1}{2}\left(x_1^{(t)} + x_2^{(t)}\right) \tag{6.109}$$

(b) update interval according sign of $f(x_m^{(t)})$:

$$I^{(t+1)} = [x_1^{(t+1)}, x_2^{(t+1)}] := \begin{cases} [x_1^{(t)}, x_m^{(t)}], & f(x_1^{(t)})f(x_m^{(t)}) < 0 \\ [x_m^{(t)}, x_2^{(t)}], & f(x_m^{(t)})f(x_2^{(t)}) < 0 \end{cases} \tag{6.110}$$

3. Repeat until convergence $m(I^{(t)}) < \varepsilon$

Convergence order $\alpha = 1$, rate $c = \frac{1}{2}$.

6.3.3 Interpolation Methods: Linear/Quadratic/Lagrange Interpolation

Interpolation is an approximation to function, thus can get approximation to solution. Interpolation can be used for both minimizing or root finding.

☐ **Regula Falsi/Linear Interpolation (Bracketing) for Root Finding:**

Idea of regula falsi linear interpolation: at root x^* of $f(x)$:

$$f(x) \approx \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x^*} (x - x^*) \tag{6.111}$$

Iterate by repeatedly constructing linear interpolation/secant and use the root as an approximation to x^*.

Algorithm *Regula Falsi Interpolation*

---

1. Initialize interval $I^{(0)} = [x_1^{(0)}, x_2^{(0)}]$ with $f(x_1^{(0)})f(x_2^{(0)}) < 0$
2. In each iteration $x^{(t)}$:

(a) Compute linear interpolation of $(x_1^{(t)}, f(x_1^{(t)})), (x_2^{(t)}, f(x_2^{(t)}))$, and compute the root of the straight line

$$x_r^{(t)} = \frac{x_1^{(t)} f(x_2^{(t)}) - x_2^{(t)} f(x_1^{(t)})}{f(x_2^{(t)}) - f(x_1^{(t)})} \tag{6.112}$$

compute $f(x_r^{(t)})$

(b) update interval according to sign of $f(x_r^{(t)})$:

$$I^{(t+1)} = [x_1^{(t+1)}, x_2^{(t+1)}] := \begin{cases} [x_1^{(t)}, x_r^{(t)}], & f(x_1^{(t)})f(x_r^{(t)}) < 0 \\ [x_r^{(t)}, x_2^{(t)}], & f(x_r^{(t)})f(x_2^{(t)}) < 0 \end{cases} \tag{6.113}$$

3. Repeat until convergence $m(I^{(t)}) < \varepsilon$

Note: for enough steps of iteration t_ξ, the iteration would be short enough such that $\mathrm{sgn}(f''(x)) = \mathrm{const}$, in which case one of $x_1^{(t)}$ or $x_2^{(t)}$ would remain fixed for $t > t_\xi$.[52]

[52] For $f''(x)f'(x) > 0$, x_2 fixed; $f''(x)f'(x) < 0$, x_1 fixed.

Convergence order $\alpha = 1$, rate $c = -\dfrac{f''(x^*)}{2f'(x^*)}(x^* - x_{\text{fixed}})$. Note that sign dependency of x_{fixed} on $f''(x)$ and $f'(x)$ ensures $c > 0$.

☐ **Secant Interpolation/Linear Interpolation (Open) for Root Finding**

Instead of limiting $x^* \in [x_1^{(t)}, x_2^{(t)}]$ (bracketing) by ensuring $f(x_1^{(t)})f(x_2^{(t)}) < 0$, we can also remove the restrict, i.e. just use the latest two points to construct secant.

Algorithm *Secant Interpolation*

---

1. Initialize two points $x^{(-1)}$, $x^{(0)}$.(interval not necessarily include potential root $\hat{x}^*$)
2. In each iteration $x^{(t)}$:
   (a) Compute linear interpolation of $(x^{(t-1)}, f(x^{(t-1)}))$, $(x^{(t)}, f(x^{(t)}))$
   (b) Use the root to update $x^{(t+1)}$:
$$x^{(t+1)} = \frac{x^{(t-1)}f(x^{(t)}) - x^{(t)}f(x^{(t-1)})}{f(x^{(t)}) - f(x^{(t-1)})} \tag{6.114}$$
3. Repeat until convergence, .e.g. $|x^{(t)} - x^{(t-1)}| < \varepsilon$

Comment: For interval small enough such that $\text{sgn}(f''(x)) = \text{const}$ and $f(x^{(t)})f(x^{(t-1)}) < 0$, this method might goes back to bracketing linear interpolation.

Convergence order $\alpha \approx 1.618$.

☐ **Parabolic Interpolation for Minimizing**

Idea of parabolic interpolation: at extreme point x^*, function f has taylor series

$$g(x) \approx g(x^*) + \frac{1}{2}\left.\frac{\mathrm{d}^2 g}{\mathrm{d}x^2}\right|_{x^*}(x - x^*)^2 \tag{6.115}$$

we can iteration by repeatedly construct parabola to approximate $f(x^*) + \frac{1}{2}\left.\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right|_{x^*}(x - x^*)^2$ and use the exterme point of the parabola.

Algorithm *Parabolic Interpolation*

---

1. First initialize three point $(x_1^{(0)}, x_2^{(0)}, x_3^{(0)})$,
2. In each iteration $x^{(t)}$:
   (a) Use $(x_1^{(t)}, x_2^{(t)}, x_3^{(t)})$ to compute corresponding $f(x)$, then use quadric fitting to obtain parabola $\Gamma^{(t)}$
   (b) Replace $\max\{x_1^{(t)}, x_2^{(t)}, x_3^{(t)}\}$ by extreme point of $\Gamma^{(t)}$ to update as $(x_1^{(t+1)}, x_2^{(t+1)}, x_3^{(t+1)})$
3. Repeat until convergence.

Convergence order $\alpha \approx 1.3247$.

☐ **Lagrange Polynomial Interpolation**

Lagrange Polynomial is a function base set: Given $n+1$ point $(x_0, y_0), \ldots, (x_n, y_n)$ $(n \geq 1)$, Lagrange polynomial:

$$\ell_i = \prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}, \quad i = 0, 1, \ldots, n \tag{6.116}$$

And Lagrange interpolation function: $L(x) = \sum_{i=0}^{n} y_i \ell_i$

$n = 1$ for linear interpolation, $n = 2$ for parabolic interpolation.

☐ **Inverse Parabolic Interpolation (IQI): Open interpoation for rooting**

Note that general parabola $y = \frac{1}{2}ax^2 + bx + c$ might have 0 or 2 root simultaneously, thus use inverse quadric function $x = \frac{1}{2}ay^2 + by + c$, i.e. inverse quadric interpolation.

Algorithm *Inverse Parabolic Interpolation*

---

1. First initialize three point $C^{(0)} = \left(x^{(-2)}, x^{(-1)}, x^{(0)}\right)$
2. In each iteration $x^{(t)}$:
   (a) Use $C^{(t)} = \left(x^{(t-2)}, x_2^{(t-1)}, x_3^{(t)}\right)$ to compute IQI function, and get root
   $$s = \sum_{\text{cycle } x^{(t-2)}, x^{(t-1)}, x^{(t)}} \frac{x^{(t-2)} f(x^{(t-1)}) f(x^{(t)})}{\left[f(x^{(t-2)}) - f(x^{(t-1)})\right]\left[f(x^{(t-2)}) - f(x^{(t)})\right]} \tag{6.117}$$
   (b) Update points
   $$C^{(t+1)} = \left(x^{(t-1)}, x^{(t)}, x^{(t+1)}\right) = \left(x^{(t-1)}, x^{(t)}, s\right) \tag{6.118}$$
3. Repeat until convergence $|x^{(t)} - x^{(t-1)}| < \varepsilon$

6.3.4 Hybrid Method: Dekker's/Brent's

☐ **Dekker's Method**

Dekker's method is a hybrid of open linear interpolation and bisection, in each step, use one of interpolation/bisection according to iteration condition to achieve both quick convergence and stability.

Algorithm *Dekker's Method*

---

1. Initialize three point $a^{(0)}$, $b^{(0)}$, $b^{(-1)} = a^{(0)}$, where interval bteween $a^{(0)}$, $b^{(0)}$ should include potential root $\hat{x}^*$, i.e. $f(a^{(0)})f(b^{(0)}) < 0$
2. In each iteration $x^{(t)}$:
   (a) $a^{(t)}$, $b^{(t)}$ is labelled as follows: label ensure $|f(a^{(t)})| \geq |f(b^{(t)})|$, thus $b^{(t)}$ is the estimate of root, while $a^{(t)}$ is the 'contrapoint' of $b^{(t)}$
   (b) compute root s of linear interpolation of $(a^{(t)}, f(a^{(t)}))$, $(b^{(t)}, f(b^{(t)}))$, and compare with midpoint $m = \dfrac{a^{(t)} + b^{(t)}}{2}$
   $$\tilde{b}^{(t+1)} = \begin{cases} s = \dfrac{a^{(t)} f(b^{(t)}) - b^{(t)} f(a^{(t)})}{f(b^{(t)}) - f(a^{(t)})}, & s \in [m, b^{(t)}] \text{ (or } [b^{(t)}, m]) \\ m = \dfrac{a^{(t)} + b^{(t)}}{2}, & s \notin [m, b^{(t)}] \text{ (or } [b^{(t)}, m]) \end{cases} \tag{6.119}$$
   (c) Then update $\tilde{a}^{(t+1)}$ as one of $a^{(t)}$ and $b^{(t)}$, such that $f(\tilde{a}^{(t+1)})f(\tilde{b}^{(t)}) < 0$, then relabel $\tilde{a}^{(t+1)}$, $\tilde{b}^{(t)}$ to $a^{(t+1)}$, $b^{(t+1)}$ according to $|f(a^{(t+1)})| > |f(b^{(t+1)})|$

3. Repeat until convergence $|b^{(t)} - b^{(t-1)}| < \varepsilon$

Comment: In step 3, the choice between bisection and open interpolation take advantage of quick convergence of open method, also ensure stability by using bisection for ill secant root s. However for interval small enough, this method might also goes back to bracketing linear interpolation, then $b^{(t)}$ convergence very slow.

☐ **Brent's Method**

Brent's Method is an improvement of Dekker's Method:

- Avoid convergence problem of $b^{(t)}$ in the case of bracketing linear interpolation by checking $|b^{(t)} - b^{(t-1)}| > \delta$ before linear interpolation, otherwise use bisection
- Further adding IQI interpolation if $a^{(t)}$, $b^{(t)}$, $b^{(t-1)}$ are distinct for quicker convergence, root for IQI:

$$s' = \sum_{\text{cycle } a^{(t)}, b^{(t)}, b^{(t-1)}} \frac{a^{(t)} f(b^{(t)}) f(b^{(t-1)})}{\left[f(a^{(t)}) - f(b^{(t)})\right]\left[f(a^{(t)}) - f(b^{(t-1)})\right]} \tag{6.120}$$

▷ `R.` **Code**

```
uniroot()
```

6.3.5 Fixed Point Iteration: Univariate

Idea: Contraction mapping thm.: for function $f : X \to X$ satisfying

$$d(f(x), f(y)) \leq \beta d(x, y),\ \beta < 1 \tag{6.121}$$

then such f has a unique fixed point x^* such that $f(x^*) = x^*$, and convergence is ensured:

$$d(f^{\{n\}}(x), x^*) \leq \frac{\beta^n}{1-\beta} d(f(x), x^*) \tag{6.122}$$

For univariate function, requires $|f'(x)| < 1$(at least at x near x^*)

To minimize $f(x)$, i.e. find root of $f'(x) = g(x)$, i.e. find fixed point of $G(x) \equiv \alpha f'(x) + x = x$, requires $|G'(x)| = |\alpha f''(x) + 1| < 1$.

Note: We can also use inverse function of $\alpha f'(x) + x$, and further use $G_1(x) = rG(x) + (1-r)x$ to find fixed point.

Iteration: use $\hat{x}^* = x^{(n)} = G^{\{n\}}(x) = \underbrace{G(G(G(\ldots G(G}_{n}(x))\ldots)))$, until $|x^{(n)} - x^{(n-1)}| < \varepsilon$

Basically, fixed point iteration is the same as parallel chord method: use the root of $y - g(x^{(t)}) = -\dfrac{1}{\alpha}(x - x^{(t)})$ as $x^{(t+1)}$.

Convergence order is α in $G(x) = \alpha f'(x)_x$

6.3.6 Fixed Point Iteration: Multivariate Linear

For solution of $Ax = b$ using fixed point iteration, where $AA^* = A^*A$(normal matrix), requires:

$$\rho(A) = \max |\lambda| < 1 \tag{6.123}$$

- Jacobi Method: Decompose $A = D + E$, where D is diagonal part

$$\underset{n\times n}{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} = D + E = \begin{bmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & 0 \end{bmatrix} \tag{6.124}$$

Then fixed point iteration: using $(D + E)x = b \Rightarrow x^{(t+1)} = D^{-1}(b - Ex^{(t)})$

$$x_i^{(t+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j\neq i} a_{ij} x_j^{(t)} \right) \tag{6.125}$$

- Gauss-Seidel Method: Decompose $A = L + U$

$$\underset{n\times n}{A} = L + U = \begin{bmatrix} a_{11} & 0 & \dots & 0 \\ a_{21} & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ 0 & 0 & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} \tag{6.126}$$

Then fixed point iteration: using $(L + U)x = b \Rightarrow Lx^{(t+1)} = (b - Ux^{(t)})$, iteration:

$$x_i^{(t+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(t+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(t)} \right) \tag{6.127}$$

- Successive Over-Relaxation Method (SOR Method): Decompose $A = D + L + U$

$$\underset{n\times n}{A} = D + L + U = \begin{bmatrix} a_{11} & 0 & \dots & 0 \\ 0 & a_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_{nn} \end{bmatrix} + \begin{bmatrix} 0 & 0 & \dots & 0 \\ a_{21} & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & 0 \end{bmatrix} + \begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ 0 & 0 & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} \tag{6.128}$$

Then fixed point iteration: using $\omega(D + L + U)x = \omega b \Rightarrow (D + \omega L)x = \omega b - [\omega U + (\omega - 1)D])x$, move non-diagonal elements to R.H.S.

$$x_i^{(t+1)} = (1-\omega)x_i^{(t)} + \frac{\omega}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(t+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(t)} \right), \qquad \omega \in (0, 2) \tag{6.129}$$

Comment: SOR iteration step is the ω weighted average of $x^{(t)}$ and Gauss-Seidel iteration.

6.3.7 Nelder-Mead Method

For multivariate function $g(x)$, with $x \in \mathbb{R}^n$, usually use Nelder-Mead Method, or Simplex Search Method. Simplex is a generalization of triangle/tetrahedron to any arbitrary dimension, and Nelder-Mead method is conducted by iterating simplex.

Algorithm *Nelder-Mead Method*

---

1. First initialize simplex $C^{(0)}$ by preset p_0 and $\vec{\lambda}$:

$$C^{(0)} = \{x_0^{(0)}, x_1^{(0)}, \dots, x_n^{(0)}\}, x_0^{(0)} = p_0,\ x_i^{(0)} = p_0 + \lambda_i \hat{e}_i \tag{6.130}$$

2. In each iteration $x^{(t)}$:

   (a) First sort $\{x_i^{(t)}\}$ according to $g(x_i^{(t)})$ as

$$g(x_{(0)}^{(t)}) \le g(x_{(1)}^{(t)}) \le \dots \le g(x_{(n)}^{(t)}) \tag{6.131}$$

   (b) Compute centroid of $\complement_{C^{(t)}}^{x_{(n)}^{(t)}} = \{x_{(0)}^{(t)}, x_{(1)}^{(t)}, \dots, x_{(n-1)}^{(t)}\}$

$$x_g^{(t)} = \frac{1}{n}\sum_{i=0}^{n-1} x_{(i)}^{(t)} \tag{6.132}$$

   And compute the reflection point of $x_{(n)}^{(t)}$:

$$x_r^{(t)} := x_g^{(t)} + (x_g^{(t)} - x_{(n)}^{(t)}) \tag{6.133}$$

   (c) Compute $g_{(0)}^{(t)} = g(x_{(0)}^{(t)})$, $g_{(n-1)}^{(t)} = g(x_{(n-1)}^{(t)})$, $g_{(n)}^{(t)} = g(x_{(n)}^{(t)})$, $g_r^{(t)} = g(x_r^{(t)})$ and compare:

   - $g_r^{(t)} < g_{(0)}^{(t)}$: reflection point $x_r^{(t)}$ is a good trial for minimizing, further try a farther point

$$x_{2r}^{(t)} := x_g^{(t)} + 2(x_g^{(t)} - x_{(n)}^{(t)}) \tag{6.134}$$

     then iteration according to $g_{2r}^{(t)}$:

$$C^{(t+1)} = \{x_0^{(t+1)}, x_1^{(t+1)}, \dots, x_n^{(t+1)}\} \equiv \begin{cases} \{x_{(0)}^{(t)}, x_{(1)}^{(t)}, \dots, x_{(n-1)}^{(t)}, x_{2r}^{(t)}\}, & g_{2r}^{(t)} < g_r^{(t)} \\ \{x_{(0)}^{(t)}, x_{(1)}^{(t)}, \dots, x_{(n-1)}^{(t)}, x_r^{(t)}\}, & g_{2r}^{(t)} \ge g_r^{(t)} \end{cases} \tag{6.135}$$

   - $g_{(0)}^{(t)} \le g_r < g_{(n-1)}^{(t)}$: better simplex but not necessarily the best, just use

$$C^{(t+1)} = \{x_0^{(t+1)}, x_1^{(t+1)}, \dots, x_n^{(t+1)}\} \equiv \{x_{(0)}^{(t)}, x_{(1)}^{(t)}, \dots, x_{(n-1)}^{(t)}, x_r^{(t)}\} \tag{6.136}$$

   - $g_{(n-1)}^{(t)} \le g_r^{(t)}$: $x_r^{(t)}$ might not optmize the simplex, conduct shrinkage:

$$x_s^{(t)} := \begin{cases} x_g^{(t)} + 0.5(x_g^{(t)} - x_{(n)}^{(t)}), & g_{(n-1)}^{(t)} \le g_r^{(t)} < g_{(n)}^{(t)} \\ x_g^{(t)} - 0.5(x_g^{(t)} - x_{(n)}^{(t)}), & g_{(n)}^{(t)} \le g_r^{(t)} \end{cases} \tag{6.137}$$

     if $g_s^{(t)} \le g_{(n)}^{(t)}$, suggesting a successful shrinkage, use $g_s^{(t)}$ for iteration

$$C^{(t+1)} = \{x_0^{(t+1)}, x_1^{(t+1)}, \dots, x_n^{(t+1)}\} \equiv \{x_{(0)}^{(t)}, x_{(1)}^{(t)}, \dots, x_{(n-1)}^{(t)}, x_s^{(t)}\},\ g_s^{(t)} \le g_{(n)}^{(t)} \tag{6.138}$$

     otherwise we have to update the whole simplex:

$$x_0^{(t+1)} = x_0^{(t)},\ x_i^{(t+1)} = x_0^{(t)} + \frac{1}{2}(x_i^{(t)} - x_0^{(t)}) \tag{6.139}$$

Section 6.4 Numeric Optimization Algorithm II

To minimize some arbitrary function $f(x)$, the idea of gradient iteration method is to update $x^{(t)}$ based on (minus) gradient $-\nabla f(x)$, with some modification on direction $p^{(t)} = T(-\nabla f(x))$ and step length $\alpha^{(t)}$

$$x^{(t+1)} = x^{(t)} + \alpha^{(t)} T\left(-\nabla f(x^{(t)})\right) = x^{(t)} + \alpha^{(t)} p^{(t)} \tag{6.140}$$

- Modifying Direction $p^{(t)}$:
  - Gradient Descent: $p^{(t)} = -\nabla f\left(x^{(t)}\right)$
  - Newton-Raphson Method: use Hessian matrix $p^{(t)} = -\left[H(x^{(t)})\right]^{-1} \nabla f\left(x^{(t)}\right)$
  - Fisher Scoring Method: for statistics problem, use fisher information $I\left(x^{(t)}\right) = -E_Y\left(H(x^{(t)})\right)$, $p^{(t)} = I\left(x^{(t)}\right)^{-1} \nabla f\left(x^{(t)}\right)$
  - Quasi-Newton Method: usually use secant condition to approximate Hessian $\hat{H}^{(t)} = M^{(t)}$ or $\hat{H^{-1}}^{(t)} = B^{(t)}$, with various updating SR-1/DFP/BFGS/L-BFGS/Broyden Class
  - Steepest Descent: general form based on various norm choice.
  - Stochastic Gradient Descent (SGD): modification for large sample
  - Conjugate Gradient Method: Use the 'perpendicular' property of conjugate vector for quick updating of p_k
- Modifying Step-Length $\alpha^{(t)}$:
  - Fixed step-length: $\alpha^{(t)} = \alpha$
  - Backtracking line search: $\alpha^{(t)} = \dfrac{\alpha}{2^{n(t)}}$
  - Exact line search: $\alpha^{(t)} = \arg\min_{\alpha} f\left(x^{(t)} + \alpha p^{(t)}\right)$
  - Trust Region Method: use Hessian matrix $H(x^{(t)})$, but restrict direction & step-length with trust region $\|\alpha^{(t)} p^{(t)}\| \leq \Delta^{(t)}$

6.4.1 Gradient Descent Method

The simplest choice for $T(\cdot)$ is identity $p^{(t)} = -\nabla f\left(x^{(t)}\right)$, because negative gradient direction is the (local) descent direction. Iteration:

$$x^{(t+1)} = x^{(t)} - \alpha^{(t)} \nabla f\left(x^{(t)}\right) \tag{6.141}$$

Note: for such gradient method, step-length should be carefully specified, use proper fixed step-length or backtracking/exact line search.

Convergence order $\alpha_{\text{conv}} = 1$.

6.4.2 Newton-Raphson Method

Idea: For minimizing problem $x^* = \arg\min f(x)$[53], using iteration method with an initial value $x^{(0)}$, we hope to find iteration step $x^{(t+1)} - x^{(t)}$ such that $x^{(t+1)}$ can approach x^* quickly. We can try to use the taylor series at $x^{(t)}$ to

[53] Here uses different notation from previous part to avoid confusion of $g(x)$ as link function.

$O(x^2)$ and try the minimizer of the quadric function:

$$f(x) \approx \tilde{f}_{x^{(t)}}(x) = f(x^{(t)}) + (x - x^{(t)})^T \nabla\, f(x)|_{x^{(t)}} + \frac{1}{2}(x - x^{(t)})^T \nabla\nabla\, f(x)|_{x^{(t)}}\, (x - x^{(t)}) \tag{6.142}$$

minimizer $\dfrac{\partial \tilde{f}(x)}{\partial x} = 0$:

$$\frac{\partial \tilde{f}}{\partial x} = \nabla\, \tilde{f}(x)\Big|_{x^{(t)}} + \nabla\nabla\, \tilde{f}(x)\Big|_{x^{(t)}} (x - x^{(t)}) = 0 \Rightarrow x^{(t+1)} - x^{(t)} = \left(\nabla\nabla \tilde{f}(x)\right)^{-1} \nabla \tilde{f}(x)\Big|_{x^{(t)}} \tag{6.143}$$

Use the above solution as the iteration step:

$$x^{(t+1)} = x^{(t)} - \left[H^{(t)}\right]^{-1} \nabla f(x^{(t)}) \tag{6.144}$$

where $H^{(t)}$ is the Hessian matrix $H^{(t)} \equiv \dfrac{\partial^2 f(x)}{\partial x \partial x^T}\Big|_{x^{(t)}}$

Convergence order $\alpha_{\text{conv}} = 2$.

☐ **Main difficulties of Newton-Raphson method:**

- Calculation of $H(f(x^{(t)}))^{-1}$, a task of second derivative + marix inverse.
- As an open method, Newton-Raphson method is unstable and sensitive to initial value: more initial trials suggested
- Positive/Negative Definition of Hessian $\dfrac{\partial f}{\partial x \partial x^T}$ is not guarenteed, while positive/negative definition would lead to local minimum/maximum respectively, i.e. descent not guarenteed.

6.4.3 Fisher's Scoring Method in MLE

For MLE optmizing problem in statistics using Newton-Raphson Method, we can use properties of log-likelihood $l(\theta; \vec{x})$ to help overcome the difficulty of calculating H^{-1}. This method is called Fisher's Scoring Method/Iteratively Re-weighted Least Squares (IRLS).

Notation: for simplication, the following part uses $\nabla f(x) := f'(x)$ (a vector), $\nabla\nabla f(x) := f''(x)$ (a matrix)

☐ **MLE Maxmizing ⇔ minus of MLE Minimizing**

MLE maximizing problem:

$$\theta^* = \arg\max l(\theta; \vec{x}) = \arg\max \ln \prod_{x_i} f(x_i; \theta) \tag{6.145}$$

Newton-Raphson iteration gives

$$\theta^{(t+1)} = \theta^{(t)} - l''(\theta^{(t)}; x)^{-1} l'(\theta^{(t)}; x) \tag{6.146}$$

Note that here $l'(\theta)$ is Score Function (equation. 2.50), and $l''(\theta)$ is relative to Fisher Information (equation. 2.52).[54]

[54] Detail see section. 2.2.3 & section. 2.2.4, page 27

- Score Function

$$S(\theta; \vec{x}) = \frac{\partial \ln f(\vec{x}; \theta)}{\partial \theta} = \frac{\partial l(\theta; \vec{x})}{\partial \theta} = \sum_{i=1}^{n} \frac{\partial \ln f(x_i; \theta)}{\partial \theta} \tag{6.147}$$

- Fisher Information

$$I(\theta) = \mathbb{E}\left[\frac{\partial \ln f(\vec{x}; \theta)}{\partial \theta} \frac{\partial \ln f(\vec{x}; \theta)}{\partial \theta^T}\right] = \mathbb{E}\left[-\frac{\partial^2 \ln f(\vec{x}; \theta)}{\partial \theta \partial \theta^T}\right] \tag{6.148}$$

Note that Fisher Information is the **expectation** of $-l''(\theta)) := J(\theta$, the idea of Fisher scoring method is the estimate $l''(x)$ using Fisher information:

$$\theta^{(t+1)} = \theta^{(t)} - l''(\theta; x)^{-1} l'(\theta; x) \longrightarrow \theta^{(t+1)} = \theta^{(t)} + I(\theta^{(t)})^{-1} l'(\theta^{(t)}; x) \tag{6.149}$$

How does Fisher Scoring improve Newton-Raphson method?

- Note that $l(\theta; \vec{x}) = \sum_{i=1}^{n} l(\theta; x_i) \Rightarrow l''(\theta; \vec{x}) = \sum_{i=1}^{n} l''(\theta; x_i)$, need much more computation for large n, while Fisher Information is a reasonable 'average' of $l''(\theta, x_i)$ and total Information is just the sum of each I_i

$$I(\theta) = nI_1(\theta) = n\mathbb{E}_{\xi}(\frac{\partial^2 l(\theta; \xi)}{\partial\theta\partial\theta^T}) \tag{6.150}$$

- Fisher Information $I(\theta)$ is always positive definite, thus improve stability.

☐ **More Specific Case: Scaled Exponential Family** $f(y; \vec{\theta}, \phi) = \exp\left(\frac{y'\theta - b(\theta)}{a(\phi)} + c(y; \phi)\right)$ where θ is the canonical parameter, declaring location.

This form of exponential family distribution posses some good properties (when approaching expectation and variance), and is one of the basic distribution assumption in Generalized Linear Model, which is an important MLE task. Detail about GLM and scaled exponential family see section. 3.7.

Further note that here we demand θ as canonical parameter, which is not necessarily the parameter μ we use. Assume θ as function of μ as $\theta = g(\mu)$.[55]

Properties:

- Log-likelihood:

$$l(\theta, \phi; y) = \frac{y'\theta - b(\theta)}{a(\phi)} + c(y; \phi) \tag{6.151}$$

- Expectation: equation. 3.187

$$\mathbb{E}(Y) = b'(\theta) \tag{6.152}$$

- Variance: equation. 3.188

$$var(Y) = a(\phi)b''(\theta) \tag{6.153}$$

- Score function:

$$S(\theta; y) = \frac{\partial l(\theta, \phi; y)}{\partial\theta} = \frac{y - b'(\theta)}{a(\phi)} \tag{6.154}$$

$$S(\mu; y) = \frac{\partial l}{\partial\theta}\frac{\mathrm{d}g(\mu)}{\mathrm{d}\mu} = \frac{y - b'(g(\mu))}{a(\phi)} g'(\mu) \tag{6.155}$$

- $J(\theta)$ or $J(\mu)$:

$$J(\theta) = -l''(\theta) = \frac{b''(\theta)}{a(\phi)} \tag{6.156}$$

$$J(\mu) = -\frac{\partial^2 l(\mu)}{\partial\mu\partial\mu^T} = \frac{\partial g}{\partial\mu} b''(g(\mu)) \frac{\partial g}{\partial\mu^T} + \left(\frac{\partial}{\partial\mu} \otimes \frac{\partial}{\partial\mu^T} g\right)(b'(g(\mu)) - y) \tag{6.157}$$

[55] Here use notation in GLM, where $\theta = \eta = g(\mu)$.

- Fisher Information:

$$I(\theta) = \mathbb{E}(J(\theta)) = \frac{b''(\theta)}{a(\phi)} \tag{6.158}$$

$$I(\mu) = \mathbb{E}(J(\mu)) = \frac{1}{a(\phi)}\frac{\partial g}{\partial \mu} b''(g(\mu))\frac{\partial g}{\partial \mu^T} \tag{6.159}$$

☐ **Fisher Scoring and GLM: Iterative Re-weighted Least Square (IRLS)**

Recall in GLM in section. 3.7

$$\mu_i \sim g^{-1}(x_i'\beta) \text{ or } g(\mu_i) \sim x'\beta \tag{6.160}$$

where minimizing task is

$$\hat{\beta} = \arg\max \sum_i l(\mu; x_i, y_i) = \arg\max \sum_i l(\beta; x_i, y_i) \tag{6.161}$$

where $l(\mu; x, y)$ satisfies $y_i \sim f(\mu_{y_i} = g(^{-1}(x_i'\beta))$. Use $\mathbb{E}(Y) = b'(\theta)$ we have

$$\mu = \mathbb{E}(Y) = g^{-1}(\eta) = g^{-1}(x'\beta) = b'(\theta) \tag{6.162}$$

Note that in GLM model we should have chosen canonical link equation. 3.198 such that $g^{-1} = b'$, then

$$\theta = \eta = x'\beta = g(\mu) \leadsto g^{-1}(\theta) = g^{-1}(\eta) = g^{-1}(x'\beta) = \mu = E(Y) \tag{6.163}$$

i.e. we could get: (Here Y and X for sample matrix notation $\vec{y}$ and $\mathbf{X}$)

$$S(\beta; Y) = \frac{\partial l(\beta)}{\partial \beta} = \frac{X^TY - X^Tg^{-1}(X\beta)}{a(\phi)} \tag{6.164}$$

$$I(\beta) = \frac{1}{a(\phi)}\frac{\partial g}{\partial \beta} b''(\theta)\frac{\partial g}{\partial \beta^T} = \frac{1}{a(\phi)} X'WX \tag{6.165}$$

$$W(\theta) := b''(\theta) = \left.\frac{\partial g^{-1}(\theta)}{\partial \theta}\right|_{\theta = X\beta} = \frac{var(Y)}{a(\phi)} \tag{6.166}$$

Then we can use above result to modify Newton-Raphson Algorithm as

$$\beta^{(t+1)} = \beta^{(t)} + I(\beta^{(t)})^{-1}S(\beta) = \beta^{(t)} + (X'W^{(t)}X)^{-1}X'(Y - g^{-1}(X\beta^{(t)})) \tag{6.167}$$

where

$$W^{(t)} = b''(\xi)\big|_{\xi = X\beta^{(t)}} \tag{6.168}$$

$$g^{-1}(\xi) = b'(\xi) \tag{6.169}$$

Further comment: iteration can be written

$$\beta^{(t+1)} = (X'W^{(t)}X)^{-1}X'W^{(t)}\left(X\beta^{(t)} + W^{-1(t)}(Y - g^{-1}(X\beta^{(t)}))\right) \tag{6.170}$$

where $Z = X\beta^{(t)} + W^{-1}(Y - g^{-1}(X\beta^{(t)}))$ can be expressed as the taylor series of $Z = g(Y)$ at $\hat{Y} = g^{-1}(X\beta)$:

$$Z = g(Y) \approx g(g^{-1}(X\beta)) + \frac{\partial g}{\partial \mu}(Y - g^{-1}(X\beta)) \tag{6.171}$$

$$= X\beta + W^{-1}(Y - g^{-1}(X\beta)) \tag{6.172}$$

i.e. each step of iteration is a weighted generalized linear regression $Z \approx g(Y) \sim X\beta$

☐ **Useful choise of General Linear Model and MLE iteration**

Note: for conciseness, the following part would use the most commonly used parameter, and canonical variable $\theta = \eta = x'\beta$

Regression data: (y_i, x_i), $i = 1, 2, \ldots, n$

- Simple Linear Regression: Normal Distribution

$$Y_i \sim N(x_i'\beta, \sigma^2) \qquad f(y; \mu, \sigma^2) = \exp\left\{\frac{y\mu - \frac{1}{2}\mu^2}{\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)\right\} \tag{6.173}$$

  – Link function:

$$g(y) = y \Leftrightarrow g^{-1}(x'\beta) = x'\beta \tag{6.174}$$

  – Canonical variable $\theta = x'\beta = \mu$ and its function

$$b(\theta) = \frac{1}{2}\theta^2 \qquad a(\sigma^2) = \sigma^2 \tag{6.175}$$

$$\mathbb{E}(Y) = b'(\theta) = \theta \tag{6.176}$$

$$var(Y) = a(\phi)b''(\theta) = \sigma^2 \tag{6.177}$$

  – Log-likelihood:

$$l(\beta, \sigma^2; y, x) = \frac{yx'\beta - \frac{1}{2}\beta' x x'\beta}{\sigma^2} - \frac{y^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2) \tag{6.178}$$

  – Gauss-Raphson Iteration:

$$\frac{\partial l}{\partial \beta} = \frac{1}{\sigma^2}\sum_{i=1}^{n}\big(x_i(y_i - x_i'\beta)\big) \tag{6.179}$$

$$\frac{\partial l}{\partial \beta \partial \beta^T} = -\frac{1}{\sigma^2}\sum_{i=1}^{n} x_i x_i' \tag{6.180}$$

  iteration step:

$$\beta^{(t+1)} = \beta^{(t)} + (X'X)^{-1}X'(Y - X\beta) \tag{6.181}$$

  – Fisher' Scoring Iteration:

$$W(\beta) = b''(\mu) = I_{p+1} \tag{6.182}$$

$$I(\beta) = \frac{1}{a(\sigma^2)}X'WX = \frac{1}{\sigma^2}X'X \tag{6.183}$$

  iteration step: the same as G-R method

$$\beta^{(t+1)} = \beta^{(t)} + (X'X)^{-1}X'(Y - X\beta) \tag{6.184}$$

- Logistic Regression: Binomial Distribution

$$Y_i \sim B(n_0, \text{logistic}(x'\beta)) \qquad f(y; n_0, \pi) = \exp\left\{y\ln\frac{\pi}{1-\pi} + n_0\ln(1-\pi) + \ln\binom{n_0}{y}\right\} \tag{6.185}$$

– Link function:

$$g(y) = \ln \frac{y}{1-y} = \text{logit}(y) \Leftrightarrow g^{-1}(x'\beta) = \frac{1}{1+e^{-x'\beta}} = \text{logistic}(x'\beta) \tag{6.186}$$

– Canonical variable $\theta = x'\beta = \text{logit}(\pi)$

$$b(\theta) = n_0 \ln(1-\pi) = n_0 \ln \frac{1}{1+e^{\theta}} \qquad a(\phi) = 1 \tag{6.187}$$

$$\mathbb{E}(Y) = b'(\theta) = n_0 \frac{1}{1+e^{-\theta}} = n_0\pi \tag{6.188}$$

$$var(Y) = a(\phi)b''(\theta) = n_0 \frac{e^{-\theta}}{(1+e^{-\theta})^2} = n_0\pi(1-\pi) \tag{6.189}$$

– Log-likelihood:

$$l(n_0, \beta; y, x) = yx'\beta + n_0 \ln(1 - g^{-1}(x'\beta)) + \ln \binom{n_0}{y} \tag{6.190}$$

– Gauss-Raphson Iteration:

$$\frac{\partial l}{\partial \beta} = \sum_{i=1}^{n} x_i \left(y_i - n_0 \text{logistic}(x_i'\beta)\right) \tag{6.191}$$

$$\frac{\partial l}{\partial \beta \partial \beta^T} = \sum_{i=1}^{n} x_i x_i' \frac{n_0 e^{-x_i'\beta}}{(1+e^{-x_i'\beta})^2} = \sum_{i=1}^{n} x_i x_i' n_0 g^{-1}(x'\beta)(1-g^{-1}(x'\beta)) \tag{6.192}$$

iteration step:

$$\beta(t+1) = \beta^{(t)} - \left(\frac{\partial l}{\partial \beta \partial \beta^T}\right)^{-1} \frac{\partial l}{\partial \beta}\bigg|_{\beta^{(t)}} \tag{6.193}$$

– Fisher's Scoring Iteration:

$$W(\beta) = \frac{var(Y)}{a(\phi)} = n_0 g^{-1}(X\beta)(1-g^{-1}(X\beta)) \tag{6.194}$$

$$I(\beta) = X'WX = X'\text{diag}\{n_0 g^{-1}(x_i'\beta)(1-g^{-1}(x_i'\beta))\}X \tag{6.195}$$

- Poisson Regression: Poisson Distribution

$$Y_i \sim P(e^{x'\beta}) \qquad f(y;\lambda) = \exp\{y \ln \lambda - \lambda - \ln(y!)\} \tag{6.196}$$

– Link function:

$$g(y) = \ln y \Leftrightarrow g^{-1}(x'\beta) = e^{x'\beta} \tag{6.197}$$

– Canonical variable $\theta = x'\beta = \ln \lambda$

$$b(\theta) = \lambda = e^{\theta} \qquad a(\phi) = 1 \tag{6.198}$$

$$\mathbb{E}(Y) = b'(\beta) = e^{\theta} = \lambda \tag{6.199}$$

$$var(Y) = a(\phi)b''(\theta) = e^{\theta} = \lambda \tag{6.200}$$

6.4.4 Linear Modification to Step Length

In minimizing methods, the key idea is usually approximate original $g(x)$ with some $\tilde{g}(x)$, and the idea of restricting step length is to avoid severe deviation of $\tilde{g}$ from g, the most direct method is to adjust step length on a given direction:

$$x^{(t+1)} = x^{(t)} + \alpha^{(t)} p^{(t)} \tag{6.201}$$

we should choose proper scale of $a^{(t)}$ adapted to the craggedness of $g(x)$ for better convergence.

- Fixed step-length: Fix $\alpha^{(t)} = \alpha$ (usually $\alpha = 1$)
- Backtracking: Starting from e.g. $\alpha_0^{(t)} = 1$ and calculate corresponding $g\left(x^{(t)} + \alpha_i^{(t)} p^{(t)}\right)$, update $\alpha_{i+1}^{(t)} = \alpha_i^{(t)}/2$ until $g\left(x^{(t)} + \alpha_i^{(t)} p^{(t)}\right) < g\left(x^{(t)}\right)$, i.e.

$$\alpha^{(t)} = \max \frac{\alpha_0}{2^n}, \; s.t. g\left(x^{(t)} + \alpha_i^{(t)} p^{(t)}\right) < g\left(x^{(t)}\right) \tag{6.202}$$

- Exact line search:

$$\alpha^{(t)} = \arg\min_{\alpha} g\left(x^{(t)} + \alpha p^{(t)}\right) \tag{6.203}$$

  Special case for quadric form

  Properties:

  - For exact line search, contiguous direction step are perpendicular, i.e.

$$\left.\frac{\partial f\left(x^{(t)} + \alpha p^{(t)}\right)}{\partial \alpha}\right|_{\alpha^{(t)}} = 0 = \left.\nabla f^T\right|_{x^{(t+1)}} p^{(t)} \Rightarrow p^{(t+1)} \perp p^{(t)} \tag{6.204}$$

  - $\alpha^{(t)}$ in special case for quadric form $f(x) = \frac{1}{2} x^T A x - b^T x + c$, denote 'residual' $r^{(t)} \equiv A x^{(t)} - b = \nabla f\left(x^{(t)}\right)$

$$\alpha^{(t)} = \arg\min f\left(x^{(t)} + \alpha p\right) = -\frac{p^T\left(A x^{(t)} - b\right)}{p^T A p} = -\frac{p^T r^{(t)}}{p^T A p} \tag{6.205}$$

$$\xlongequal{\text{for } p = -\nabla f^{(t)} = -r^{(t)}} \frac{r^{(t)T} r^{(t)}}{r^{(t)T} A r^{(t)}} \tag{6.206}$$

More general modification based on quadric form see section. 6.4.7, Trust Region Method.

6.4.5 Quasi Newton Method

One of the main difficulty of Newton-Raphson method is calculation of Hessian $H\left(x^{(t)}\right)$ (as well as its inverse). We can use some estimation method for $M^{(t)} \equiv \hat{H}^{(t)}$, for equivalently for $B^{(t)} \equiv \left[\hat{H}^{(t)}\right]^{-1}$[56]

Updating:

$$x^{(t+1)} = x^{(t)} - \alpha^{(t)} \left[M^{(t)}\right]^{-1} \nabla f\left(x^{(t)}\right) = x^{(t)} - \alpha^{(t)} B^{(t)} \nabla f\left(x^{(t)}\right) \tag{6.207}$$

☐ **Discrete Newton Method**

[56]Notation different from lecture note. Here always use H for Hessian $H \equiv \nabla\nabla f$

Numerical finite differential for $M^{(t)}$:

$$M_{ij}^{(t)} = \frac{f_i'\left(x^{(t)} + h_{ij}^{(t)}\hat{e}_j\right) - f_i'\left(x^{(t)}\right)}{h_{ij}^{(t)}} \tag{6.208}$$

This basic numeric method for Hessian has heavy calculation burden, and cannot ensure positive definition of Hessian, **Not** recommended.

□ **Quasi Newton Method: SR1, DFP, BFGS, L-BFGS, Broyden Class**

Instead of 'recalculating' $M^{(t+1)}$ (or $B^{(t+1)}$) in each step, we can 'update' $M^{(t+1)}$ based on known $M^{(t)}$, $x^{(t+1)}$, $x^{(t)}$, $\nabla f^{(t+1)}$, $\nabla f^{(t)}$. And Update of $x^{(t+1)}$ as

$$x^{(t+2)} = x^{(t+1)} - \left[M^{(t+1)}\right]^{-1} \nabla f^{(t+1)} \tag{6.209}$$

Calculation of second derivative is avoided. Note that in $M^{(t+1)}$, in total n^2 elements are needed, thus we usually has some basic assumptions/conditions for $M^{(t+1)}$ which should be inherited in iteration

- Symmetry:

$$M^{(t+1)} = \left(M^{(t+1)}\right)^T \Leftrightarrow B^{(t+1)} = \left(B^{(t+1)}\right)^T \tag{6.210}$$

- Secant Condition/Quasi-Newton Condition:

  Define

$$y^{(t)} \equiv \nabla f^{(t+1)} - \nabla f^{(t)} \qquad s^{(t)} \equiv x^{(t+1)} - x^{(t)} \tag{6.211}$$

  Secant condition:

$$y^{(t)} = M^{(t+1)} s^{(t)} \Leftrightarrow s^{(t)} = B^{(t+1)} y^{(t)} \tag{6.212}$$

- Curvature Condition/Strong Convex Condition (on function property)

$$\langle s^{(t)}, y^{(t)} \rangle \geq \xi > 0 \tag{6.213}$$

With these two constraint, degree of freedom of $M^{(t+1)}$ is reduced to $\dfrac{n(n-1)}{2}$

In the following part in this subsubsection, we will usually ignore the superscipt $\cdot^{(t)}$ or use subscript $\cdot_t$ if necessary.

- SR-1 Method/Davidon Update: Rank-1 updated

$$M_{(t+1)} = M_{(t)} + \frac{(y - M_{(t)}s)(y - M_{(t)}s)^T}{(y - M_{(t)}s)^T s} \tag{6.214}$$

$$B_{(t+1)} = B_{(t)} + \frac{(s - B_{(t)}y)(s - B_{(t)}y)^T}{(s - B_{(t)}y)^T y} \tag{6.215}$$

  Note: SR-1 update cannot guarenteed the positive definition of $M_{(t+1)}$ and $B_{(t+1)}$. But this method can be used together with Trust Region method to avoid the disadvantage.

- DFP Method & BFGS Method:

  Idea: We want to pick the Hessian M nearest to $M_{(t)}$, with constraints above, i.e.

$$M_{(t+1)} = \arg\min_M \|M - M_{(t)}\| \qquad s.t. M = M^T,\ y = Ms \tag{6.216}$$

  where norm $\|\cdot\|$ can take different form, each giving a corresponding quasi-Newton update. Here we take weighted frobenius norm

$$\|A\|_W = \|W^{-1/2} A W^{-1/2}\|_F \qquad y = Ws \tag{6.217}$$

  Note: Here we take any W with secant condition for a scale-invariant norm (because W would also looks like some 'hessian'[57])

  Solution[58]:

$$M_{(t+1)} = \left(I - \frac{ys^T}{y^Ts}\right) M_{(t)} \left(I - \frac{sy^T}{y^Ts}\right) + \frac{yy^T}{y^Ts} \tag{6.224}$$

  And inverse using Sherman-Morrison formula $\left(A + u^Tv\right)^{-1} = A^{-1} - \dfrac{A^{-1}uv^TA^{-1}}{1 + v^TA^{-1}u}$ (Note: tough calculation, haven't tried) is the DFP updating:

$$B_{(t+1)} = M_{(t+1)}^{-1} = B_{(t)} - \frac{B_{(t)}yy^TB_{(t)}}{y^TB_{(t)}y} + \frac{ss^T}{y^Ts} \tag{DFP}$$

★ Similarly, using dual minimizing problem

$$B_{(t+1)} = \arg\min_B \|B - B_{(t)}\|_{W^{-1}} \qquad s.t. B = B^T,\ s = By \tag{6.225}$$

---

[57] One of possible form of W can take

$$W = \int_0^1 \nabla\nabla f\left(x_{(t)} + \tau s\right) \mathrm{d}\tau \tag{6.218}$$

[58] Solution of minimizing problem using Lagrange multiplier: Note that weighted frobenius norm is

$$\|M - M_t\|_W^2 = tr\left(W^{-1/2}(M - M_{(t)})W^{-1}(M - M_{(t)})W^{-1/2}\right) \tag{6.219}$$

with constraints $M = M^T$, $y = Ms$, given $y = Ws$, $M_{(t)} = M_{(t)}^T$. Minimizing Lagrange function taken as

$$\Xi(M, \lambda, \Lambda) = tr\left(W^{-1/2}(M - M_{(t)})W^{-1}(M - M_{(t)})W^{-1/2}\right) - 4\lambda^T(Ms - y) - 4tr\left(\Lambda(M - M^T)\right) \tag{6.220}$$

$$\arg\min \Xi(M, \lambda, \Lambda) \Rightarrow \begin{cases} \dfrac{\partial \Xi}{\partial M} = 2W^{-1}(H - H_{(t)})^TW^{-1} - 4\lambda s^T - 4(\Lambda^T - \Lambda) = 0 \\ \dfrac{\partial \Xi}{\partial 4\lambda} = Ms - y = 0 \\ \dfrac{\partial \Xi}{\partial 4\Lambda} = M^T - M = 0 \end{cases} \tag{6.221}$$

Solve: fisrt eliminate $\Lambda - \Lambda^T$ into $\lambda s^T - s\lambda^T$, then eliminate λs^T, finally eliminate $s\lambda^T$, solution:

$$M_{(t+1)} = M_{(t)} + \frac{y - M_{(t)}s}{y^Ts}y^T + \frac{y}{y^Ts}\left(\frac{s^TM_{(t)}sy^T}{y^Tsy^Ts} - \frac{s^TM_{(t)}}{y^Ts}\right) \tag{6.222}$$

$$= \left(I - \frac{ys^T}{y^Ts}\right) M_{(t)} \left(I - \frac{sy^T}{y^Ts}\right) + \frac{yy^T}{y^Ts} \tag{6.223}$$

Solution:

$$B_{(t+1)} = \left(I - \frac{sy^T}{y^Ts}\right) B_{(t)} \left(I - \frac{ys^T}{y^Ts}\right) + \frac{ss^T}{y^Ts} \tag{BFGS}$$

Also we can inverse to get estimation of hessian in BFGS updating:

$$M_{(t+1)} = M_{(t)} - \frac{M_{(t)}ss^TM_{(t)}}{s^TM_{(t)}s} + \frac{yy^T}{y^Ts} \tag{6.226}$$

Note that our final goal is to evaluate $B_{(t+1)}$ to get step direction

$$p_{(t+1)} = -B_{(t+1)}\nabla f_{(t+1)} \tag{6.227}$$

$$B_{(t+1)} = \begin{cases} B_{(t)} + \dfrac{(s - B_{(t)}y)(s - B_{(t)}y)^T}{(s - B_{(t)}y)^Ty} & \text{(SR1)} \\ B_{(t)} - \dfrac{B_{(t)}yy^TB_{(t)}}{y^TB_{(t)}y} + \dfrac{ss^T}{y^Ts} & \text{(DFP)} \\ \left(I - \dfrac{sy^T}{y^Ts}\right) B_{(t)} \left(I - \dfrac{ys^T}{y^Ts}\right) + \dfrac{ss^T}{y^Ts} & \text{(BFGS)} \end{cases} \tag{6.228}$$

Comment: DFP updating and BFGS updating can both update $(M^{(t+1)}, B^{(t+1)})$ from $(M^{(t)}, B^{(t)})$, with symmetry condition and secant condition. But such updating has $dof = \dfrac{n(n-1)}{2} > 0$, thus we can have multiple choice of updating, in which DFP and BFGS get such update from minimizing weight norm. In practical terms, **BFGS is usually more suitable than DFP in general optimization problem**.

A guess from their minimizing problem: BFGS is more 'direct' by minimizing $\|B - B^{(t)}\|_{W^{-1}}$, without the inverse of minimizer matrix as in DFP.

☐ **More methods based on DFP and BFGS:**

- Broyden Class: linear combination of DFP and BFGS

$$B_{(t+1)} = M_{(t+1)}^{-1} \qquad M_{(t+1)} = (1 - \phi_{(t)})M_{(t+1)}^{\text{BFGS}} + \phi_{(t)}M_{(t+1)}^{\text{DFP}} \tag{6.229}$$

  Set: $\phi = 1$ for DFP, $\phi = 0$ for BFGS, $\phi = \dfrac{s^Ty}{s^Ty - s^TM_{(t)}s}$ for SR-1

- L-BFGS Method: For high dimension $n = \dim(x) \gg 1$, storage of $M_{(t)}$ or $B_{(t)}$ take $\sim n^2$, which could be unacceptable. Thus instead of storing $B_{(t)}$, $y_{(t)}$ and $s_{(t)}$, we can store $y_{(t_i)}$, $s_{(t_i)}$ $\forall t_i < t$, or at least as more t_i as possible.

6.4.6 Steepest Descent*

Steepest Descent Method

6.4.7 Trust Region Method

Approximation quadric form $\tilde{f}$ at iteration $x^{(t)}$

$$\tilde{f}_{x^{(t)}}(x) = f(x^{(t)}) + \left(x - x^{(t)}\right)^T \nabla f^{(t)} + \frac{1}{2}\left(x - x^{(t)}\right)^T M^{(t)} \left(x - x^{(t)}\right) \tag{6.230}$$

Trust Region: within $\|x - x^{(t)}\| \leq \Delta^{(t)}$, $\tilde{f}_{x^{(t)}}$ is similar enough to g, and we minimize $\tilde{f}_{x^{(t)}}$ within trust region.

☐ **Iteration:**

- Preset parameters:

$$\text{Region Radius}: \Delta^{(t)} > 0 \tag{6.231}$$

$$\text{TR step quality measure}: \eta_\nu (= 0.9),\ \eta_s < \eta_\nu (= 0.1) \tag{6.232}$$

$$\text{region update}: \gamma_i \geq 1 (= 2),\ \gamma_d (= 0.5) \tag{6.233}$$

and approximation function (usually use quadric form)

$$\tilde{f}_{x^{(t)}}(x) \left(= f(x^{(t)}) + \left(x - x^{(t)}\right)^T \nabla f^{(t)} + \frac{1}{2}\left(x - x^{(t)}\right)^T M^{(t)} \left(x - x^{(t)}\right) \right) \tag{6.234}$$

- In each iteration step (t), solve constraint minimizing problem

$$x_{\text{cm}} = \arg\min_x \tilde{f}_{x^{(t)}}(x), \quad s.t. \|x - x^{(t)}\| \leq \Delta^{(t)} \tag{6.235}$$

and the quality of reduction: $\rho^{(t)}$:

$$\rho^{(t)} = \frac{f^{(t)} - f(x_{\text{cm}})}{f^{(t)} - \tilde{f}(x_{\text{cm}})} \tag{6.236}$$

- Update $x^{(t+1)}$ and $\Delta^{(t+1)}$ based on quality $\rho^{(t)}$

$$\begin{cases} x^{(t+1)} = x_{\text{cm}},\ \Delta^{(t+1)} = \gamma_i \Delta^{(t)} & \rho^{(t)} \geq \eta_\nu \\ x^{(t+1)} = x_{\text{cm}},\ \Delta^{(t+1)} = \Delta^{(t)} & \eta_s \leq \rho^{(t)} < \eta_\nu \\ x^{(t+1)} = x^{(t)},\ \Delta^{(t+1)} = \gamma_d \Delta^{(t)} & \rho^{(t)} < \eta_s \end{cases} \tag{6.237}$$

6.4.8 Conjugate Gradient Method

Note that in Gauss-Raphson method, our iteration step was obtained by minimizing the taylor series to $O(x^2)$ in equation. 6.142,

$$f(x) \approx \tilde{f}_{x^{(t)}}(x) = f(x^{(t)}) + (x - x^{(t)})^T \nabla\ f(x)|_{x^{(t)}} + \frac{1}{2}(x - x^{(t)})^T \nabla\nabla\ f(x)|_{x^{(t)}}\,(x - x^{(t)}) \tag{6.238}$$

or, as a more specific problem: get x^* by minimizing function

$$x^* = \arg\min_x f(x) = \frac{1}{2}x^T A x - b^T x + c \tag{6.239}$$

which has analytical solution $Ax^* = b$, and we could solve this equation using algebraic methods in section. 6.2. Here Conjugate Gradient Methods uses iteration method to solve it, which can be used in Newton-Raphson/Fisher Scoring etc. to help find $\hat{H}^{(t)} p^{(t)} = -\nabla f^{(t)}$. Or use some modified conjugate gradient method directly on $f(xx)$.

☐ **Conjugate vectors of A**

Note: Here we assume $\underset{n\times n}{A}$ is symmetric positive definite (SPD). SPD of A allows us to define an inner product based on A:

$$\langle \xi_i, \xi_j \rangle_A = \xi_i^T A \xi_j \tag{6.240}$$

and conjugate vectors of A are vector set that are 'orthonormal' in the sense of $\langle\cdot,\cdot\rangle_A$:

$$\xi_i^T A\xi_j = \delta_{ij},\ \forall \xi_i, \xi_j \in \text{CV set} \tag{6.241}$$

Further if A is full-rank and conjugate vector set has n independent vector, it can span the whole space span$\{\xi_1, \xi_2, \ldots, \xi_n\} = \mathbb{R}^n$, thus we can expand any vector $x - x^{(0)}$ on $\{\xi_i\}$:

$$x = x^{(0)} + \sum_{i=1}^{n} c_i\xi_i \tag{6.242}$$

and express $f(x)$ as function of c_i, using orthonormal condition $\xi_i' A\xi_j = \delta_{ij}$

$$\begin{aligned}
f(x) =& \frac{1}{2}x^T Ax - b^T x + c && (6.243)\\
=& \frac{1}{2}(x^{(0)} + \sum_{i=1}^{n} c_i\xi_i)^T A(x^{(0)} + \sum_{i=1}^{n} c_i\xi_i) - b^T(x^{(0)} + \sum_{i=1}^{n} c_i\xi_i) + c && (6.244)\\
=& \frac{1}{2}\sum_{i=1}^{n} c_i^2 + \sum_{i=1}^{n} c_i(Ax^{(0)} - b)^T\xi_i + f\left(x^{(0)}\right) && (6.245)\\
=& \left(\sum_{i=1}^{n} \frac{1}{2}c_i^2 + c_i(Ax^{(0)} - b)^T\xi_i\right) + f\left(x^{(0)}\right) && (6.246)
\end{aligned}$$

i.e. we can minimize the quadric form by minimizing on each direction separately.

□ **Conjugate Direction Construction**

General procedue: Using a linear-independent vector set $\{\nu_i\}$ and use a process similar to Gauss-Elimination to get $\{\xi_i\}$:

$$\begin{aligned}
\xi_k =& \nu_k - \sum_{i=1}^{k-1} \frac{\xi_i^T A\nu_k}{\xi_i^T A\xi_i}\xi_i && (6.247)\\
=& \left(I - \sum_{i=1}^{k-1} \frac{\xi_i\xi_i^T A}{\xi_i^T A\xi_i}\right)\nu_k = \prod_{i=1}^{k-1}\left(I - \frac{\xi_i\xi_i^T A}{\xi_i^T A\xi_i}\right)\nu_k && (6.248)
\end{aligned}$$

Note that here we only use the condition $\xi_i^T A\xi_j = \delta_{ij}$, and $\{\nu_i\}$ is arbitrary. To avoid the storage spend of $O(n^2)$, we could choose special way in descent such that conjugate perpendicular information of $\xi_{i<k}$ are automatically 'stored' in ξ_k, and we would only need storage $O(n)$:

- Conjugate Gradient for Quadric Form: In each descent steps k

$$x_{k+1} = x_k + \alpha_k\xi_k, \qquad \xi_k = \nu_k - \sum_{i=1}^{k-1} \frac{\xi_i^T A\nu_k}{\xi_i^T A\xi_i}\xi_i \tag{6.249}$$

  choose α_k by exact line search $\alpha_k = -\frac{r_k^T\xi_k}{\xi_k^T A\xi_k} = -\frac{\nabla f_k^T\xi_k}{\xi_k^T A\xi_k}$, $r_k = Ax_k - b = \nabla f_k$, and $\nu_k = -\nabla f(x_k)$[59], and using the fomula:

$$\alpha_i A\xi_i = A(x_{i+1} - x_i) = r_{i+1} - r_i = \nabla f_{i+1} - \nabla f_i \tag{6.252}$$

[59] Such that $\nu_k = -\nabla f_k \perp$ span$\{\xi_1, \ldots, \xi_{k-1}\}$= span$\{\nu_1, \ldots, \nu_{k-1}\}$, then.

$$\begin{aligned}
\nu_k =& -\nabla f_k \perp \nu_i,\ \forall i < k && (6.250)\\
\nu_k =& -\nabla f_k \perp \xi_i,\ \forall i < k && (6.251)
\end{aligned}$$

and the orthogonality of ξ, ∇f, ξ_k can be expressed as

$$\xi_k = -\nabla f(x_k) - \sum_{i=1}^{k-1} \frac{(\nabla f_{i+1} - \nabla f_i)^T \nabla f_k}{(\nabla f_{i+1} - \nabla f_i)^T \xi_i} \xi_i \tag{6.253}$$

$$= -\nabla f(x_k) + \frac{(\nabla f_k - \nabla f_{k-1})^T \nabla f_k}{\nabla f_{k-1}^T \nabla f_{k-1}} \xi_{k-1} \tag{PR}$$

$$= -\nabla f(x_k) + \frac{\|\nabla f_k\|^2}{\|\nabla f_{k-1}\|^2} \xi_{k-1} \tag{FR}$$

For general minimizing problem, we can either use conjugate gradient just for solving $\hat{H}^{(t)} p^{(t)} = -\nabla f^{(t)}$ in each step (t), or more directly use the following conjugate method directly on the general $f(x)$: take different α and coefficient of vector as modification to the non-quadric part of f

$$x_{k+1}^{(t)} = x_k^{(t)} + \alpha_k^{(t)} p_k^{(t)} \tag{6.254}$$

$$p_k^{(t)} = -\nabla f(x_k^{(t)}) + \beta_k^{(t)} p_{k-1}^{(t)} \tag{6.255}$$

where:

- General Form of Conjugate Gradient: In each sub-step $(t)k$, replace $A_k^{(t)} = A^{(t)}$ by $\nabla\nabla f\left(x_k^{(t)}\right)$, i.e.

$$\alpha_k^{(t)} = -\frac{\nabla f(x_k^{(t)})^T p_k}{p_k^{(t)T} \nabla\nabla f(x_k^{(t)}) p_k^{(t)}} \tag{6.256}$$

$$\beta_k^{(t)} = \frac{\nabla f(x_k^{(t)})^T \nabla\nabla f(x_k^{(t)}) p_k^{(t)}}{p_{k-1}^{(t)T} \nabla\nabla f(x_k^{(t)}) p_{k-1}^{(t)}} \tag{6.257}$$

$$k = 1, 2, \ldots, n \tag{6.258}$$

- Fletcher-Reeves Method:

$$\alpha_k^{(t)} = \arg\min_{\alpha} f\left(x_k^{(t)} + \alpha p_k^{(t)}\right) \tag{6.259}$$

$$\beta_k^{(t)} = \frac{\|\nabla f(x_k^{(t)})\|^2}{\|\nabla f(x_{k-1}^{(t)})\|^2} \tag{6.260}$$

$$k = 1, 2, \ldots, n \tag{6.261}$$

- Polak-Ribière Method:

$$\alpha_k^{(t)} = \arg\min_{\alpha} f\left(x_k^{(t)} + \alpha p^{(t)}\right) \tag{6.262}$$

$$\beta_k^{(t)} = \frac{\left(\nabla f(x_k^{(t)}) - \nabla f(x_{k-1}^{(t)})\right)^T \nabla f(x_k^{(t)})}{\|\nabla f(x_{k-1}^{(t)})\|^2} \tag{6.263}$$

$$k = 1, 2, \ldots, n \tag{6.264}$$

Section 6.5 Expectation Maximization Algorithm

Motivation: use MLE to estimate some model parameter θ for model $\{x_i\}$ i.i.d. $\sim f(x|\theta)$. Difficulty: for complex model

Main appication: Probability Generative Model, observed value x_i is generated from distributon $f(x|z_i,\theta_i,\theta_z)$ dependent on **unobserved** random $z \sim g(z|\theta_z)$(usually z is discrete, denoted $z_\nu = z_\alpha, \dots z_\gamma$). Where we know the form of $f(x,z|\theta_{z_\nu},\theta_z)$, but form of $f(x|\theta_{z_\nu},\theta)$ might be hard to solve, thus we use an iterative method to deal with the latent variable z so that we can use the known form $f(x,z|\theta_{z_\nu},\theta)$.

6.5.1 Requisite Knowledge

- Kullback-Leibler Divergence: mearures the difference of distribution $p(x)$ from distribution $q(x)$

$$\mathrm{KL}(q||p) \equiv -\int q(x)\log\frac{p(x)}{q(x)}\,\mathrm{d}x \tag{6.265}$$

  Note: non-exchange for p, q.

  Property: $\mathrm{KL}(q||p) \geq 0, \forall p(x)$, take equal when $p(x)=q(x)$

- Jensen Inequality: For **concave** function $h(x)$ and random variable $X \sim f$

$$\mathbb{E}_f\left(h(X)\right) \leq h\left(\mathbb{E}_f(X)\right) \tag{6.266}$$

6.5.2 Derivation

Notation: $\theta = (\theta_{z_\nu},\theta_z)$, sample $X=(x_1,x_2,\dots,x_N)$. Expectation of function of ramdom variable $h(Y)$ on distribution $q(y)$ as $E_{(q_y)}\left(h(Y)\right)$.

Target: MLE of $l(\theta|X) \equiv \sum_{i=1}^N \log f(x_i|\theta)$. i.e. get $\theta^* = \arg\max_\theta l(\theta|X)$.

□ **Key Formula**

But due to the untraceablility of $f(x|\theta)$, we have to expand to the full form $f(x,z|\theta)$, and use a mathematic trick of $E_q(\cdot)$, where $q(z)$ is any arbitrary distribution of z.

$$\begin{aligned}
f(x|\theta) =& f(x,z|\theta)f(z|x,\theta) \Rightarrow \qquad (6.267)\\
\Rightarrow \log f(x|\theta) = E_{q(z)}\left(\log f(x|\theta)\right) =& E_{q(z)}\left(\log f(x,z|\theta)f(z|x,\theta)\right) \qquad (6.268)\\
=& \int q(z)\log f(x,z|\theta)f(z|x,\theta)\,\mathrm{d}z \qquad (6.269)\\
=& \int q(z)\log\frac{f(x,z|\theta)}{q(z)}\,\mathrm{d}z + \mathrm{KL}\left(q||f(z|x,\theta)\right) \qquad (6.270)\\
\geq& \int q(z)\log\frac{f(x,z|\theta)}{q(z)}\,\mathrm{d}z, \quad \forall x = x_1,x_2,\dots,x_N \qquad (6.271)
\end{aligned}$$

where $\int q(z)\log\frac{f(x,z|\theta)}{q(z)}\,\mathrm{d}z$ is also called ELBO (Evidence Lower Bound) of $\log f(x|\theta)$. And we could similarly get the ELBO of log-likelihood:

$$l(\theta|X) = \sum_{i=1}^N \log f(x_i|\theta) \geq \sum_{i=1}^N \int_z q_i(z)\log\frac{f(x_i,z|\theta)}{q_i(z)}\,\mathrm{d}z \equiv \mathrm{ELBO}(q,\theta), \quad q=\{q_i\} \tag{6.272}$$

i.e. ELBO provides a lower bound estimate for $l(\theta|X)$, thus we can instead maximize $\mathrm{ELBO}(q,\theta)$, using coordiante ascent is the Maximization-Maximization Algorithm:.[60]

$$q \text{ Maximum}: q^{(t+1)} = \arg\max_{q(z)} \text{ELBO}(q, \theta^{(t)}) = p(z|x, \theta^{(t)}) \tag{6.273}$$

$$\theta \text{ Maximum}: \theta^{(t+1)} = \arg\max_{\theta} \text{ELBO}(q^{(t+1)}, \theta) \tag{6.274}$$

Further if we take can derive and use the form of $p(z|x,\theta)$ (sometimes this posterior is also untraceable), then θ maximization step becomes

$$\theta^{(t+1)} = \arg\max_{\theta} \text{ELBO}\left(p(z|x,\theta^{(t)}),\theta\right) = \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log\frac{f(x_i,z|\theta)}{p(z|x_i,\theta^{(t)})}\,\mathrm{d}z \tag{6.275}$$

$$= \arg\max_{\theta} \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log f(x_i,z|\theta)\,\mathrm{d}z \equiv Q(\theta|\theta^{(t)}) \tag{6.276}$$

$$= \arg\max_{\theta} \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log f(x_i,z|\theta)\,\mathrm{d}z \tag{6.277}$$

and naturally q maximization Step becomes computing $Q(\theta|\theta^{(t)}) = \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log f(x_i,z|\theta)\,\mathrm{d}z$, i.e. the Expectation of $f(x_i,z|\theta)$ on the posterior $p(z|x_i,\theta^{(t)})$, gather as Expectation-Maximization Algorithm:

Algorithm *Expectation-Maximization*

$$\text{E}_{\text{xpectation}}\text{-Step}: Q(\theta|\theta^{(t)}) = \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log f(x_i,z|\theta)\,\mathrm{d}z = \sum_{i=1}^{N} E_{p(z|x_i,\theta^{(t)})}\left[\log f(x_i,z|\theta)\right] \tag{6.278}$$

$$\text{M}_{\text{aximization}}\text{-Step}: \theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)}) = \arg\max_{\theta} \sum_{i=1}^{N}\int_z p(z|x_i,\theta^{(t)}) \log f(x_i,z|\theta)\,\mathrm{d}z \tag{6.279}$$

E-M Algorithm can guarentee ascent of ELBO, and finally can ensure convergence (at least to a local maximum).

An application of E-M Algorithm is Gaussian Mixture Model for Clustering, detail see section. 4.7.3.

☐ **Limitation and Improvement**

- Note that for generative model, we used a set of latent variable z, further we need an $\int_z \,\mathrm{d}x$ in $Q(\theta|\theta^{(t)})$, thus E-M requires low-dimensionality of z (e.g. in GMM, z is one-dimensional).
- Slow convergence near extreme point, use acceleration improvement, e.g. Louis acceleration.
- In q-Maximization step, the form of q might be untraceable (i.e. $p(z|x,\theta)$ untraceable). For such function extreme value problem, use VEM (Variational Expectation Maximization) / VBEM(Variational Bayesian Expectation Maximization)

Section 6.6 Statistical Simulation

Statistic model inference problem can be solved using simulation, i.e. Monte-Carlo simulation. We can use the model-based random numbers to analyze model.

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[60] where one of the 'coordinate' is the function space $q(z)$

- Simulation is well-adapted, especially for high-dimensional problems
- Low-precision, usually sd $\sim O(\frac{1}{\sqrt{N}})$.
- Simulation method is also usually used for validation of model reliability.

▷ `R.` **Code**

Remember to sed random generator seed before simulation.

```
set.seed(INI_NUM)
```

6.6.1 Random Number Generation

Motivation: In many simulation models, we need to generate sets of random number with some distribution, **however** they are not totally 'random' because of repeatability need.

Idea: use a 'seed' to generate pseudo ranom number, where within each seed, numbers are random. The random number sequence can be repeated by setting the same seed.

☐ **Linear Congruential Method for** $U(0,1)$

Linear Congruential Method (LCM) is the most commonly used method for generating uniform distribution $U(0,1)$, which is the basic for more complex distribution.

Algorithm *Linear Congruential for Uniform Distribution*

1. Set seed X_0 and pick proper a, c, m for LCM
2. Repeat for iterative i:

   (a) compute X_{i+1}

$$X_{i+1} \equiv aX_i + c(\operatorname{mod} m) \tag{6.280}$$

   (b) Random number normalized to $(0,1)$

$$R_{i+1} = \frac{X_{i+1}}{m} \tag{6.281}$$

Choice of a, c, m: LCM sequence has period m thus m should large , and choice of a, c should avoid early period value, and let R_i distribute uniformly in $(0,1)$. Useful choice:

	a	c	m
Lehmer's	23		10^8+1
RANDU	$2^{16}+3$	1	2^{31}
IBM	16807		$2^{31}-1$

☐ **Improvement of LCG**

Key problem is the periodically structure of generated X_i, i.e. when some $X_{\tilde{i}}$ return to X_0, then the following $X_{\tilde{i}+i} = X_i$ will repeat. Idea: modify the generation rule, e.g. use groups m of LCM X_{im} with differnet period P_m to generate R_i. Example: L' Ecuyer-CMRG Algorithm.

$$X_i = \left(\sum_{j=1}^{m}(-1)^{j+1}X_{ij}\right) \bmod m \quad R_i = \begin{cases} \frac{X_i}{m} & X_i > 0 \\ \frac{X_i}{m} + 1 & X_i < 0 \\ 1 - \frac{1}{m} & X_i = 0 \end{cases} \tag{6.282}$$

Note (Guess): why we want $X_i \in (0,1)$ rather than $[0,1]$. $(0,1)$ is homeomorphous with $\mathbb{R}$, which would be convenient for generate more distribution on $\mathbb{R}$.

More improvement: use general form

$$X_{i+1} = g(X_i, X_{i-1}, \ldots) \bmod m \tag{6.283}$$

where in $g(\ldots)$ use more X_j, or take different function form.

☐ **Random Variate Generation**

Further for any arbitrary distribution generation, which is 'variate' of uniform distribution[61]

Target: generate random number sequence with some distribution ($f(x)$ or $F(x)$ known). Denote random number sequence with $U(0,1)$ distribution as U_i

- Quantile Method/Inverse Transform Method: For distributions with traceable CDF $F(x) \in (0,1)$.

$$X_i = F_X^{-1}(U_i) \tag{6.284}$$

  Proof:

$$\mathbb{P}\left(x < X < x + \mathrm{d}x\right) = \mathbb{P}\left(F(x) < U < F(x + \mathrm{d}x)\right) \tag{6.285}$$

$$= \frac{\partial F(x)}{\partial x}\mathrm{d}x = f(x)\,\mathrm{d}x \tag{6.286}$$

- Acceptance-Rejection Method: For $F(x)$ untraceable, only $f(x)$ known, e.g. Normal Distribution.

  First decompose $f(x)$ as

$$f(x) = \frac{p(x)g(x)}{\int p(x)g(x)\,\mathrm{d}x} \tag{6.287}$$

  where $g(x)$ is some distribution that we can generate, $p(x) \in [0,1]$. Then X_{n_k} sequence $\sim f(x)$ can be generated as follows:

  1. Propose a $x_k \sim g(x)$ and a $u_k \sim U(0,1)$
  2. Decide whether accept/reject x_k to be X_{n_k}:

$$\begin{cases} p(x_k) \geq u_k & \text{Reject} \\ p(x_k) < u_k & \text{Accept} \end{cases} \tag{6.288}$$

[61]关于 variate 的中译，笔者想到一个有趣的翻译是国际象棋术语“变例”variation，原指一类开局方法的衍生分支，这里或许可以指其他分布随机数可由均匀分布随机数衍生而来这一特点。

Proof:

$$\mathbb{P}(\text{Accept}|x) = \frac{f(x)}{g(x)\int p(\xi)g(\xi)\,\mathrm{d}\xi} \Rightarrow \mathbb{P}(\text{Accept}) = \int_x \mathbb{P}(\text{Accept}|x)g(x)\,\mathrm{d}x = \frac{1}{\int p(\xi)g(\xi)\,\mathrm{d}\xi} \tag{6.289}$$

Using Bayesian Rule:

$$\mathbb{P}(x_k|\text{Accept}) = \frac{\mathbb{P}(\text{Accept}|x_k)g(x_k)}{\mathbb{P}(\text{Accept})} = f(X_{n_k}) \tag{6.290}$$

Intuitively view: figure $f(x)$ lies under $g(x)$. If for each x we accept it with probability $\frac{f(x)}{g(x)}$, then figure $g(x)$ is 'cut' into $f(x)$, $\int p(x)g(x)\,\mathrm{d}x$ acts as the normalize constant, which corresponds to 'accept rate' controlling generate frequancy.

We should choose a proper $g(x)$ which is similar to $f(x)$, so that $\int p(x)g(x)\,\mathrm{d}x$ could be large and the algorithm is efficient.

▷ `R.` **Code**

Use the following command for all distributions supported in `R. stats::`. More distributions based on packages see https://CRAN.R-project.org/view=Distributions

```
?Distributions
```

6.6.2 Numerical Integration With Simulation

Motivation: In Bayesian statistics we usually use the following expression to calculate some posterior:

$$f(z|x) = \frac{f(x|z)f(z)}{\displaystyle\int_z f(x|z)f(z)\,\mathrm{d}z} \tag{6.291}$$

Key difficulty is calculation of the normalize integration $\int_z f(x|z)f(z)\,\mathrm{d}z = E_{f(z)}[f(x|z)]$, where $f(z)$ is the prior of z. Usually such integration needs numeric calculation. Statistical simulation using sampling is one of the methods.

Target: calculate integration

$$I(h) = \int_{x\in\mathcal{X}} h(x)\,\mathrm{d}x \tag{6.292}$$

- Hit-and-Miss Method: if $\mathcal{X}\otimes h(x)$ is bounded in e.g. $[a,b]\otimes[0,M]$. We can generate uniform distribution (x,y) in the region, and count # points under $h(x)$, proportion of accept denoted $\hat{p}$, then

$$\hat{I} = M(b-a)\hat{p} \tag{6.293}$$

such estimation is guarenteed by CLT:

$$\hat{I}_{\mathrm{H}} \xrightarrow{\mathscr{L}} N\left(I, \frac{[M(b-a)]^2 p(1-p)}{N}\right) \tag{6.294}$$

- Mean Value Method: generate uniform distribution in e.g. $\mathcal{X}=[a,b]$, and calculate function value at each sample item $h(u_i)$, estimator

$$\hat{I} = \frac{N}{a-b}\sum_{i=1}^{N} h(u_i), \qquad w.r.t.\ u_i\sim U(a,b) \tag{6.295}$$

with CLT:

$$\hat{I}_{\mathrm{M}} \xrightarrow{\mathscr{L}} N\left(I, \frac{(b-a)^2 var(h(U))}{N}\right) \tag{6.296}$$

Note: $var(\hat{I}_{\mathrm{H}}) > var(\hat{I}_{\mathrm{M}})$. Intuitively, more points are used in mean value method, thus is more precise.

Random simulation has good performance for high-dimensional case by avoiding curse of dimensionality.

☐ **Importance Sampling Estimator**

Improvement of mean value estimator: Note that in mean value with uniform distribution, variance

$$var(\hat{I}_{\mathrm{M}}) = \frac{(b-a)^2}{N} var(h(U)) \tag{6.297}$$

could be large if $h(x)$ varies dramatically. To avoid the disadvantage, we could use some other distribution of $x_i \sim p(x)$, the integration

$$I = \int_{x\in\mathcal{X}} h(x)\,\mathrm{d}x = \int_{x\in\mathcal{X}} \frac{h(x)}{p(x)} p(x)\,\mathrm{d}x = \mathbb{E}_{p(x)}\left[\frac{h(x)}{p(x)}\right] \tag{6.298}$$

Estimator use

$$\hat{I}_{g(x)} = \frac{1}{N}\sum_{i=1}^{N} \frac{h(x_i)}{g(x_i)}, \qquad w.r.t.\, x_i \sim g(x) \tag{6.299}$$

Variance

$$var(\hat{I}_{g(x)}) = \frac{1}{N} var\left(\frac{h(X)}{g(X)}\right) \tag{6.300}$$

i.e. if $\dfrac{h(x)}{g(x)} \approx$ const, the estimator can be more precise.

- An application of importance sampling: estimating expectation of function of r.v. $E_{f(z)}(\phi(z))$, where r.v. with $f(z)$ distribution is hard to generate. We can generate another random number series $x_i \sim q(x)$:

$$I(\phi, h) = \int \phi(z) f(z)\,\mathrm{d}z = \int \phi(x)\frac{f(x)}{q(x)} q(x)\,\mathrm{d}x = \mathbb{E}_{q(x)}\left(\phi(x)\frac{f(x)}{q(x)}\right) \tag{6.301}$$

$$= \int \phi(x) W(x) q(x)\,\mathrm{d}x, \quad W(x) \equiv \frac{f(x)}{q(x)} \tag{6.302}$$

Use Estimator:

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} \phi(x_i) W(x_i) \tag{6.303}$$

As a worse case where we only have an unnormalized $\tilde{f}(x)$, with the normalize integration $f(x) = \dfrac{\tilde{f}(x)}{\int f(\xi)\,\mathrm{d}\xi} = \frac{1}{c}\tilde{f}(x)$ incomputable. Use property of weight $\tilde{W}(x) \equiv \dfrac{\tilde{f}(x)}{g(x)}$:

$$\int \tilde{W}(x) g(x)\,\mathrm{d}x = \int \tilde{f}(\xi)\,\mathrm{d}\xi = c \Rightarrow \hat{c} = \frac{1}{N}\sum_{i=1}^{N} \tilde{W}(x_i) \tag{6.304}$$

Estimator:

$$\hat{I} = \frac{\sum_{i=1}^{N} \phi(x_i)\tilde{W}(x_i)}{\sum_{i=1}^{N} \tilde{W}(x_i)}, \quad \tilde{W}(x_i) = \frac{\tilde{f}(x_i)}{g(x_i)} \tag{6.305}$$

Comment: Idea of importance sampling estimation is to put more point at where $h(x)$ has large function value to get better fit of integration, i.e. smaller variance.

6.6.3 Bootstrap

In statistic inference for distribution $x \sim f(x;\theta)$, $\theta \in \Theta$, we want to estimate some statistic ϕ by estimator $\hat{\phi}$, including e.g. mean $E(\hat{\phi})$, standard error SE $= \sqrt{var(\hat{\phi})}$. In section. 2.3 we used pivot variable method to estimate statistics: parametric method, model required. Difficluty: strange distribution/strange statistics $\to$ use non-parametric method, e.g. bootstrap method.

□ **Bootstrap Method**

Conduct bootstrap given sample $X = (X_1, X_2, \ldots, X_N)$, X_i i.i.d. $\sim f(x;\theta)$.

1. Use sample X to estimate population distribution as $\hat{f}(x)$. e.g. empirical CDF.
2. Repeatedly sample from $\hat{f}(x)$ to get B samples of size n:

$$X^{(b)} = (X_1^{(b)}, X_2^{(b)}, \ldots, X_n^{(b)}), \quad b = 1, 2, \ldots, B \tag{6.306}$$

3. For each sample $X^{(b)}$ estimate a statistic $\hat{\phi}^{(b)}$
4. $\{\hat{\phi}^{(b)}\}$, $b = 1, 2, \ldots, B$ is the distribution estimation of $\hat{\phi}$ based on $\hat{f}(x)$, i.e. sample of statistics. We could use this sample of statistics to estimate e.g. SE($\hat{\phi}$), or get interval estimation of $\hat{\phi}$.

$$\hat{\phi}_{\text{boot}} = \frac{1}{B}\sum_{b=1}^{B}\hat{\phi}^{(b)} \tag{6.307}$$

□ **Bias Correction**

The above estimator is the unbiased estimator for $\hat{\phi}$. However in the sense of minimizing MSE, usually $\tilde{\phi} \equiv \hat{\phi} - bi\hat{a}s(\phi)$ is a better estimator. Bias $b = \hat{\phi} - \phi$ can be estimated as

$$\hat{b} = \hat{\phi}_{\text{boot}} - \hat{\phi} \tag{6.308}$$

where $\hat{\phi}$ is calculated by using the original sample X. And MSE estimator is:

$$\tilde{\phi} = \hat{\phi} - \hat{b} = 2\hat{\phi} - \hat{\phi}_{\text{boot}} = 2\hat{\phi} - \frac{1}{B}\sum_{b=1}^{B}\hat{\phi}^{(b)} \tag{6.309}$$

6.6.4 Markov Chain Monte Carlo Method

Markov Chain Monte Carlo (MCMC) aims at solving integration and simulation problems by sampling from some distribution. MCMC can deal with complex distribution in high dimensional, an example is Gibbs distribution

$$\mathbb{P}(s) = \frac{e^{-\beta E(s)}}{\sum_{\sigma} e^{-\beta E(\sigma)}}, s \in \text{phase space} \tag{6.310}$$

In this case, partition function is almost impossible to calculate, what we could obtain is just the unnormalized distribution.

□ **Markov chain**

Denote phase space $\mathcal{X} \ni x$. We could design such a process X_t to **transit from one state to another**, i.e. a conditional probability

$$\mathbb{P}(X_{t+1} = x | X_0 = x_0, X_1 = x_1, \ldots, X_t = x_t) \tag{6.311}$$

a markov process is a memoryless one in which future only depends on the current one step, i.e.

$$\mathbb{P}\left(X_{t+1}=x|X_0=x_0,X_1=x_1,\ldots,X_t=x_t\right)=\mathbb{P}\left(X_{t+1}=x|X_t=x_t\right) \tag{6.312}$$

for discrete version $x\in\{1,2,\ldots\}$, we could denote it into a discrete-time stochastic process that is time-homogeneous

$$p_{ij}:=\mathbb{P}\left(X_{t+1}=j|X_t=i\right),\quad \sum_j p_{ij}=1 \tag{6.313}$$

which could be denoted in matrix form $P=\{p_{ij}\}$

Further, n-step transition denoted

$$p_{ij}^{(n)}:=\mathbb{P}\left(X_{t+n}=j|X_t=i\right) \tag{6.314}$$

$$=\sum_k p_{ij}^{(n-1)}p_{kj} \tag{6.315}$$

$$=\sum_{k_1,k_2,\ldots,k_{n-1}} p_{ik_1}p_{k_1k_2}\cdots p_{k_{n-1}j} \tag{6.316}$$

$$=P^n \tag{6.317}$$

Stationary Distribution π_∞ of a markov satisfies

$$\pi_\infty=P\pi_\infty=P^n\pi_\infty \tag{6.318}$$

Convergence and Ergodic Thm.: An ergodic markov chain converges to a unique stationary distribution π_∞

$$\pi_{infty}=\lim_{n\to\infty}P^n\pi_0 \tag{6.319}$$

where π_0 is an arbitrary initial distribution.

Detailed Balance Condition of stationart distribution π:

$$\pi(i)p_{ij}=\pi(j)p_{ji} \tag{6.320}$$

is a sufficient condition for stationary distribution.

MCMC aims at designing a proper chain p_{ij}, starting from some arbitrary state π_0, and after some transitions t we would expect $\pi_{t+n}\to\pi_\infty$, $n=1,2,\ldots$.

□ **MCMC Algorithms for Unnormalized distribution**

To sample from an unnormalized distribution $\tilde{p}$, i.e. $p=\dfrac{\tilde{p}(x)}{\int\tilde{p}(\xi\,\mathrm{d}\xi)}$, but normalizer $Z=\int\tilde{p}(\xi\,\mathrm{d}\xi)$ is impossible to calculate, we could only get relative probability ratio of states.

- Metropolis-Hastings Algorithm:

Algorithm *MCMC*

---

1. A pre-selected conditional distribution $q(\cdot|x)$ is used as **proposal distribution**. In each step t, a new state is proposed as

$$Y\sim q(\cdot|X_t),\text{ i.e.}\mathbb{P}\left(Y=y|X_t\right)=q(y|X_t) \tag{6.321}$$

2. Acceptance ratio $\alpha_{Y|X_t}$ is the probability to accept the proposal as the new state

$$\alpha(Y|X_t) = \min\left\{1, \frac{\tilde{p}(Y)q(X_t|Y)}{\tilde{p}(X_t)q(Y|X_t)}\right\} \tag{6.322}$$

3. Increment of $t \to t+1$ if accept.

Comment:

- Detailed balanced condition of M-H Algorithm

$$\begin{aligned}
p(x)p_{xy} =& p(x)q(y|x)\alpha(y|x) && (6.323)\\
=& p(x)q(y|x)\min\left\{1, \frac{p(y)q(x|y)}{p(x)q(y|x)}\right\} && (6.324)\\
=& \min\left\{p(x)q(y|x), p(y)q(x|y)\right\} && (6.325)\\
=& p(y)q(x|y)\min\left\{\frac{p(x)q(y|x)}{p(y)q(x|y)}, 1\right\} && (6.326)\\
=& p(y)p_{yx} && (6.327)
\end{aligned}$$

  i.e. $p_{xy} = q(y|x)\alpha(y|x)$ is the transition matrix to generate the stationary distribution as $\pi_\infty = p(x)$

- Choice of proposal $q(\cdot|x)$ is flexible, but should be properly chosen for higher acceptance to increase efficiency.

Chapter. VII 可靠性数据与生存分析部分

Instructor: Jiangdian Wang

Key focus of reliability data and survival analysis: Study the 'survival time' T before some 'failure event'. Basically the research problem is the distribution of T, including topics on descriptive statistics, estimation and hypothesis testing. Further for actual cases, T might be censored, i.e. the observe time is not exact; and we may also wonder the influence of covariants z.

Section 7.1 Reliability Data

The main feature of reliability data is **censoring**, to be distinguished from the exact numbers in usual statistical inference. Censor means we cannot observe the exact **event time** T. Instead, a **censoring time** C is observed, together with a censoring type, e.g.

$$\text{Right Censoring: } T_{\text{actual}} > C \tag{7.1}$$

$$\text{Left Censoring: } T_{\text{actual}} < C \tag{7.2}$$

$$\text{Interval Censoring: } C_l < T_{\text{actual}} < C_r \tag{7.3}$$

$$\cdots \tag{7.4}$$

7.1.1 Right Censor Data and Representation

In most parts of this course we focus on right censor data, i.e. dataset contains both event time T and right censor time T^+:

$$\text{Event Time: } T_1, \dots, T_{n_1} \tag{7.5}$$

$$\text{Right Censor: } T_1^+, \dots, T_{n_r}^+ \tag{7.6}$$

$$\tag{7.7}$$

Or we could use an indicator δ to express whether a time is event (1) or right censored (0):

$$(T_i, \delta_i; z_i),\ i = 1, 2, \dots n_1 + n_r \tag{7.8}$$

where z_i for covariants.

Usually we assume that event and censor are independent $T \perp\!\!\!\perp C$

7.1.2 Life Table Data

Life table collect survival data at ordinal, uniformly-spaced time points, where each row contains # items at risk, # events, ...

Section 7.2 Survival Model and Statistical Inference

7.2.1 Survival Function and Hazard

Key focus of survival analysis problem is the distribution of T (note that in actual cases we need to make use of both event time T_i and censored data T_i^+ to estimate the distribution of T). The distribution feature can be described in various approaches: PDF $f(t)$, CDF $F(t)$, Survival Function $S(t)$, Hazard Function $\lambda(t)$, Cumulative Hazard Function $\Lambda(t)$:

- Continuous Case: $t \in \mathbb{R}^+$
  - Survival Function $S(t)$:
$$S(t) \equiv 1 - F(t) = \int_t^\infty f(\tau)\,\mathrm{d}\tau, \qquad f(t) = -\frac{\mathrm{d}S(t)}{\mathrm{d}t} \tag{7.9}$$
  - Hazard Function $\lambda(t)$ (or in some materials denoted $h(t)$): mortality at t:
$$\lambda(t) = \lim_{h\to 0} \frac{\mathbb{P}[t \le T < t+h | T \ge t]}{h} = \frac{f(t)}{S(t)} = -\frac{\mathrm{d}\log S(t)}{\mathrm{d}t} \tag{7.10}$$
  - Cumulative Hazard Function $\Lambda(t)$ (or in some materials denoted $H(t)$):
$$\Lambda(t) = \int_0^t \lambda(\tau)\,\mathrm{d}\tau = -\log S(t) \tag{7.11}$$
$$S(t) = e^{-\Lambda(t)} = e^{-\int_0^t \lambda(\tau)\,\mathrm{d}\tau} \tag{7.12}$$
- Discrete Case: $t \in \{t_1, t_2, \ldots, t_n\}$
  - PMF: $p(t)$ is defined on
$$t \in \mathcal{T}, \quad p(t) \in (\mathcal{T} \to [0,1]^n]) \tag{7.13}$$
  - Survival Function: Note that CDF $F(t)$ is right continuous, then $S(t) = 1 - F(t)$ is left continuous:
$$S(t) = \mathbb{P}(T > t) = \sum_{t_i > t} p(t_i), \qquad p(t_i) = S(t_{i-1}) - S(t_i) = \lambda(t_i) S(t_{i-1}) \tag{7.14}$$

    Decomposition of survival function into hazard production
$$\begin{aligned} S(t) =& \mathbb{P}(T > t) = P(T > t \cap T > t_j), \quad \forall t_j < t \\ =& \mathbb{P}(T > t | T > t_j) \cdot \mathbb{P}(T > t_j) \\ =& \mathbb{P}(T > t | T > t_j) \cdot \mathbb{P}(T > t_j | T > t_{j-1}) \cdot \mathbb{P}(T > t_{j-1}) \\ =& \mathbb{P}(T > t | T > t_j) \cdot \frac{S(t_j)}{S(t_{j-1})} \cdot \mathbb{P}(T > t_{j-1}) \\ =& \prod_{0 < t_j \le t} \frac{S(t_j)}{S(t_{j-1})} \\ =& \prod_{0 < t_j \le t} [1 - \lambda(t_j)] \end{aligned} \tag{7.15}$$
  - Hazard Function $\lambda(t)$:
$$\lambda(t_i) = \mathbb{P}(T = t_i | T \ge t_i) = \frac{p(t_i)}{S(t_{i-1})} = 1 - \frac{S(t_i)}{S(t_{i-1})} \tag{7.16}$$

☐ **Properties of survival function and hazard function & More concepts and definition**

- Mean Survival Time:

$$\mu \equiv \mathbb{E}(T) = \begin{cases} \int_0^\infty \tau f(\tau)\,\mathrm{d}\tau = \int_0^\infty S(\tau)\,\mathrm{d}\tau \\ \sum_{i=1}^n t_i p(t_i) \end{cases} \tag{7.17}$$

- Mean Residual Life Time (mrl):

$$\mathrm{mrl}(t) = \mathbb{E}[T - t | T \geq t_0] = \frac{\int_t^\infty S(\tau)\,\mathrm{d}\tau}{S(t)} \tag{7.18}$$

- Considering that $T > 0$ and $\lim_{t\to\infty} F(t) \to 0$, $S(t)$ has following properties

$$S(0) = 1 \qquad S(\infty) = 0 \tag{7.19}$$

- For independent survival time $T_1, , T_2$, define $T = \min\{T_1, T_2\}$, then

$$\lambda_T(t) = \lambda_1(t) + \lambda_2(t) \tag{7.20}$$

- Hazard Rate: for two survival r.v. T_1, T_2, the hazard rate at t

$$\text{hazard ratio}(t) = \frac{\lambda_1(t)}{\lambda_2(t)} \tag{7.21}$$

7.2.2 Parametric Statistical Inference to Survival Function

Usually the parametric inference is based on a hypothetical distribution, then we conduct estimation using the parametric distribution, or conduct hypothesis testing on parameter(s).

☐ **Common Survival Distribution Prior**

In parametric model, there are some commonly used distribution models

- Exponential $T \sim \varepsilon(\lambda)$

$$f(t) = \lambda e^{-\lambda t} \tag{7.22}$$

$$F(t) = 1 - e^{-\lambda t} \tag{7.23}$$

$$S(t) = e^{-\lambda t} \tag{7.24}$$

$$\lambda(t) = -\frac{\mathrm{d}\log S(t)}{\mathrm{d}t} = \lambda \tag{7.25}$$

$$H(t) = \lambda t \tag{7.26}$$

$$\mathbb{E}(T) = \frac{1}{\lambda} \tag{7.27}$$

$$var(T) = \frac{1}{\lambda^2} \tag{7.28}$$

- Weibull $T \sim W(p, \lambda) = [\varepsilon(\lambda^p)]^{1/p}$, degrade to exponential $\varepsilon(\lambda)$ when $p = 1$[62]

$$f(t) = p\lambda^p t^{p-1} e^{-(\lambda t)^p} \tag{7.29}$$
$$F(t) = 1 - e^{-(\lambda t)^p} \tag{7.30}$$
$$S(t) = e^{-(\lambda t)^p} \tag{7.31}$$
$$\lambda(t) = p\lambda^p t^{p-1} \tag{7.32}$$
$$H(t) = (\lambda t)^p \tag{7.33}$$
$$\mathbb{E}(T) = \frac{1}{\lambda}\Gamma(1 + \frac{1}{p}) \tag{7.34}$$
$$var(T) = \frac{1}{\lambda^2}\left[\Gamma(1 + \frac{2}{p}) - (\Gamma(1 + \frac{1}{p}))^2\right] \tag{7.35}$$
$$t_{0.5} = \left[\frac{\log 2}{\lambda^p}\right]^{1/p} \tag{7.36}$$

- Gamma $T \sim \Gamma(\alpha, \lambda)$. Degrade to exponential $\varepsilon(\lambda)$ when $\alpha = 1$, to $2\lambda T \sim \chi^2_{2\alpha}$ when $2\alpha \in \mathbb{N}$

$$F(t) = \frac{\lambda^\alpha}{\Gamma(\alpha)} t^{\alpha-1} e^{-\lambda t} \tag{7.37}$$
$$\mathbb{E}(T) = \frac{\alpha}{\lambda} \tag{7.38}$$
$$var(T) = \frac{\alpha}{\lambda^2} \tag{7.39}$$

- Log-Normal $T \sim \text{LN}(\mu, \sigma^2) = \exp\left[N(\mu, \sigma^2)\right]$.

$$f(t) = \frac{\phi(\frac{\log(t) - \mu}{\sigma})}{t\sigma} \tag{7.40}$$
$$F(t) = \Phi\left(\frac{\log(t - \mu)}{\sigma}\right) \tag{7.41}$$
$$S(t) = 1 - \Phi\left(\frac{\log(t - \mu)}{\sigma}\right) \tag{7.42}$$
$$\mathbb{E}(T) = e^{\mu + \frac{\sigma^2}{2}} \tag{7.43}$$
$$var(T) = e^{2\mu + \sigma^2}(e^{\sigma^2} - 1) \tag{7.44}$$

- Generalized Gamma $T \sim \text{GG}(\alpha, p, \lambda)$, degrade to Weibull when $\alpha = p$, to Gamma when $p = 1$

$$f(t) = p\lambda(\lambda t)^{\alpha-1} e^{-(\lambda t)^p} \Big/ \Gamma(\frac{\alpha}{p}) \tag{7.45}$$
$$\mathbb{E}(T) = \frac{\Gamma((\alpha + 1)/p)}{\lambda\Gamma(\alpha/p)} \tag{7.46}$$

□ Likelihood for Censored Data

When dealing with censored data, we put a basic assumption that $T \parallel C$ so that we can consider their distribution

[62] Weibull distribution could also be parameterized as $W(p, \gamma)$, where $\gamma = 1/\lambda$ is the scale factor.

separately:

$$\text{General Notation:} \begin{cases} f(t) \\ F(t) \\ S(t) \\ \lambda(t) \end{cases} \quad T: \begin{cases} f_T(t) \\ F_T(t) \\ S_T(t) \\ \lambda_T(t) \end{cases} \quad C: \begin{cases} f_C(t) \\ F_C(t) \\ S_C(t) \\ \lambda_C(t) \end{cases} \tag{7.47}$$

Probability that we observe either T or C, or equivalently observe $(\tilde{T}, \delta)$:

$$\mathbb{P}(\tilde{T}, \delta) = \begin{cases} f_T(t)S_C(t), & \text{case event} \\ f_C(t)S_T(t), & \text{case censor} \end{cases} \tag{7.48}$$

$$= [f_T(t)S_C(t)]^{\delta} [f_C(t)S_T(t)]^{1-\delta} \tag{7.49}$$

$$\propto f_T(t)^{\delta} S_T(T)^{1-\delta} = \lambda_T(t)^{\delta} S_T(t) \tag{7.50}$$

Likelihood for estimating survival $S(t)$ can be taken as the part of T:

$$L(\theta; \tilde{t}, \delta) = \prod_{i=1}^{n} f_T(\tilde{t}_i; \theta)^{\delta_i} S_T(\tilde{t}_i; \theta)^{1-\delta_i} = \prod_{i=1}^{n} \lambda_T(\tilde{t}_i; \theta)^{\delta_i} S_T(\tilde{t}_i; \theta) \tag{7.51}$$

$$= \prod_{e\in\mathcal{E}} f(\tilde{t}_e; \theta) \prod_{r\in\mathcal{R}} S(\tilde{t}_r; \theta) \tag{7.52}$$

where $\mathcal{E}$ denotes indices of event data, $\mathcal{R}$ for indices of right censored data. This form can be generalized to more kinds of censoring, e.g. left censor $\mathcal{L}$, interval censor $\mathcal{I} = \{(t_{i,l}, t_{i,r})\}_{i=1}^{n_{\mathcal{I}}}$:

$$L(\theta; \tilde{t}, \delta) = \prod_{e\in\mathcal{E}} f(\tilde{t}_e; \theta) \prod_{r\in\mathcal{R}} S(\tilde{t}_r; \theta) \prod_{l\in\mathcal{R}} [1 - S(\tilde{t}_l; \theta)] \prod_{(t_{i,l}, t_{i,r})\in\mathcal{I}} [S(\tilde{t}_{i,l}; \theta) - S(\tilde{t}_{i,r}; \theta)] \tag{7.53}$$

then use proper methods to maximize the Likelihood / conduct hypothesis testing. Following are some knowledeg recap for inference concerning likelihood:

☐ **Likelihood Function**

Knowledge on likelihood function see section. 2.2.4. Some recap:

$$\text{Likelihood: } L(\theta; X_1, X_2, \ldots, X_n) = \prod_{i=1}^{n} f(X_i; \theta) \tag{7.54}$$

$$\text{Log-Likelihood: } \ell(\theta; X_1, X_2, \ldots, X_n) = \sum_{i=1}^{n} \log\{f(X_i; \theta)\} \tag{7.55}$$

$$\text{Score: } U(\theta; X_1, X_2, \ldots, X_n) = \frac{\partial \ell(\theta; X_1, X_2, \ldots, X_n)}{\partial\theta} = \sum_{i=1}^{n} \frac{\partial \log\{f(X_i; \theta)\}}{\partial\theta} \tag{7.56}$$

$$\text{Fisher Information: } I(\theta) = -\mathbb{E}\left[\frac{\partial^2 \log f(\vec{X}; \theta)}{\partial\theta\partial\theta^T}\right] = -n\mathbb{E}_{\vec{X}}\left[\frac{\partial^2 \log f(X_i; \theta)}{\partial\theta\partial\theta^T}\right] = n\bar{I}(\theta) \tag{7.57}$$

$$\bar{I} = I_i(\theta) = -\mathbb{E}\left[\frac{\partial^2 \log f(X_i; \theta)}{\partial\theta\partial\theta^T}\right] \tag{7.58}$$

$$\text{Observed Information: } I_n(\theta) = J(\theta) = -\sum_{i=1}^{n} \frac{\partial^2 \log f(X_i; \theta)}{\partial\theta\partial\theta^T} \tag{7.59}$$

Note: Fisher is an expectation of function of r.v., not random.

Properties:

$$\mathbb{E}_{\vec{X}}\left[U(\theta;\vec{X})\right] = 0 \tag{7.60}$$

$$I(\theta) = -\mathbb{E}_{\vec{X}}\left[\frac{\partial^2 \log f(\vec{X};\theta)}{\partial\theta\partial\theta^T}\right] \tag{7.61}$$

$$= \mathbb{E}_{\vec{X}}\left[\frac{\partial \log f(\vec{X};\theta)}{\partial\theta}\frac{\partial \log f(\vec{X};\theta)}{\partial\theta^T}\right] = \mathbb{E}_{\vec{X}}\left[U(\theta;\vec{X})U(\theta;\vec{X})^T\right] \tag{7.62}$$

$$var_{\vec{X}}\left[U(\theta;\vec{X})\right] = \mathbb{E}_{\vec{X}}\left[\left(U(\theta;\vec{X}) - \mathbb{E}_{\vec{X}}\left[U(\theta;\vec{X})\right]\right)\left(U(\theta;\vec{X}) - \mathbb{E}_{\vec{X}}\left[U(\theta;\vec{X})\right]\right)^T\right] \tag{7.63}$$

$$= \mathbb{E}_{\vec{X}}\left[U(\theta;\vec{X})U(\theta;\vec{X})^T\right] = I(\theta) \tag{7.64}$$

$$\tag{7.65}$$

By CLT, considering U as a function of r.v.: (for a given θ and the data generated from the distribution with **this** parameter θ, i.e. $U(\theta) = U\left(\theta;\vec{X}(\theta)\right)$)

$$\sqrt{n}\left\{\bar{U}(\theta) - \mathbb{E}(U(\theta))\right\} = \frac{1}{\sqrt{n}}U(\theta) \xrightarrow{\mathscr{L}} N(0, \frac{I(\theta)}{n}) \tag{7.66}$$

and by taking MLE estimation $\hat{\theta}^{MLE} \xrightarrow{p} \theta^*$, we can estimate the distribution (Note that MLE Estimator requires $U(\theta) = 0$)

$$J(\hat{\theta})^{-1/2}\left(U(\hat{\theta}) - \mathbb{E}(U(\hat{\theta}))\right) = J(\hat{\theta})^{-1/2}U(\hat{\theta}) \xrightarrow{\mathscr{L}} N(0,1) \tag{7.67}$$

☐ **Statistical Inference on Parameter θ**

Statistical Inference concerning θ can be conducting using the above functions of θ

- Score Test: Use the distribution of score function directly: we can construct

$$J(\theta_0)^{-1/2}U(\theta_0;\vec{X}(\theta)) \xrightarrow[H_0]{\mathscr{L}} N(0,1) \tag{7.68}$$

explanation: under $H_0 : \theta = \theta_0$, we should have $\hat{\theta} \to \theta = \theta_0$, which would lead to

$$J(\theta_0)^{-1/2}U(\theta_0;\vec{X}(\theta_0)) \xrightarrow{\mathscr{L}} N(0,1) \tag{7.69}$$

however if $\hat{\theta} \to \theta \neq \theta_0$, then

$$\mathbb{E}\left[U(\theta_0;\vec{X}(\theta))\right] \neq 0 \tag{7.70}$$

which would lead to a different distribution, thus we can test the assumption $H_0 : \theta = \theta_0$ using equation. 7.68. Conduct hypothesis testing utilizing the fractiles of $N(0,1)$

- Wald Test: Use the Taylor Series of $U(\theta)$ to the 1st order

$$U(\theta) \approx -J(\hat{\theta})(\theta - \hat{\theta}) \Rightarrow J(\hat{\theta})^{1/2}(\hat{\theta} - \theta) \approx J(\hat{\theta})^{-1/2}U(\hat{\theta}) \xrightarrow{\mathscr{L}} N(0,1) \tag{7.71}$$

i.e.

$$\hat{\theta} \xrightarrow{\mathscr{L}} N(\theta, J(\hat{\theta})^{-1}) \tag{7.72}$$

which can be utilized to construct testing statistics/interval estimations.

- Likelihood Ratio Test: Use the Taylor Series of $\ell(\theta)$ to the 2nd order, and take $\hat{\theta}=\hat{\theta}^{MLE}$ so that $\ell'(\hat{\theta})=0$

$$\ell(\theta)\approx\ell(\hat{\theta})-\frac{1}{2}(\theta-\hat{\theta})^TJ(\theta)(\theta-\hat{\theta})\Rightarrow 2(\ell(\hat{\theta})-\ell(\theta))\approx(\theta-\hat{\theta})^TJ(\theta)(\theta-\hat{\theta})\xrightarrow{\mathscr{L}}\chi_p^2 \tag{7.73}$$

where p is the dimension of θ

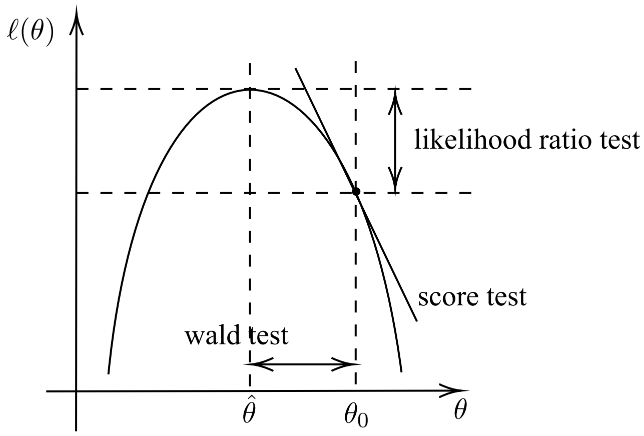


图 5: Illustration of Tests on $\ell(\theta)$-θ Plot

7.2.3 Non-Parametric Estimation to Survival Function

In this part we only focus on right censor data $(\tilde{T}_i,\delta_i)$, $\delta_i=0$ for right censoring.

☐ **Kaplan-Meier Estimator**

Idea of KM Estimator: Separate time into segments by censor/event time t_i, and decompose survival function into products of hazard within segments, using equation. 7.15 which is:

$$\hat{S}(t)=\hat{\mathbb{P}}(T>t)=\prod_{t_i\le t}\hat{\mathbb{P}}(T>t_i|T>t_{i-1}) \tag{7.74}$$

$$=\hat{\mathbb{P}}(T>t|T>t_i)\prod_{t_i\le t}\left[1-\hat{\mathbb{P}}(t_i\ge T>t_{i-1}|T>t_{i-1})\right] \tag{7.75}$$

$$=\left(1-\hat{\lambda}(t_i)\right)\prod_{t_i\le t}\left(1-\hat{\lambda}(t_{i-1})\right) \tag{7.76}$$

$$=\prod_{t_i\le t}\left[1-\hat{\lambda}(t_i)\right] \tag{7.77}$$

where $\hat{\lambda}(t_i)$ are relatively easy to estimate with censoring considered. r_i for # at risk: not censored/event till t_i, d_i for # event (death). We can model $\hat{\lambda}_i$ as

$$d_i|r_i\sim B(r_i,\lambda_i)\xrightarrow{\mathscr{L}}N(r_i\lambda_i,r_i\lambda_i(1-\lambda_i)) \tag{7.78}$$

and obtain the MLE estimation of $\hat{\lambda}_i|r_i,d_i$[63]

[63]Here we use the Δ method for estimating the variance of function of r.v.: if $X\sim f(\mu,\sigma^2)$:

$$g(X)\approx g(\mu)+g'(\mu)(X-\mu)\Rightarrow var(g(X))\approx[g'(\mu)]^2var(X)\leftarrow[g'(X)]^2var(X) \tag{7.79}$$

$$\hat{\lambda}_i = \frac{d_i}{r_i} \tag{7.80}$$

$$var(\hat{\lambda}_i) = var(\frac{d_i}{r_i}) = \frac{\hat{\lambda}_i(1-\hat{\lambda}_i)}{r_i} \tag{7.81}$$

$$\hat{S}(t) = \prod_{t_i \le t} \left[1 - \hat{\lambda}(t_i)\right] = \prod_{t_i \le t} \left[1 - \frac{d_i}{r_i}\right] \tag{KM Estimator}$$

$$var(\hat{S}(t)) = var\left\{\exp\left[\log S\hat{(t)}\right]\right\} \tag{7.82}$$

$$\approx [\hat{S}(t)]^2 var\left[\log \hat{S}(t)\right] \tag{7.83}$$

$$= [\hat{S}(t)]^2 \sum_{t_i \le t} var\left[\log(1-\hat{\lambda}_i)\right] \tag{7.84}$$

$$= [\hat{S}(t)]^2 \sum_{t_i \le t} \frac{1}{(1-\hat{\lambda}_i)^2} var(\hat{\lambda}_i) \tag{7.85}$$

$$= [\hat{S}(t)]^2 \sum_{t_i \le t} \frac{d_i}{r_i(r_i - d_i)} \tag{Greenwood' Formula}$$

$$= [\hat{S}(t)]^2 var(\hat{\Lambda}(t)) \tag{7.86}$$

Interval Estimation of $\hat{S}(t)$ can be conducted using pointwise interval/confidence band:

- Plain pointwise approach:

$$\hat{S}(t) \pm N_{1-\frac{\alpha}{2}} \sigma[\hat{S}(t)] \tag{7.87}$$

- Log-Log pointwise approach (`R.` default): using $\hat{L}(t) = \log\left[-\log \hat{S}(t)\right] = \log\left[\hat{\Lambda}(t)\right]$

$$\hat{S}(t) \times e^{\pm N_{1-\frac{\alpha}{2}} \sigma(\hat{L}(t))} \tag{7.88}$$

  where

$$\sigma(\hat{L}(t)) = \sqrt{\frac{1}{[\log \hat{S}(t)]^2} \sum_{t_i \le t} \frac{d_i}{r_i(r_i - d_i)}} \tag{7.89}$$

- EP confidence band approach
- HW confidence band approach

Estimator of mean survival time:

$$\hat{\mu}_\tau = \int_0^\tau \hat{S}(t)\, \mathrm{d}t \tag{7.90}$$

$$var(\hat{\mu}_\tau) = \sum_{t_i} \left[\int_{t_i}^\tau \hat{S}(t)\, \mathrm{d}t\right]^2 \frac{d_i}{r_i(r_i - d_i)} \tag{7.91}$$

□ **Nelson-Aalen Estimator**

Idea of NA Estimator: estimate $\hat{\Lambda}(t)$ first, then obtain Fleming-Harrington Estimator $\hat{S}_{FH}(t) = e^{-\hat{\Lambda}(t)}$:

$$\hat{\Lambda}(t) = \sum_{t_i \le t} \hat{\lambda}(t_i) = \sum_{t_i \le t} \frac{d_i}{r_i} \tag{7.92}$$

$$var(\hat{\Lambda}(t)) = \sum_{t_i \le t} \frac{d_i(r_i - d_i)}{r_i^2(r_i - 1)} \tag{7.93}$$

$$\hat{S}_{FH}(t) = \exp\left[-\hat{\Lambda}(t)\right] \tag{7.94}$$

☐ **Survival Function of Life Table**

A key difference of survival data of life table is that we cannot know the exact event time/censor time, locating in $[t_{i-1}, t_i)$, in this case we usually estimate d_i, r_i using

$$d_i' = d_i \tag{7.95}$$

$$r_i' = r_i - \frac{c_i}{2} \tag{7.96}$$

where c_i is # censor in $[t_i, t_{i+1})$, r_i is # censoring at the begeining of interval, i.e. t_{i-1}. And construct KM/NA estimator:

$$\hat{S}_{KM}(t) = \prod_{t_i \leq t} \left(1 - \frac{d_i}{r_i'}\right) \tag{7.97}$$

$$var(\hat{S}_{KM}(t)) = \left[\hat{S}_{KM}(t)\right]^2 \sum_{t_i \leq t} \frac{d_i}{r_i'(r_i' - d_i)} \tag{7.98}$$

$$\hat{\lambda}(t_{\text{mid}\, i}) = = \frac{\hat{f}(t_i)}{\hat{S}(t_i)} = \frac{d_i}{(t_i - t_{i-1})(r_i' - \frac{d_i}{2})} = \frac{d_i}{(t_i - t_{i-1})(r_i - \frac{c_i + d_i}{2})} \tag{7.99}$$

where mid i means the mid point of $[t_{i-1}, t_i)$, i.e. $\dfrac{t_{i-1} + t_i}{2}$

7.2.4 Hypothesis Testing to Group Comparison

Key focus: how to judge the difference between two survival function $S_1(t)$, $S_2(t)$, or even when there are more than two groups.

☐ **Mantel-Haenszel Logrank Test** [64]

Idea of logrank test: adapt contingency table to censor table

表 4: 2×2 contingency table

	Event δ		
Group	Yes(1)	No(0)	Total
0	d_0	$r_0 - d_0$	r_0
1	d_1	$r_1 - d_1$	r_1
Total	d	$r - d$	r

- Recap: Pearson's χ^2 test: assign n sample into k groups, and conduct test on p_i, $i = 1, 2, \ldots, k$, denote that v_i samples are assigned to the i^{th} groups, then

$$K_n = \sum_{i=1}^{k} \frac{(v_i - np_i)^2}{np_i} \xrightarrow{\mathscr{L}} \chi^2_{df} \tag{7.100}$$

In the above example, $df = k - 1$. In 2×2 contingency table, $df = 1$ because we assume d, r, r_0, r_1 are fixed.

[64] Note: Log means 'time record' here, rather than logarithm.

Pearson's χ^2 statistics for 2×2 contingency table:

$$\chi_P^2 = \sum_{\text{4 grids}} \frac{(\text{obs} - \text{expe})^2}{\text{expe}} \tag{7.101}$$

$$= \frac{(d_0 - r_0 \frac{d}{r})^2}{r_0 \frac{d}{r}} + \text{etc} \tag{7.102}$$

$$= \frac{\left[d_0 - r_0 \frac{d}{r}\right]^2}{r_0 r_1 d(r-d)/r^3} \sim \chi_1^2 \tag{7.103}$$

- Recap: Mental-Haenszel test, based on the Hypergeometric distribution that

$$d_0 \sim H(r_0, d, r) \Rightarrow \begin{cases} \mathbb{E}(d_0) = r_0 \frac{d}{r} \\ var(d_0) = \frac{r_0 r_1 d(r-d)}{r^2(r_0 - 1)} \end{cases}, \quad d_1, r_0 - d_0, r_1 - d_1 \text{ similar} \tag{7.104}$$

and construct

$$\chi_{MH}^2 = \frac{\left(\sum_{\text{4 grids}} \text{obs} - \mathbb{E}(\text{obs})\right)^2}{\sum_{\text{4 grids}} var(\text{obs})} = \frac{\left[d_0 - r_0 \frac{d}{r}\right]^2}{\frac{r_0 r_1 d(r-d)}{r^2(r-1)}} \sim \chi_1^2 \tag{7.105}$$

χ_{MH}^2 and χ_P^2 are equal for lare r.

$$\chi_{MH}^2 = \frac{r-1}{r} \chi_P^2 \tag{7.106}$$

- Cochran-Mantel-Haenszel log-rank test

For survival data $t_1, t_2, \ldots, t_K$, we can construct a contingency table $\mathcal{C}_i$ at each time, and test on the $K \times 2 \times 2$ contingency table sequence:

表 5: 2×2 contingency table, $j = 1, 2, \ldots, K$

	Event δ		
Group	Yes(1)	No(0)	Total
0	d_{0j}	$r_{0j} - d_{0j}$	r_{0j}
1	d_{1j}	$r_{1j} - d_{1j}$	r_{1j}
Total	d_j	$r_j - d_j$	r_j

and get the CMH statistics for testing $H_0 : \theta_{t_1} = \theta_{t_2} = \ldots = \theta_{t_K} = 1$, θ for odds ratio between group 0/1.

$$\chi_{CMH}^2 = \frac{\left[\sum_{j=1}^K (d_{0j} - r_{0j} \frac{d_j}{r_j})\right]^2}{\sum_{j=1}^K \frac{r_{0j} r_{1j} d_j (r_j - d_j)}{r_j^2 (r_j - 1)}} \sim \chi_1^2 \tag{7.107}$$

where the K contingency tables are treated independent, but they are still ordinal beacuse r_j contains information of history $d_{t_i < t_j}$, $c_{t_i < t_j}$

Properties & Special Cases & Extension of CMH logrank test:

- No tied death $d_j = 1$:

$$\chi_{CMH}^2 = \frac{\left[\sum_{j=1}^K (d_{0j} - r_{0j} \frac{d_j}{r_j})\right]^2}{\sum_{j=1}^K \frac{r_{0j} r_{1j} d_j (r_j - d_j)}{r_j^2 (r_j - 1)}} = \frac{\left[\sum_{j=1}^K (d_{0j} - r_{0j} \frac{d_j}{r_j})\right]^2}{\sum_{j=1}^K \frac{r_{0j} r_{1j}}{r_j^2}} \sim \chi_1^2, \quad d_{0j} \in \{0, 1\} \tag{7.108}$$

- Intuition of obs $-\mathbb{E}$ (obs):

$$\begin{aligned}\text{obs}-\mathbb{E}(\text{obs}) \approx & d_{0j}-d_j\frac{r_{0j}}{r_j} & (7.109)\\ = & \frac{r_{0j}r_{1j}}{r_j}\left(\hat{\lambda}_{0j}-\hat{\lambda}_{1j}\right) & (7.110)\end{aligned}$$

- Attach weight $w_i \geq 0, i=1,2,\ldots,K$ to $\mathcal{C}_i$:

$$\chi^2_{CMH,w}=\frac{\left[\sum_{j=1}^K w_j(d_{0j}-r_{0j}\frac{d_j}{r_j})\right]^2}{\sum_{j=1}^K w_j^2\frac{r_{0j}r_{1j}d_j(r_j-d_j)}{r_j^2(r_j-1)}}\sim\chi^2_1 \quad (7.111)$$

bu choosing differnet kinds of weight $\vec{w}$ we could get variants of CMH test.

  - $w_i=1$ for log-rank test. Focus more on difference at large t
  - $w_i=r_i$ for generalized Wilcoxon rank sum test. Focus more on difference at small t.

Note: weighted log-rank test should be used when **no cross** btw. $S_1(t)$ and $S_2(t)$. Kink-of-Weight to choose depends on H_1.

☐ **Generalized Wilcoxon Rank Sum Test**

- Wilcoxon Two-Sample Rank Sum Test: Knowledge of Wilcoxon two-sample rank sum test see section. 2.4.6. Recap: to test the distribution difference of $\vec{X}=(X_1,X_2,\ldots,X_n)$ and $\vec{Y}=(Y_1,Y_2,\ldots,Y_m)$, we mix them together and rank as $\vec{Z}=(Z_{(1)},Z_{(2)},\ldots,Z_{(m+n)})$. Rank of X_i:

$$\begin{aligned}R_i \equiv & \text{rank}(X_i) \text{ in } \vec{Z},\quad i=1,2,\ldots,n & (7.112)\\ R\equiv & \sum_{i=1}^n R_i & (7.113)\end{aligned}$$

A rank sum statistic to test:

$$\frac{R-\mathbb{E}(R)}{\sqrt{var(R)}}\sim N(0,1) \quad (7.114)$$

$$\begin{cases}\mathbb{E}(R)=\dfrac{n(m+n+1)}{2}\\ var(R)=\dfrac{mn(m+n+1)}{12}\end{cases} \quad (7.115)$$

Rank sum statistic can be written in a Mann-Whitney form that can be generalized:

$$U_{ij}=U(X_i,Y_j)\equiv\begin{cases}+1 & ,\text{case } X_i>Y_j\\ 0 & ,\text{case } X_i=Y_j\\ -1 & ,\text{case } X_i<Y_j\end{cases},\qquad U=\sum_{i,j}^{n,m}U_{ij} \quad (7.116)$$

$$R=\frac{n(m+n+1)}{2}+\frac{U}{2} \quad (7.117)$$

- Mann-Whitney-Wilcoxon rank sum test for censored data:

Notation: we still mix $X=\{(\tilde{t}_{1i},\delta_{1i})\}_{i=1}^n$ and $Y=\{(\tilde{t}_{2j},\delta_{2j})\}_{j=1}^m$ to get:

$$Z_{\text{mix}}=\left\{(\tilde{t}_i,\delta_i)\right\}_{i=1}^{m+n} \quad (7.118)$$

and the Mann-Whitney form for Z_{mix}:

$$U_{ij} = U(Z_i, Z_j) \equiv \begin{cases} +1 & \text{, case } \tilde{t}_i > \tilde{t}_j,\ \delta_j = 1 \\ 0 & \text{, case } \tilde{t}_i = \tilde{t}_j \text{ or } \delta_j = 0 \\ -1 & \text{, case } \tilde{t}_i < \tilde{t}_j,\ \delta_j = 1 \end{cases}, \quad i = 1, 2, \ldots, m+n.\ j = 1, 2, \ldots, m+n. \tag{7.119}$$

and the Extended Wilcoxon rank sum statistic:

$$W = \sum_{i \text{ if } Z_i \in X}^{m+n} \sum_{j=1}^{m+n} U_{ij} \tag{7.120}$$

Under $H_0 : X \sim Y$, distribution features

$$\mathbb{E}(W) = 0 \tag{7.121}$$

$$v\hat{a}r(W) = \frac{mn}{(m+n)(m+n-1)} \sum_{i=1}^{m+n} \left(\sum_{j=1}^{m+n} U_{ij} \right)^2 \tag{7.122}$$

– choose $w_i = r_i$ in weighted log-rank test, and nominator becomes

$$\sum_{j=1}^{K} r_j (d_{0j} - r_{0j} \frac{d_j}{r_j}) = \sum_{j=1}^{K} \left[(r_{1j} - d_{1j}) d_{0j} - (r_{0j} - d_{0j}) d_{1j} \right] \tag{7.123}$$

$$= \sum_{j=1}^{K} \left[\#_{Y > t_j} \times \#_{X = t_j} - \#_{X > t_j} \times \#_{Y = t_j} \right] \tag{7.124}$$

$$= \#_{Y > X} - \#_{Y < X} \tag{7.125}$$

$$= -W \tag{7.126}$$

in which $\chi^2_{w_i = r_i, CMH}$ test is the same as generalized Wilcoxon rank sum test.

Section 7.3 Survival Model with Covariants

To research on the dependence of T with regard to covariants z. Survival data with covariants: $X = (\tilde{t}_i, \delta_i, z_i)$

7.3.1 Cox's Proportion Hazard Model

Basic assumption on dependence form: T hazard part and covariants part are Separatable:

$$\lambda(t|z) = \lambda_0(t) g(z) \Leftrightarrow S(t|z) = [S_0(t)]^{g(z)}, \quad S_0(t) = e^{-\int_0^t \lambda_0(\tau)\, \mathrm{d}\tau} \tag{7.127}$$

further a linear form $g(z) = \beta^T z$ is used;

$$\lambda(t|z) = \lambda_0(t) \exp\left[\beta^T z\right] \tag{7.128}$$

Basic Assumptions of Cox's PH Model:

- constant regression coefficient β;
- linear dependent of covariants $\beta' z$;

- exponential link function $e^{\cdot}$

in this proportion hazard model, the ratio of hazard only depend on β:

$$\log\left\{\frac{\lambda_{z_i}(t)}{\lambda_0(t)}\right\} = \beta^T z_i \parallel t \tag{7.129}$$

The unknown components are $\lambda_0(t), \beta$, where the $\lambda_0(t)$ lies in the $dim \to \infty$ space, and causes difficulty in conducting inference. Solution: decompose full likelihood into two parts, in which one of them, **Partial Likelihood** is only function of β:

$$L(\beta, \lambda_0(\cdot); X) = \prod_i \left[\left(\lambda_0(t_i)e^{\beta^T z_i}\right)_i^{\delta} \left(e^{-\int_0^{t_i}\lambda_0(\tau)\,\mathrm{d}\tau}\right)^{e^{\beta^T z_i}}\right] \tag{7.130}$$

$$= L_{PH}(\beta; X) L_{res}(\beta, \lambda_0; X) \tag{7.131}$$

and we could focus on L_{PH} for further inference.

Note: the feasibility of partial likelihood comes from the form of proportion hazard.

☐ **Partial Likelihood without Tie**

Derivation: First we assert t_i in ascending order and without tie: $t_1 < t_2 < \ldots < t_n$, and we use an discrete estimated form of $\lambda_0(t_i) = \lambda_i$

$$\int_0^{t_i} \lambda_0(\tau)\,\mathrm{d}\tau \approx \sum_{j=1}^{i} \lambda_j \tag{7.132}$$

then we could use a trick to reformulate $\ell(\beta, \lambda_1, \ldots, \lambda_n; X)$ as[65]

$$\ell(\beta, \lambda_1, \ldots, \lambda_n) = \sum_{i=1}^{n}\left\{\delta_i(\log\lambda_i + \beta' z_i) - \sum_{j=1}^{i}\lambda_j e^{\beta' z_i}\right\} \tag{7.134}$$

$$= \sum_{i=1}^{n}\left\{\delta_i(\log\lambda_i + \beta' z_i) - \lambda_i \sum_{j=i}^{n} e^{\beta' z_j}\right\} \tag{7.135}$$

and use MLE with regard to λ_i to get an estimate to λ_i:

$$\frac{\partial \ell(\beta, \lambda_1, \ldots, \lambda_n)}{\partial \lambda_i} = 0 \Rightarrow \lambda_i(\beta) = \frac{\delta_i}{\sum_{j=1}^{n} e^{\beta' z_j}} \quad \forall i \tag{7.136}$$

---

[65] Illustration for $\sum_{i=1}^{n}\lambda_i \sum_{j=i}^{n} e^{\beta' z_j} = \sum_{i=1}^{n}\sum_{j=1}^{i}\lambda_j e^{\beta' z_i}$

$$\begin{array}{cc}
\begin{pmatrix}
\lambda_1 e^{\beta' z_1} & & & & \\
\lambda_1 e^{\beta' z_2} & \lambda_2 e^{\beta' z_2} & & & \\
\lambda_1 e^{\beta' z_3} & \lambda_2 e^{\beta' z_3} & \lambda_3 e^{\beta' z_3} & & \\
\vdots & \vdots & \vdots & \ddots & \\
\lambda_1 e^{\beta' z_n} & \lambda_2 e^{\beta' z_n} & \lambda_3 e^{\beta' z_n} & \cdots & \lambda_n e^{\beta' z_n}
\end{pmatrix}
&
\begin{array}{l}
\leftarrow \sum_{j=1}^{1}\lambda_j e^{\beta' z_1} \\
\leftarrow \sum_{j=1}^{2}\lambda_j e^{\beta' z_2} \\
\leftarrow \sum_{j=1}^{3}\lambda_j e^{\beta' z_3} \\
\leftarrow \vdots \\
\leftarrow \sum_{j=1}^{n}\lambda_j e^{\beta' z_n}
\end{array}
\\
\begin{array}{ccccc}
\uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\
\lambda_1 \sum_{j=1}^{n} e^{\beta' z_j} & \lambda_2 \sum_{j=2}^{n} e^{\beta' z_j} & \lambda_3 \sum_{j=3}^{n} e^{\beta' z_j} & \therefore & \lambda_n \sum_{j=n}^{n} e^{\beta' z_j}
\end{array}
&
\sum_{i=1}^{n}\lambda_i \sum_{j=i}^{n} e^{\beta' z_j} = \sum_{i=1}^{n}\sum_{j=1}^{i}\lambda_j e^{\beta' z_i}
\end{array} \tag{7.133}$$

then we could get the partial likelihood

$$L(\beta, \lambda_1(\beta), \ldots, \lambda_n(\beta)) = \prod_{i=1}^{n} \lambda_i(\beta)^{\delta_i} e^{\delta_i \beta' z_i} e^{-\sum_{j=1}^{n} e^{\beta' z_i}} \tag{7.137}$$

$$= e^{-\sum_i \delta_i} \prod_{i=1}^{n} \left(\frac{e^{\beta' z_i}}{\sum_{j:t_j \geq t_i} e^{\beta' z_j}} \right)^{\delta_i} \tag{7.138}$$

$$PL(\beta) \equiv \prod_{i=1}^{n} \left(\frac{e^{\beta' z_i}}{\sum_{j:t_j \geq t_i} e^{\beta' z_j}} \right)^{\delta_i} \tag{7.139}$$

$$P\ell = \sum_{i=1}^{n} \delta_i \left[\beta' z_i - \log \left(\sum_{j:t_j \geq t_i} e^{\beta' z_j} \right) \right] \tag{7.140}$$

$$U(\beta) = \sum_{i=1}^{n} \delta_i \left[z_i - \frac{\sum_{j:t_j \geq t_i} z_j e^{\beta' z_j}}{\sum_{j:t_j \geq t_i} e^{\beta' z_j}} \right] \tag{7.141}$$

$$J(\beta) = \sum_{i=1}^{n} \delta_i \left[\sum_{j:t_j \geq t_i}^{n} \frac{e^{\beta' z_j}}{\sum_{l:t_l \geq t_j} e^{\beta' z_l}} \left(z_j - \frac{\sum_{l:t_l \geq t_j} z_l e^{\beta' z_l}}{\sum_{l:t_l \geq t_j} e^{\beta' z_l}} \right)^2 \right] \tag{7.142}$$

The above statistics can be use for further inference.

$$J(\beta_0)^{-1/2} U(\beta_0) \xrightarrow{\mathscr{L}} N(0,1) \tag{7.143}$$

$$(\hat{\beta} - \beta_0) \xrightarrow{\mathscr{L}} N(0, J(\hat{\beta})^{-1}) \tag{7.144}$$

$$2(\ell(\hat{\beta}) - \ell(\beta)) \xrightarrow{\mathscr{L}} \chi_p^2 \tag{7.145}$$

□ **Modification for Partial Likelihood with Tie**

There are various modification for tied data case. In PL without tie, the $\frac{e^{\beta' z_i}}{\sum_{j:t_j \geq t_i} e^{\beta' z_j}}$ term are usually changed to adapt for the case of. Intuition:

$$\frac{e^{\beta' z_i}}{\sum_{j:t_j \geq t_i} e^{\beta' z_j}} = \frac{\lambda(t_i|z_i)}{\sum_{j:t_j \geq t_i} \lambda(t_j|z_j)} \approx \mathbb{P}\left(i^{\text{th}}\text{event} | 1\text{out of } \#\{j : t_j \geq t_i\} \right) \tag{7.146}$$

Notation: $\mathcal{R}_i$ for all datapoints at risk at time t_i, $\mathcal{D}_i$ for event cases at time t_i, $\mathcal{D}_i \subset \mathcal{R}_i$

- Cox's modification: 索引 Cox's Modification

$$\mathbb{P}\left(\mathcal{D}_i \text{ events} \middle| |\mathcal{D}_i| \text{out of } \#\{j : t_j \geq t_i\} \right) = \frac{e^{\sum_{l \in \mathcal{D}_i} \beta' z_l}}{\sum_{\text{all possible } |\mathcal{D}_j| = |\mathcal{D}_i|} e^{\sum_{l \in \mathcal{D}_j} \beta' z_j}} \tag{7.147}$$

drawback: $\sim O(|\mathcal{D}_i|!)$ complexity

$$PL(\beta) = \prod_{i=1}^{n} \left\{ \frac{e^{\sum_{l \in \mathcal{D}_i} \beta' z_l}}{\sum_{\text{all possible } |\mathcal{D}_j| = |\mathcal{D}_i|} e^{\sum_{l \in \mathcal{D}_j}} e^{\sum_{l \in \mathcal{D}_j} \beta' z_l}} \right\} \tag{7.148}$$

- Breslow's approximation:

$$\mathbb{P}\left(\mathcal{D}_i \text{event} \middle| |\mathcal{D}_i| \text{out of } \#\{j : t_j \geq t_i\} \right) \approx \frac{e^{\sum_{l \in \mathcal{D}_i} \beta' z_l}}{\left(\sum_{l \in \mathcal{R}_i} e^{\beta' z_l} \right)^{|\mathcal{D}_i|}} \tag{7.149}$$

or directly write the PL as

$$PL(\beta) = \prod_{i=1}^{n} \left\{ \prod_{j \in \mathcal{D}_i} \frac{e^{\beta' z_j}}{\sum_{l \in \mathcal{R}_i} e^{\beta' z_l}} \right\} \tag{7.150}$$

- Efron's approximation: usually better than Breslow's, default method in `coxph()`

$$PL(\beta)=\prod_{i=1}^{n}\left\{\frac{e^{\sum_{l\in\mathcal{D}_i}\beta' z_l}}{\prod_{j=1}^{|\mathcal{D}_i|}\left(\sum_{l\in\mathcal{R}_i}e^{\beta' z_l}-\frac{j-1}{|\mathcal{D}_i|}\sum_{l\in\mathcal{D}_i}e^{\beta' z_l}\right)}\right\} \tag{7.151}$$

☐ **Extension for Time-Dependent Variable**

Model:

$$\begin{cases}\lambda(t)= & \lambda_0(t)e^{\beta' z(t)}\\ \lambda(t)= & \lambda_0(t)e^{\beta(t)' z}\end{cases} \tag{7.152}$$

☐ **Diagnostic Methods for PH Assumption**

- log-log plots: for categorical z_1, z_2, use relation

$$\log\left[-\log S(t,z_1)\right]-\log\left[-\log S(t,z_2)\right]=\beta'(z_1-z_2)\perp\!\!\!\perp t \tag{7.153}$$

Plot of $\log\left[\log\hat{S}(t,z)\right]$ should be 'parallel' curves.

- Check the coherence bet. observed data v.s. expected data.

- Goodness-of-fit using Schoenfeld residuals 索引 Schoenfeld Residual

$$\hat{r}_i = z_i-\sum_{j\in\mathcal{R}_i}z_k\cdot p(\hat{\beta},z_k)=z_i\bar{z}_i \tag{7.154}$$

$$p(\beta,z_k):=\frac{e^{\beta' z_k}}{\sum_{j\in\mathcal{R}_k}e^{\beta' z_j}} \tag{7.155}$$

- (Generalized) Cox-Snell Residual for overall goodness-of-fit:

Recall: for r.v. $T\sim f(t)$, $S(t)=\int_t^\infty f(\tau)\,\mathrm{d}\tau$. function of r.v. has distribution:

$$S(T)\sim U(0,1)\Rightarrow\Lambda(T)\sim\varepsilon(1) \tag{7.156}$$

define Cox-Snell Residual:

$$\hat{\Lambda}(z_i)=-\log\hat{S}(z_i) \tag{7.157}$$

the set $\{\hat{\Lambda}(z_i)\}$ could be viewed as a sample from $\varepsilon(1)$, we could test on the distribution, e.g. plot the cumulative hazard **of residual** v.s. residual to check $\Lambda(e)=e$.

- Delta-Beta Residual for infulential: for $\beta=(\beta_0=1,\beta_1,\ldots)$, define

$$\hat{\Delta}_{ij}=\hat{\beta}_j-\hat{\beta}_{j(\wedge i)} \tag{7.158}$$

where $\wedge i$ for estimator with the i^{th} subject removed. Plot the scatter plot of $\hat{\Delta}_{ij}$ to locate influential.

☐ **Experiment Design for Log-rank Test under PH Assumption**

Question: how many events are needed for the testing $H_0:\beta=0 \leftrightsquigarrow H_a:\beta=\beta_a$?

Using log-rank statistics equation. 7.108 in z-test form, under condition 1. no ties $d_j = 0, 1, 2$. β_a is small enough for taylor expansion:[66]

$$T_{CMH} = \frac{\sum_{j=1}^{K}\left(d_{0j} - r_{oj}\frac{d_j}{r_j}\right)}{\sqrt{\sum_{j=1}^{K}\frac{r_{0j}r_{1j}d_j(r_j-d_j)}{r_j^2(r_j-1)}}} \xrightarrow{\mathscr{L}} N(\beta_a\sqrt{d\theta(1-\theta)}, 1) \tag{7.160}$$

where $d = \sum_{j=1} d_j$, θ is the prevalence of group 1.

Power of the test: denote γ for probability of type II error

$$\mathbb{P}\left(T_{CMH} > N_{\alpha/2}|H_a\right) = 1-\gamma \Rightarrow \mu := \beta_a\sqrt{d\theta(1-\theta)} \approx N_{\alpha/2} + N_\gamma \tag{7.161}$$

Minimum number of events:

$$d = \frac{(N_{\alpha/2} + N_\gamma)^2}{\beta_a^2\theta(1-\theta)} \tag{7.162}$$

7.3.2 Accelerated Failure Time Model

Basic form of AFT Model (Accelerated Failure Tome Model) for categorical covariants:

$$S(t; z=1) = S(\gamma t; z=2) \Leftrightarrow \mathbb{P}\left(T_1 > t\right) = \mathbb{P}\left(T_2 > \gamma t\right) \tag{7.163}$$

Usually we attach some assumptions on function form of $S(t, z)$, usually take (parameter denoted α):

- Exponential:

$$S(t) = e^{-\lambda t}, \quad \lambda(t) = \lambda \tag{7.164}$$

$$\Rightarrow t = -\frac{1}{\lambda}\log S(t) \tag{7.165}$$

$$\Rightarrow \gamma := e^{\alpha' z} = \frac{1}{\lambda} = e^{-\beta' z} \tag{7.166}$$

  i.e. Exponential AFT model in which $\gamma = e^{\alpha' z}$ is equivalent to PH model with $\lambda = e^{\beta' z}$, and $\beta = -\alpha$

- Weibull:

$$S(t) = e^{-\lambda t^p}, \quad \lambda(t) = \lambda p t^{p-1} \tag{7.167}$$

$$\Rightarrow t = -\frac{1}{\lambda^{1/p}}\log S(t) \tag{7.168}$$

$$\Rightarrow \gamma := e^{\alpha' z} = \frac{1}{\lambda^{1/p}} = e^{-\beta' z/p} \tag{7.169}$$

  i.e. Weibull AFT model with $\gamma = e^{\alpha' z}$ is equivalent to PH model with $\lambda = e^{\beta' z}$, and $\beta = -\alpha p$

- General Case: In different groups z, survivial time

$$T_i = T_0 e^{\alpha' z_i + \varepsilon_i/p}, \quad \varepsilon_i \sim \varepsilon(1) S_i(t) = \qquad \mathbb{P}\left(T_i \geq t\right) \tag{7.170}$$

$$= \mathbb{P}\left(\log T_0 + \alpha' z_i + \frac{\varepsilon_i}{p} \geq \log t\right) \tag{7.171}$$

$$= S_{\varepsilon(1)}\left(p(\log t - \log T_0 - \alpha' z_i)\right) \tag{7.172}$$

[66] Proof key:

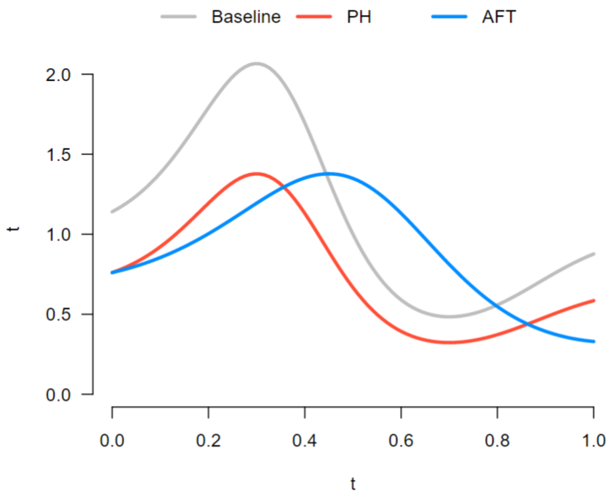
$$d_{0j} \sim B(p_{0j}), \quad p_{0j} = \frac{r_{0j}\lambda_0}{r_{0j}\lambda_0 + r_{1j}\lambda_0 e^{\beta_a}} \tag{7.159}$$

and at small β_a, take approximation $\theta \approx r_{1j}/r_j$

□ AFT Model and PH Model

An intuition for parameters in AFT model and PH model:

$$\mathrm{PH}: \lambda_i(t) = \lambda_0(t)e^{\eta_i}$$
$$\mathrm{AFT}: \lambda_i(t) = \lambda_0(e^{-\eta_i}t)e^{-\eta_i}$$



Usually AFT model depends on a parametric model, whlie PH model only depends on the PH assumption.

▷ `R.` **Code**

An example:

```
coxph(formula = Surv(start, stop, event) ~ rx + number + size + factor(
    enum), data = bladder2)
```

Chapter. VIII 生物统计学概论部分

Instructor: Tianying Wang

Biostatistics is discipline to apply statistical methods to biological problems, including medicine, biology experiment, public health, etc. This section would focus on basic quantative skills to be used in advanced biostatistics research.

Section 8.1 Factor Model and ANOVA

A major question in biostatistics is to study the difference between groups, i.e. explanatory variable X is categorical. A 'way' to conduct grouping is called a **factor** , e.g. $\{\alpha_i\}$ where each i correponds to a **level** of the factor.

To compare groups, e.g. to determine whether there is significant difference between Y of each group, ANOVA is used. The key thought is to analyze difference value and variance and see whether the difference is large enough to 'exceed' variance.

☐ **Factor Notation**

Response Y is denoted by its subsript to declare its group and index in this group, e.g. Y_{ijkl} indicates it is the l^{th} sample in group (i, j, k)

8.1.1 Single Factor Model and One-Way ANOVA

☐ **Cell Mean Model**

$$Y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \text{ i.i.d.} \sim N(0, \sigma^2)$$

Estimation target: $\mu_1, \ldots, \mu_r, \sigma^2$

Hypothesis testing H_0: $\mu_1 = \ldots = \mu_r = \mu$, v.s. H_1 : at least 1 μ_i is different.

Estimation:

$$\hat{\mu}_i = \bar{Y}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i} Y_{ij} \tag{8.1}$$

$$s_i^2 = \frac{1}{n_i - 1}\sum_{j=1}^{n_i}(Y_{ij} - \bar{Y}_{i\cdot})^2 \tag{8.2}$$

$$s^2 = \frac{\sum_{i=1}^r (n_i - 1)s_i^2}{\sum_{i=1}^r (n_i - 1)} = \frac{\sum_{i=1}^r (n_i - 1)s_i^2}{n_T - r} \tag{8.3}$$

Key of ANOVA: Decomposition of variation SS:

$$\text{SST} = \sum_{i=1}^r \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{\cdot\cdot})^2 = \sum_{i=1}^r \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_{i\cdot} + \bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot}\right)^2 \tag{8.4}$$

$$= \sum_{i=1}^r + \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i\cdot})^2 + \sum_{i=1}^r (\bar{Y}_{i\cdot} - \bar{Y}_{\cdot\cdot})^2 \tag{8.5}$$

$$= \text{SSE} + \text{SSR} \tag{8.6}$$

☐ **Factor Model**

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad \varepsilon_{ij} \text{ i.i.d. } \sim N(0, \sigma^2) \tag{8.7}$$

Estimation target: $\mu, \alpha_1, \ldots, \alpha_r, \sigma^2$, w.r.t. $\sum_{i=1}^{r} \alpha_i = 0$.

Hypothesis tesing: $H_0: \alpha_1 = \ldots = \alpha_r = 0$, v.s. H_1 : at least 1 $\alpha_i \neq 0$

Estimation:

$$\hat{\mu} = \bar{Y}_{i\cdot} = \frac{1}{n_i} \sum_{j=1}^{n_i} Y_{ij} \tag{8.8}$$

$$s_i^2 = \frac{1}{n_i - 1} \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_{i\cdot}\right)^2 \tag{8.9}$$

$$s^2 = \frac{\sum_{i=1}^{r} (n_i - 1) s_i^2}{n_T - r} \tag{8.10}$$

8.1.2 Fixed Effect and Random Effect

When divided into groups/naturally assigned in groups, we need to specify whether the factor levels are specially chosen (fixed effect) of randomly chosen from a ‘population of levels’ (random effect).

- Fixed Effect: whether there is a difference between / estimating the value of mean value μ_i of each specific levels
- Random Effect: whether the overall behaviour of μ_i comes from a ‘random distribution’

Comment on fised / random in actual model building and statistical inference:

- whether a factor is fixed or random should be determined by how the data are obtained and the research problem to be studied, i.e. determining fixed / random model does **not** come from mathematics.
- for effect of interaction term, say $(\alpha\beta)_{ij}$ as the interaction effect of factor α_i and β_j, then $(\alpha\beta)_{ij}$ would be random once one of α_i or β_j is random.

Here use a one-way factor model as example:

□ **Fixed Effect:**

$$Y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad \varepsilon_{ij} \text{ i.i.d. } \sim N(0, \sigma^2) \tag{8.11}$$

Estimation target: $\mu, \alpha_1, \ldots, \alpha_r, \sigma^2$, w.r.t. $\sum_{i=1}^{r} \alpha_i = 0$.

Hypothesis tesing: $H_0: \alpha_1 = \ldots = \alpha_r = 0$, v.s. H_1 : at least 1 $\alpha_i \neq 0$

Estimation:

$$\hat{\mu} = \bar{Y}_{i\cdot} = \frac{1}{n_i} \sum_{j=1}^{n_i} Y_{ij} \tag{8.12}$$

$$s_i^2 = \frac{1}{n_i - 1} \sum_{j=1}^{n_i} \left(Y_{ij} - \bar{Y}_{i\cdot}\right)^2 \tag{8.13}$$

$$s^2 = \frac{\sum_{i=1}^{r} (n_i - 1) s_i^2}{n_T - r} \tag{8.14}$$

ANOVA table:

Source of Var	SS	dof	MS	$\mathbb{E}$ (MS)
α_i	$\mathrm{SS}\alpha=\sum_{i=1}^r n_i\left(\bar{Y}_{i\cdot}-\bar{Y}_{\cdot\cdot}\right)^2$	$r-1$	$\frac{\mathrm{SS}\alpha}{r-1}$	$\sigma^2+\frac{\sum_{i=1}^r n_i\alpha_i^2}{r-1}$
σ^2	$\mathrm{SSE}=\sum_{i=1}^r\sum_{j=1}^{n_i}\left(Y_{ij}-Y_{i\cdot}\right)^2$	n_T-r	$\frac{\mathrm{SSE}}{n_T-r}$	σ^2

表 6:

F statistics for $H_0:\alpha_1=\ldots=\alpha_r=0$:

$$F=\frac{\mathrm{MS}\alpha}{\mathrm{MSE}}\sim F_{r-1,n_T-r} \tag{8.15}$$

☐ **Random Effect**

$$Y_{ij}=\mu+\alpha_i+\varepsilon_{ij}\quad \alpha_i \text{ i.i.d. } \sim N(0,\sigma_\alpha^2),\quad \varepsilon_{ij} \text{ i.i.d. } \sim N(0,\sigma^2) \tag{8.16}$$

Estimation target: $\mu,\sigma_\alpha^2,\sigma^2$

Hypothesis testing $H_0:\ \sigma_\alpha^2=0$, v.s. $H_1:\sigma_\alpha^2\neq 0$

Estimation:

$$\hat{\mu}=\bar{Y}_{i\cdot}=\frac{1}{n_i}\sum_{j=1}^{n_i}Y_{ij} \tag{8.17}$$

$$s_i^2=\frac{1}{n_i-1}\sum_{j=1}^{n_i}\left(Y_{ij}-\bar{Y}_{i\cdot}\right)^2 \tag{8.18}$$

$$s^2=\frac{\sum_{i=1}^r(n_i-1)s_i^2}{n_T-r} \tag{8.19}$$

ANOVA table:

Source of Var	SS	dof	MS	$\mathbb{E}$ (MS)
α_i	$\mathrm{SS}\alpha=\sum_{i=1}^r n_i\left(\bar{Y}_{i\cdot}-\bar{Y}_{\cdot\cdot}\right)^2$	$r-1$	$\frac{\mathrm{SS}\alpha}{r-1}$	$\sigma^2+n\sigma_\alpha^2$
σ^2	$\mathrm{SSE}=\sum_{i=1}^r\sum_{j=1}^{n_i}\left(Y_{ij}-Y_{i\cdot}\right)^2$	n_T-r	$\frac{\mathrm{SSE}}{n_T-r}$	σ^2

表 7:

F statistics for $H_0:\alpha_1=\ldots=\alpha_r=0$:

$$F=\frac{\mathrm{MS}\alpha}{\mathrm{MSE}}\sim F_{r-1,n_T-r} \tag{8.20}$$

8.1.3 Two Factor Model and Two-Way ANOVA

Two factor model with interation term:

$$Y_{ijk}=\mu+\alpha_i+\beta_j+(\alpha\beta)_{ij}+\varepsilon_{ijk}$$

$$Y_{ijk}-\bar{Y}_{...}=\left(\bar{Y}_{i..}-\bar{Y}_{...}\right)+\left(\bar{Y}_{.j.}-\bar{Y}_{...}\right) \tag{8.21}$$
$$+\left(\bar{Y}_{ij.}-\bar{Y}_{i..}-\bar{Y}_{.j.}+\bar{Y}_{...}\right)+\left(Y_{ijk}-\bar{Y}_{ij.}\right) \tag{8.22}$$
$$\alpha_i+\beta_j+(\alpha\beta)_{ij}+\varepsilon_{ijk}=((\mu+\alpha_i)-\mu)+((\mu+\beta_j)-\mu) \tag{8.23}$$
$$+((\mu+\alpha_i+\beta_j+(\alpha\beta)_{ij})-(\mu+\alpha_i)-(\mu+\beta_j)+\mu)+(\varepsilon_{ijk}) \tag{8.24}$$

Here for convenience and clarity, when applying model with more factors, we use terms like $(\alpha\beta)_{ij}$ to avoid confusion of too many symbols.

8.1.4 General Case for Factor Model

e.g. three factors model

$$Y_{ijkl}=\mu+\alpha_i+\beta_j+\gamma_k+(\alpha\beta)_{ij}+(\alpha\gamma)_{ik}+(\beta\gamma)_{jk}+(\alpha\beta\gamma)_{ijk}+\varepsilon_{ijkl}$$

□ **Montgomery's Method for Restricted Model**

Montgomery describe a useful trick to form the ANOVA table and to find correponding $\mathbb{E}\,(\mathrm{MS})$ (EMS), and finally help construct proper F^* statistics. Here an explicit example of three factor (1F+2R) model is provided to illustrate the procedure.

Model we use here as example:

$$Y_{ijkl}=\mu+\alpha_i+\beta_j+\gamma_k+(\alpha\beta)_{ij}+(\alpha\gamma)_{ik}+(\beta\gamma)_{jk}+(\alpha\beta\gamma)_{ijk}+\varepsilon_{ijkl} \tag{8.25}$$
$$i=1,2,\ldots,a \tag{8.26}$$
$$j=1,2,\ldots,b \tag{8.27}$$
$$k=1,2,\ldots,c \tag{8.28}$$
$$l=1,2,\ldots,n \tag{8.29}$$

where a is for fixed effect, b and c are for random effect.

model parameter:

$$\theta=\{\mu,\alpha_i^{i=1,\ldots,a},\sigma^2_\beta,\sigma^2_\gamma,\sigma^2_{\alpha\beta},\sigma^2_{\alpha\gamma},\sigma^2_{\beta\gamma},\sigma^2_{\alpha\beta\gamma},\sigma^2\} \tag{8.30}$$

1. Prepare the framework of the EMS table, including:
   - column: list groups, and their random/fixed, and their number of levels.
   - row: terms in the model
   - error term written as $\varepsilon_{(ijk)l}$, i.e. random term index excluded from the bracket.

Random/Fix	F	R	R	R	
# level	a	b	c	n	
Index	i	j	k	l	$\mathbb{E}$ (MS)
α_i					
β_j					
γ_k					
$(\alpha\beta)_{ij}$					
$(\alpha\gamma)_{ik}$					
$(\beta\gamma)_{jk}$					
$(\alpha\beta\gamma)_{ijk}$					
$\varepsilon_{(ijk)l}$					

2. For each row, copy the number of observations under each column subscripts, if the column subscript does not appear in the index subscripts of the term. e.g. $(\alpha\beta)_{ij}$ does not contain, k, l so fill in the grid $((\alpha\beta)_{ij}, k)$ with c, and fill $((\alpha\beta)_{ij}, l)$ with n.

Random/Fix	F	R	R	R	
# level	a	b	c	n	
Index	i	j	k	l	$\mathbb{E}$ (MS)
α_i		b	c	n	
β_j	a		c	n	
γ_k	a	b		n	
$(\alpha\beta)_{ij}$			c	n	
$(\alpha\gamma)_{ik}$		b		n	
$(\beta\gamma)_{jk}$	a			n	
$(\alpha\beta\gamma)_{ijk}$				n	
$\varepsilon_{(ijk)l}$					

3. 1 is filled in the row of error term $(\varepsilon_{(ijk)l}, \cdot)$

Random/Fix	F	R	R	R	
# level	a	b	c	n	
Index	i	j	k	l	$\mathbb{E}$ (MS)
α_i		b	c	n	
β_j	a		c	n	
γ_k	a	b		n	
$(\alpha\beta)_{ij}$			c	n	
$(\alpha\gamma)_{ik}$		b		n	
$(\beta\gamma)_{jk}$	a			n	
$(\alpha\beta\gamma)_{ijk}$				n	
$\varepsilon_{(ijk)l}$	1	1	1	1	

4. for remaining grids, fill 1 if the column is Fixed, or 0 if the column is Random

Random/Fix	F	R	R	R	
# level	a	b	c	n	
Index	i	j	k	l	$\mathbb{E}$ (MS)
α_i	0	b	c	n	
β_j	a	1	c	n	
γ_k	a	b	1	n	
$(\alpha\beta)_{ij}$	0	1	c	n	
$(\alpha\gamma)_{ik}$	0	b	1	n	
$(\beta\gamma)_{jk}$	a	1	1	n	
$(\alpha\beta\gamma)_{ijk}$	0	1	1	n	
$\varepsilon_{(ijk)l}$	1	1	1	1	

5. Now the L.H.S. of the table is finished. To get the $\mathbb{E}$ (MS), we will need the coefficients in front of the variance term[67]. The approach is as follows: use the fourth row $(\alpha\beta)_{ij}$ as example:

   * (e.g. focus on row $(\alpha\beta)_{ij}$)

   (a) ignore columns with the same indexes, here it would be column i and j

   (b) select rows with the same or more extra indexes, here it would be row $(\alpha\beta)_{ij}$, $(\alpha\beta\gamma)_{ijk}$, $\varepsilon_{(ijk)l}$

   (c) now the grids to be used are colored brown

   (d) for each row, multiply all used grids to form the correponding coefficient (of the variance of this row), here it would be

$$\mathbb{E}\left(\mathrm{MS}_{(\alpha\beta)}\right) = c \times n\sigma^2_{\alpha\beta} + 1 \times n\sigma^2_{\alpha\beta\gamma} + 1 \times 1\sigma^2 = \sigma^2 + cn\sigma^2_{\alpha\beta} + n\sigma^2_{\alpha\beta\gamma} \tag{8.31}$$

[67]Note the variance term is what we already know: for fixed effect it would be $\dfrac{\sum_i \alpha_i^2}{a-1}$, for random effect it would be σ^2_β

Random/Fix	F	R	R	R	
# level	a	b	c	n	
Index	i	j	k	l	$\mathbb{E}(\text{MS})$
α_i	0	b	c	n	$\sigma^2 + cn\sigma^2_{\alpha\beta} + bn\sigma^2_{\alpha\gamma} + n\sigma^2_{\alpha\beta\gamma} + bcn\frac{\sum_i \alpha_i^2}{a-1}$
β_j	a	1	c	n	$\sigma^2 + an\sigma^2_{\beta\gamma} + acn\sigma^2_{\beta}$
γ_k	a	b	1	n	$\sigma^2 + an\sigma^2_{\beta\gamma} + abn\sigma^2_{\gamma}$
$(\alpha\beta)_{ij}$	0	1	c	n	$\sigma^2 + cn\sigma^2_{\alpha\beta} + n\sigma^2_{\alpha\beta\gamma}$
$(\alpha\gamma)_{ik}$	0	b	1	n	$\sigma^2 + bn\sigma^2_{\alpha\gamma} + n\sigma^2_{\alpha\beta\gamma}$
$(\beta\gamma)_{jk}$	a	1	1	n	$\sigma^2 + an\sigma^2_{\beta\gamma}$
$(\alpha\beta\gamma)_{ijk}$	0	1	1	n	$\sigma^2 + n\sigma^2_{\alpha\beta\gamma}$
$\varepsilon_{(ijk)l}$	1	1	1	1	σ^2

6. Now we can use $\mathbb{E}(\text{MS})$ to construct correponding F^*. e.g. to test $H_0 : \alpha_1 = \alpha_2 = \ldots = \alpha_a$, test:

$$\mathbb{E}(\text{MS}_\alpha) = \sigma^2 + cn\sigma^2_{\alpha\beta} + bn\sigma^2_{\alpha\gamma} + n\sigma^2_{\alpha\beta\gamma} + bcn\frac{\sum_i \alpha_i^2}{a-1} \tag{8.32}$$

$$\mathbb{E}(\text{MS}_{\alpha\beta} + \text{MS}_{\alpha\gamma} - \text{MS}_{\alpha\beta\gamma}) = \sigma^2 + cn\sigma^2_{\alpha\beta} + bn\sigma^2_{\alpha\gamma} + n\sigma^2_{\alpha\beta\gamma} \tag{8.33}$$

$$F^*_{\alpha_i} = \frac{\text{MS}_\alpha + \text{MS}_{\alpha\beta\gamma}}{\text{MS}_{\alpha\beta} + \text{MS}_{\alpha\gamma}} \sim F_{(a-1)+(a-1)(b-1)(c-1),(a-1)(b-1)+(a-1)(c-1)} \tag{8.34}$$

8.1.5 Diagnosis

Some useful diagnosis to check assumptions:

- Levene's Test for homogeneity of variance: ▷ R. **Code**

```
dat %>% group_by(cat_1) %>% rstatix::levene_test(y ~ group)
```

- Shapiro-Wilk Test for Normality: ▷ R. **Code**

```
dat %>% group_by(cat_1) %>% rstatix::shapiro_test(y)
```

- Outlier test: ▷ R. **Code**

```
dat %>% group_by(cat_1) %>% rstatix::identify_outliers(y)
```

8.1.6 Miscellaneous Topics

Some miscellanea in design of experiment and about some advanced models:

☐ **Crossed and Nested Factors**

In multi-factor studies, we may not be able to go through all possible factor settings.

- Crossed factor: all level combinations are covered in the experiment.
- Nested factor: the levels of one factor are unique to a particular level of another factor.

☐ **Longitudinal Study**

When discrete **time** is used as factors, say $\tau_t^{t=\{t_1,\dots,t_T\}}$ in Y_{ijt} where i for treatment, j for individuals, we may notice that response Y_{ijt} is effected by individual baseline, in such case we cannot use the ordinary factor model to study the difference of trent. Instead we would use **longitudinal study** to construct model and study the trend.. e.g.

$$Y_{ijt} = \mu + \alpha_i + \beta_{j(i)} + \tau_t + \varepsilon_{ijt} \tag{8.35}$$

where $\beta_{j(i)}$ stands for indivudual difference (say, with assumption $\beta_{j(i)} \sim N(0, \sigma_\beta^2)$)

Section 8.2 Statistical Inference on Contingency Table

Contingency table is an easy way to display categorical variables, an example:

表 8: A 2×2 contingency table

	Variable Z		
Variable Y	D	$D^\complement$	Total
E	n_{11}	n_{12}	$n_{1\cdot}$
$E^\complement$	n_{21}	n_{22}	$n_{2\cdot}$
Total	$n_{\cdot 1}$	$n_{\cdot 2}$	$n_{\cdot\cdot}$

8.2.1 Quantities and Statistics from Contingency Table

☐ **Prospective Study and Retrospective Study**

Contingency table itself is symmetric w.r.t. Y, Z, but in experimental design we usually first specify and divide groups, and then conduct experiment (prospective) or conduct survey (retrospective), which would cause different conditional probability. An example in studying the effect of medicine

- Prospective Study: say, $Y = E/E^\complement$ for drug/placebo group is assigned before experiment, and then $Z = D/D^\complement$ for medicine effect is studied after treatment.

  In this case $n_{1\cdot}$, $n_{2\cdot}$ are pre-determined fixed number.

  Such design is a well-controlled experiment to study the effct, but sometimes faced with problem concerning survival analysis, see Chapter. 7 for detail. And for some problems like, e.g. Z is related to rare disease, this method is **low-efficient**.

- Retrospective Study: say, some $Z = D/D^\complement$ for medicine effect patients are selected, and then their history of taking drug or not is collected.

  In this case $n_{\cdot 1}$, $n_{\cdot 2}$ are pre-determined fixed number.

  This method is quick and convenient to conduct study, but usually we cannot control the exposure status Y accurately (because they are collected by, e.g. questionnaire)

Statistics and tests should be selected based on the data collection design (prospective/retrospective) because of different probability condition.

□ **Statistics and Estimation**

With respective probabilities in two groups $E,\ E^{\complement}$ denoted as

$$p_1 = \mathbb{P}\left(D|E\right), \qquad p_2 = \mathbb{P}\left(D|E^{\complement}\right) \tag{8.36}$$

we usully focus on the 'difference' between group E and $E^{\complement}$, there are some quantities to help measure the group difference:

$$\text{Risk difference: } \Delta = p_1 - p_2 \tag{8.37}$$

$$\text{Relative risk: } \phi = p_1 / p_2 \tag{8.38}$$

$$\text{Odds ratio: } \theta = \frac{p_1/(1-p_1)}{p_2/(1-p_2)} \tag{8.39}$$

Their estimation:

- Respective probability p_1, p_2:

$$\text{Prospective: } \begin{cases} \hat{p}_1 = \dfrac{n_{11}}{n_{1\cdot}} \\ \hat{p}_2 = \dfrac{n_{21}}{n_{2\cdot}} \end{cases} \tag{8.40}$$

$$\text{Retrospective: } \begin{cases} \hat{p}_1 = \dfrac{\rho\frac{n_{11}}{n_{\cdot 1}}}{\rho\frac{n_{11}}{n_{\cdot 1}} + (1-\rho)\frac{n_{12}}{n_{\cdot 2}}} \\ \hat{p}_2 = \dfrac{\rho\frac{n_{21}}{n_{\cdot 1}}}{\rho\frac{n_{21}}{n_{\cdot 1}} + (1-\rho)\frac{n_{22}}{n_{\cdot 2}}} \end{cases} \tag{8.41}$$

$$\text{where } \rho \text{ is the prevalence btw} D, D^{\complement} \text{ in natural condition} \tag{8.42}$$

- Relative Risk ϕ:

$$\text{Prospective: } \hat{\phi} = \frac{n_{11}/n_{1\cdot}}{n_{21}/n_{2\cdot}} \tag{8.43}$$

$$\text{Retrospective: } \hat{\phi} = \frac{\hat{p}_1}{\hat{p}_2} \tag{8.44}$$

- Odds Ratio θ:

$$\text{Prospective\&Retrospective: } \hat{\theta} = \frac{n_{11}n_{22}}{n_{21}n_{12}} \tag{8.45}$$

  which is the same in either cases.

  variance of $\hat{\theta}$: estimated at $(n_{11}, n_{12}, n_{21}, n_{22}) \sim$ Multinomial$(n_{\cdot\cdot}, \pi_{11}, \pi_{12}, \pi_{21}, \pi_{22})$:

$$\hat{var}(\log\hat{\theta}) = \frac{1}{n_{11}} + \frac{1}{n_{12}} + \frac{1}{n_{21}} + \frac{1}{n_{22}} \tag{8.46}$$

□ **Hypothesis Testing**

The mostly used hypothesis is the dependence assumption: $p_1 = p_2$, or more generally speaking for $m \times n$ table:

$$H_0 : \pi_{ij} = \pi_{i\cdot}\pi_{\cdot j}, \quad \forall i, j \tag{8.47}$$

Denote $O_{ij} = n_{ij}$ as the **O**bserved value, $E_{ij} = n_{..}\pi_{ij}$ as the **E**xpected value.[68] Expected value is calculated for the model used, under null hypothesis H_0. Example for independence test $\pi_{ij} = \pi_{i.}\pi_{.j}$:

$$\hat{\pi}_{ij} = \hat{\pi}_{i.}\hat{\pi}_{.j} = \frac{n_{i.}}{n_{..}}\frac{n_{.j}}{n_{..}} \Rightarrow E_{ij} = n_{..}\hat{\pi}_{ij} = \frac{n_{i.}n_{.j}}{n_{..}} \tag{8.54}$$

Statistics:

- **Pearson's χ^2 Test**:

$$\chi^2_P = \sum_{i=1}^{I}\sum_{j=1}^{J}\frac{(O_{ij} - E_{ij})^2}{E_{ij}} \xrightarrow{\mathscr{L}} \chi^2_{(I-1)(J-1)} \tag{8.55}$$

- **Likelihood Ratio Test**:

$$G^2 = -2\log(\Lambda) = 2\sum_{i=1}^{I}\sum_{j=1}^{J} O_{ij}\log\frac{O_{ij}}{E_{ij}} \xrightarrow{\mathscr{L}} \chi^2_{(I-1)(L-1)} \tag{8.56}$$

Some other useful tests:

- McNemar test on $\pi_{12} = \pi_{21}$ for matched pairs:

$$z^2 = \frac{(n_{12} - n_{21})^2}{n_{12} + n_{21}} \xrightarrow{\mathscr{L}} \chi^2_1 \tag{8.57}$$

[68] E_{ij} is calculated based on data and the model you choose, thus can be applied to more complexed cases, e.g. Hardy-Weinberg proportions with X^a gene grequency p

$$\mathbb{P}(X^aX^a;\text{Female}) = p^2 \tag{8.48}$$
$$\mathbb{P}\left(X^AX^a;\text{Female}\right) = 2p(1-p) \tag{8.49}$$
$$\mathbb{P}\left(X^AX^A;\text{Female}\right) = (1-p)^2 \tag{8.50}$$
$$\mathbb{P}(X^aY;\text{Male}) = p \tag{8.51}$$
$$\mathbb{P}\left(X^AY;\text{Male}\right) = (1-p) \tag{8.52}$$

In such complex case, parameter should be estimated using e.g. MLE estimation.And then calculate E_{ij}s

$$L(p) = \left[p^2\right]^{O_{a,\mathrm{F}}}\left[1-p^2\right]^{O_{A,\mathrm{F}}}[p]^{O_{a,\mathrm{M}}}[1-p]^{O_{A,\mathrm{M}}} \tag{8.53}$$

Chapter. IX 统计学习导论部分

Instructor: Sheng Yu

In this course, some key formulations/theorem in machine learning are deduced, together with core principles illustrated.

☐ **What is Machine Learning?**

> Machine learning is a field of computer science that uses statistical techniques to give computer systems the ability to ”learn” with data, without being explicitly programmed.

Examples of Machine Learning:

- Linear/Logistic Regression (Linear Model)
- Decision Tree
- Support Vector Machine
- Clustering
- Bayesian Network
- Neural Network
- Conditional Random Field
- etc.

This section will cover some of the methods above in a machine learning perspective.

Section 9.1 Linear Model

Linear model is the basic model in statistics, see Chapter. 3.

9.1.1 Linear Model in Machine Learning Perspective

In machine learning field, key feature of linear model is its affine form of variable dependence:

$$Y = f(X) + \varepsilon = \tilde{f}_\beta(X'\beta) + \varepsilon$$

where usually $X = (1, X_1, X_2, \ldots, X_p)$, $\beta = (\beta_0, \beta_1, \beta_2, \ldots, \beta_p)$.[69] Some example of linear model:

- Linear Regression:

$$Y = \beta_0 + \beta_1 x_1 + \ldots \beta_p x_p + \varepsilon = X'\beta + \varepsilon$$

- General Linear Model:

$$Y \sim f(\theta(X'\beta))$$

  in this framework,

[69] Some materials use $X = (X_1, X_2, \ldots, X_p)$, $\beta = (\beta_1, \beta_2, \ldots, \beta_p)$, and the affine dependence is $\tilde{f}(\beta_0 + X'\beta)$

– Linear regression:

$$Y \sim N(X'\beta, \sigma^2)$$

– Logistic regression:

$$Y \sim \text{Bernoulli}(\text{logistic}(X'\beta))$$

9.1.2 Linear Regression

Linear Regression:

$$Y = \beta_0 + \beta_1 x_1 + \dots \beta_p x_p + \varepsilon = X'\beta + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2)$$

usually use Squared Error Loss to eatimate (β, σ^2)

$$\mathcal{L}(Y, \hat{f}(X)) = \left(Y - \hat{f}(X)\right)^2 = \left(Y - X\hat{\beta}\right)^2$$

LSE estimator (where Y and X imply corresponding sample vector/matrix), more detail see section. 3.3:

$$\frac{\partial \mathcal{L}}{\partial \beta} = 0 \Rightarrow \hat{\beta} = (X'X)^{-1}X'Y$$

- Predict:

$$\hat{Y} = X\beta = X(X'X)^{-1}X'Y$$

- Hat Matrix:

$$H = P_X \equiv X(X'X)^{-1}X'$$

  idempotent and symmetry

$$H^2 = H, \quad H = H'$$

- Properties of $\hat{\beta}$, $\hat{\sigma^2}$:[70]

$$\begin{aligned} cov(\hat{\beta}) =& cov\left((X'X)^{-1}X'(X\beta + \varepsilon)\right) = (X'X)^{-1}\sigma^2 && (9.1)\\ var(\hat{\beta}_j) =& \frac{\sigma^2}{(n-1)S_{x_j}^2} \cdot \text{VIF}_j && (9.2)\\ cov(e) =& cov(Y - \hat{Y}) = (I - H)\sigma^2 && (9.3)\\ var(\hat{\sigma^2}) =& var(\text{MSE}) = \frac{Y'(I-H)Y}{n-(p+1)} && (9.4) \end{aligned}$$

9.1.3 Normalization Methods

In machine learning topic we would focus more on model generalization ability, so that the model can perform better on reality problems. In linear regression, we usually use normalization methods.

Basically linear model uses SE loss:

$$\mathcal{L} = \sum_{i=1}^{n}(y_i - \beta_0 - \beta' x_i)^2 = \sum_{i=1}^{n}(y_i - x_i'\beta)^2$$

we can put various normalize term (penalty) in loss or put constraint on β: (these two methods are equivalent in many cases)

[70]Definition of VIF_j see section. 3.4.7

- Ridge Regression/ℓ_2 Penalty/Tikhonov Regularization:[71]

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda\|\beta\|_2^2$$

or equivalent form

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 \tag{9.5}$$

$$s.t. \|\beta\|_2^2 \leq s \tag{9.6}$$

in either case, λ or s is hyper-parameter.

Ridge regression has closed form solution

$$\hat{\beta}^{\text{ridge}} = (X'X + \lambda I)^{-1} X'Y$$

Intuitively speaking, ridge regression help shrink $\hat{\beta}$ by an non-zero factor.

- LASSO/ℓ_1 Penalty:

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda\|\beta\|_1$$

or equivalent form

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 \tag{9.7}$$

$$s.t. \|\beta\|_1 \leq s \tag{9.8}$$

LASSO help shrink significantly large coefficients and truncate small coefficients.

- Generalized ℓ_p norm penalty:

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda\|\beta\|_2^2$$

or equivalent form

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i'\beta)^2 \tag{9.9}$$

$$s.t. \|\beta\|_2^2 \leq s \tag{9.10}$$

- Elastic Net:

$$\hat{\beta} = \arg\min_{\beta} \|Y - X\beta\|_2^2 + \lambda_1\|\beta\|_1 + \lambda_2\|\beta\|_2^2$$

equivalent form:

[71] Recall for ℓ_p norm: for n-dim vector $\vec{v} = (v_1, v_2, \ldots, v_n)$

$$\|v\|_p = \left(\sum_{i=1}^{m} |v_i|^p\right)^{1/p}$$

$$\hat{\beta} = \arg\min_{\beta} \|Y - X\beta\|^2 \tag{9.11}$$

$$s.t. \frac{\lambda_1}{\lambda_1 + \lambda_2}\|\beta\|_1 + \frac{\lambda_2}{\lambda_1 + \lambda_2}\|\beta\|_2^2 \leq s \tag{9.12}$$

picking proper hyper-parameter $(s, \lambda = \dfrac{\lambda_2}{\lambda_1 + \lambda_2})$

A note on elastic net: the boundary of elastic net $\lambda_1\|\beta\|_1 + \lambda_2\|\beta\|_2^2 = \text{const}$ is between ℓ_1 boundary and ℓ_2 boundary. Both the variable selection feature of ℓ_1 and the differnetiable feature of ℓ_2 are partially maintained.

- Adaptive LASSO:

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} \left(y_u - x_i'\beta\right)^2 + \lambda \sum_{j=1}^{p} \frac{|\beta_j|}{|\hat{\beta}_j^{\text{OLS}}|}$$

- Non-negative Garrote method.
- SCAD

Section 9.2 Basic Classification Model

Denote: Dataset $\mathcal{D} = \{(x_i, y_i), i = 1, 2, \ldots, N\}$, $x_i = [x_{i1}, x_{i2}, \ldots, x_{ip}]$, with reponse $y_i \in \mathcal{C} = \{c_1, c_2, \ldots, c_K\}$ as a K-classification problem. When $K = |\mathcal{C}| = 2$ for binary classification, in this case we usually denote $\mathcal{C}_{01} = \{0, 1\}$.

Target is to predict/classify Y from X

$$\hat{Y} = \hat{f}(X) \rightsquigarrow Y \tag{9.13}$$

9.2.1 Classification Metrics

- Accuracy

$$\mathbb{P}\left(\hat{Y} = Y\right) \hat{\to} \frac{\sum_{i=1}^{N} \mathbb{I}(\hat{y}_i = y_i)}{N} \tag{9.14}$$

- Error Rate/ Misclassification Rate

$$\mathbb{P}\left(\hat{Y} \neq Y\right) \hat{\to} \frac{\sum_{i=1}^{N} \mathbb{I}(\hat{y}_i \neq y_i)}{N} \tag{9.15}$$

- prevalence for binary classification

$$\mathbb{P}\left(Y = 1\right) \hat{\to} \frac{\sum_{i=1}^{N} y_i}{N} \tag{9.16}$$

□ Confusion Matrix and Metrics for Binary Classification

表 9: Confusion matrix for binary classification

	Predicted Value $\hat{Y}$	
Ground Truth Y	1	0
1	n_{11}	n_{10}
0	n_{01}	n_{00}

Metrics:

- True Positive Rate (TPR)/ Sensitivity/ Recall:

$$\mathbb{P}\left(\hat{Y}=1|Y=1\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)\cdot\mathbb{I}(y_i=1)}{\sum_{i=1}^{N}\mathbb{I}(y_i=1)} = \frac{n_{11}}{n_{11}+n_{10}} \tag{9.17}$$

- False Positive Rate (FPR):

$$\mathbb{P}\left(\hat{Y}=1|Y=0\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)\cdot\mathbb{I}(y_i=0)}{\sum_{i=1}^{N}\mathbb{I}(y_i=0)} = \frac{n_{01}}{n_{01}+n_{00}} \tag{9.18}$$

- True Negatie Rate (TNR)/ Specific (SPC):

$$\mathbb{P}\left(\hat{Y}=0|Y=0\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)\cdot\mathbb{I}(y_i=0)}{\sum_{i=1}^{N}\mathbb{I}(y_i=0)} = \frac{n_{00}}{n_{01}+n_{00}} \tag{9.19}$$

- False Negative Rate (FNR):

$$\mathbb{P}\left(\hat{Y}=0|Y=1\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)\cdot\mathbb{I}(y_i=1)}{\sum_{i=1}^{N}\mathbb{I}(y_i=1)} = \frac{n_{10}}{n_{11}+n_{10}} \tag{9.20}$$

-

- Positive Predictive Value (PPV)/ Precision:

$$\mathbb{P}\left(Y=1|\hat{Y}=1\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)\cdot\mathbb{I}(y_i=1)}{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)} = \frac{n_{11}}{n_{11}+n_{01}} \tag{9.21}$$

- False Discovery Rate (FDR):

$$\mathbb{P}\left(Y=0|\hat{Y}=1\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)\cdot\mathbb{I}(y_i=0)}{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=1)} = \frac{n_{01}}{n_{11}+n_{01}} \tag{9.22}$$

- Negative Predictive Value (NPV):

$$\mathbb{P}\left(Y=0|\hat{Y}=0\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)\cdot\mathbb{I}(y_i=0)}{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)} = \frac{n_{00}}{n_{10}+n_{00}} \tag{9.23}$$

- False Omission Rate (FOR):

$$\mathbb{P}\left(Y=1|\hat{Y}=0\right) \hat{\to} \frac{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)\cdot\mathbb{I}(y_i=1)}{\sum_{i=1}^{N}\mathbb{I}(\hat{y}_i=0)} = \frac{n_{10}}{n_{10}+n_{00}} \tag{9.24}$$

F_1 Score:

$$F_1 = 2\frac{\text{precision}\cdot\text{recall}}{\text{precision}+\text{recall}} \tag{9.25}$$

Receive Operating Characteristic Curve (ROC Curve) is used to examing performance of a model with threshold s:

$$\hat{Y} = \begin{cases} 1, & \text{case } \hat{f}(X) > s \\ 0, & \text{case } \hat{f}(X) \le s \end{cases} \tag{9.26}$$

for each s, the model gives a corresponding $\text{TPR}(s)$ (recall) and $\text{FPR}(s)$, all $(\text{TPR}(s), \text{FPR}(s))$ forms the ROC curve. Area Under ROC Curve (AUC) is used also as a measure of model performance.

9.2.2 Cross-Validation

In general process of train & validate, we split the data into train set and validation set, which causes insufficient usage of data. k-fold Cross-validation (CV) is proposed to oversome the problem.

1. Divide $\mathcal{D}$ into k folds
2. For each time $i = 1, 2, \ldots, k$, pick the i^{th} fold as validation set, others as train set, train the model and calculate the metric m_i
3. Average over all folds is used as final performance

$$m = \frac{\sum_{i=1}^{k} m_i}{k} \tag{9.27}$$

CV could help ease the problem of overfitting.

9.2.3 Bayes Optimal Classifier

Due to the randomness of class distribution, no classifier could reach 100% accuracy, but there is a optimal classifier (if we really know the underlying distribution) to minimizie the expected loss:

$$\mathbb{E}\left(\mathcal{L}\right) = \mathbb{E}_X \left(\sum_{k=1}^{K} \mathcal{L}(k, \hat{y}(X)) \right) \cdot \|Y = k|X\| \tag{9.28}$$

$$\Rightarrow \hat{y}(x)_{\text{optimal}} = \arg\min_j \mathcal{L}(k, j) \cdot \mathbb{P}\left(Y = k|X = x\right) \tag{9.29}$$

$$0/1 \text{ loss} = \arg\max_j \mathbb{P}\left(Y = j|X = x\right) \tag{9.30}$$

which is the Bayes Optimal Classifier $\hat{y}(x)_{\text{optimal}}$, its error rate is Bayes optimal rate.

9.2.4 k-Nearest Neighbours Approach

The k-nearest neighours (KNN) fit with threshold s:

$$\hat{f}(x) = \frac{1}{k} \sum_{i: x_i \in \mathcal{N}_k(x)} y_i \tag{9.31}$$

$$\hat{Y} = \begin{cases} 1, & \text{case } \hat{f}(X) > s \\ 0, & \text{case } \hat{f}(X) \leq s \end{cases} \tag{9.32}$$

where $\mathcal{N}_k(x)$ is the nearest k datapoints of x, various distance measure $\|\cdot\|$ could be used. k-NN method is faced with the problem of curse of dimensionality (see section. 4.3) in high dimension case. Calculation cost is at $O(N)$.

9.2.5 Density Based Classification

An intuition: samples from the same class k should be clustered, we use some distribution to represent it as $f_k(x)$. Bayes optimal criterion with prior π_k:

$$\hat{y}(x) = \arg\max_k \mathbb{P}\left(Y = k|X = x\right) = \arg\max_k \frac{f_k(x)\pi_k}{\sum_{l=1}^{K} f_l(x)\pi_l} = \arg\max_k f_k(x)\pi_k \tag{9.33}$$

☐ **Discriminant Analysis**

Detail about discriminant analysis could be found in section section. 4.6. Here are some recaps:

Discriminant analysis assume a gaussian distribution

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma_k|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu_k)'\Sigma_k^{-1}(x-\mu_k)\right\} \tag{9.34}$$

- Linear Discriminant Analysis (LDA): Assume $\Sigma_k = \Sigma, \forall k$

$$\log \frac{\mathbb{P}(k|x)}{\mathbb{P}(l|x)} = \log \frac{f_k(x)\pi_k}{f_l(x)\pi_l} \tag{9.35}$$

$$= \log \frac{\pi_k}{\pi_l} - \frac{1}{2}(\mu_k+\mu_l)'\Sigma^{-1}(\mu_k-\mu_l) + x'\Sigma^{-1}(\mu_k-\mu_l) \tag{9.36}$$

  Classification function:

$$\hat{y}(x) = \arg\max_k \delta_k(x) = \arg\max_k \log\hat{\pi}_k + x'\hat{\Sigma}^{-1}\hat{\mu}_k - \frac{1}{2}\hat{\mu}_k'\hat{\Sigma}^{-1}\hat{\mu}_k \tag{9.37}$$

$$\hat{\pi}_k = \frac{N_k}{N} \tag{9.38}$$

$$\hat{\mu}_k = \frac{\sum_{i:y_i=k} x_i}{N_k} \tag{9.39}$$

$$\hat{\Sigma} = \frac{\sum_{k=1}^{K}\sum_{i:y_i=k}(x_i-\hat{\mu}_k)(x_i-\hat{\mu}_k)'}{N-K} \tag{9.40}$$

- Quadratic Discriminant Analysis (QDA): Allow different Σ_k, Classification function:

$$\hat{y}(x) = \arg\max_k \delta_k(x) = \arg\max_k \log\hat{\pi}_k - \frac{1}{2}\log|\hat{\Sigma}_k| - \frac{1}{2}(x-\hat{\mu}_k)'\hat{\Sigma}_k^{-1}(x-\hat{\mu}_k) \tag{9.41}$$

$$\hat{\pi}_k = \frac{N_k}{N} \tag{9.42}$$

$$\hat{\mu}_k = \frac{\sum_{i:y_i=k} x_i}{N_k} \tag{9.43}$$

$$\hat{\Sigma}_k = \frac{\sum_{i:y_i=k}(x_i-\hat{\mu}_k)(x_i-\hat{\mu}_k)'}{N_k-1} \tag{9.44}$$

☐ **Naïve Bayes Classifier**

Distribution is estimated as (which is a naïve decomposition)

$$f_k(\vec{x}) = f_k(x_1)f_k(x_2)\dots f_k(x_p) \tag{9.45}$$

Classification function:

$$\hat{y}(x) = \arg\max_k \hat{\pi}_k \prod_{i=1}^{p} \hat{f}_k(x_i) = \arg\max_k \sum_{i=1}^{k} \pi_k \log\hat{f}_k(x_i) \tag{9.46}$$

9.2.6 Logistic Regression

Logistic Regression calculates $\mathbb{P}(Y|X)$ directly. Detail theory see section. 3.7. Here are some recaps:

$$y|x \sim \text{Binom}\left(1, \frac{e^{x'\beta}}{1+e^{x'\beta}}\right) \tag{9.47}$$

$$\mathbb{P}(Y=1|X=x) = \frac{e^{x'\beta}}{1+e^{x'\beta}} := \text{logit}(x'\beta) \tag{9.48}$$

Classify with thres hold s.

☐ **Multiple Classification**

$$\mathbb{P}(Y=k|X=x) = \frac{e^{x'\beta_k}}{1+\sum_{l=1}^{K-1} e^{x'\beta_l}}, \quad k=1,2,\ldots,K-1 \tag{9.49}$$

$$\mathbb{P}(Y=K|X=x) = \frac{1}{1+\sum_{l=1}^{K-1} e^{x'\beta_l}} \tag{9.50}$$

Comment on Logistic Regression:

- Classification core $x'\beta$ is linear, so logistic regression is still a linear classifier.
- Classification paramter βs are usually obtained using MLE. Detail see section. 6.4.3.

$$\beta^{(t+1)} = \beta^{(t)} - \left(\frac{\partial^2 \ell(\beta)}{\partial\beta\partial\beta'}\right)\frac{\partial \ell(\beta)}{\partial\beta} \tag{9.51}$$

$$= \beta^{(t)} + (X'WX)^{-1}X'(Y - \text{logit}(X,\beta^{(t)})), \quad W = \text{diag}\left\{\text{logit}(X,\beta^{(t)}) \odot (1-\text{logit}(X,\beta^{(t)}))\right\} \tag{9.52}$$

▷ R. **Code**

```
library(glmnet)
glmnet(x, y, family="binomial") # two-class
glmnet(x, y, family="multinomial") # multi-class
glmnet(x, y, family="binomial", alpha, lambda) # with penalty
```

☐ **Logistic Regression as Loss-Penalization Method**

Logistic Regression with ℓ_2 norm regularized term is

$$\arg\min_{\beta} \sum_{i=1}^{N} \log \mathbb{P}(Y \neq y_i | X = x_i; \beta) + \frac{\lambda}{2}\|\beta\|^2 \tag{9.53}$$

$$= \arg\max_{\beta} \sum_{i=1}^{N} \log[1+e^{y_i f(x_i)}] + \frac{\lambda}{2}\|\beta\|^2, \quad y_i \in \{+1,-1\} \tag{9.54}$$

where $f(\cdot)$ is classification function, $\beta_0 + x'\beta$ for linear classification.

Section 9.3 Support Vector Machine

Support vector machine (SVM) classifier was one of the most successful classification model in 2010±, mainly because of the kernel trick method in extending feature space.

First we will consider the linear classification case, i.e. dataset $\mathcal{D} = \{(\vec{x}_i, y_i), i = 1,2,\ldots,N\}$ are devided by a linear boundary $x'\beta + \beta_0$, where label $y_i \in \{1,-1\}$.

9.3.1 Derivation of Basic Optimize Problem

☐ **Hard Margin SVM**

The intuition of SVM is to determine the classification boundary by ensuring all the points are 'far away enough' from the boundary.

$$\begin{aligned}\underset{\beta,\beta_0,M}{\arg\max} \quad & M \\ s.t. \quad & \frac{1}{\|\beta\|} y_i(x_i'\beta + \beta_0) \geq M \quad i = 1, 2, \ldots, N\end{aligned}$$

where M for 'Margin', which indicates the distance of point from boundary. L.H.S. of inequality is the distance from x_i to boundary.[72]

However note that the *dof* of this problem is 1, i.e. all $(\beta_0, \beta) \propto (\beta_0^*, \beta^*)$ give the same result. We could omit this *dof* by putting an extra constraint, here a convenient one is used: $\|\beta\| = \dfrac{1}{M}$. i.e.

$$\begin{aligned}\underset{\beta,\beta_0:M=1/\|\beta\|}{\arg\min} \quad & \frac{1}{2}\|\beta\|^2 \\ s.t. \quad & y_i(x_i'\beta + \beta_0) \geq 1 \quad i = 1, 2, \ldots, N\end{aligned}$$

□ **Soft Margin SVM**

To tackle the case when $y_i(x_i'\beta+\beta_0) \geq 1$ cannot always been satisfied, use soft margin by inducing a 'slack variable' ξ_i for each point, indicating the proportion of distance that the point enters the margin, see figure. 6

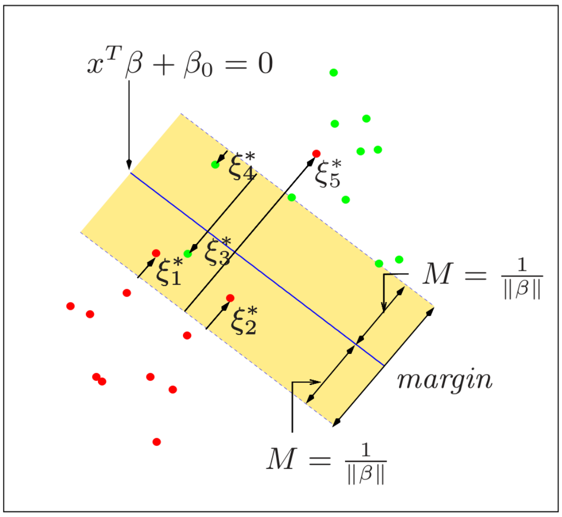


图 6: Support Vector Machine Illustration

[72]*proof:* denote some point on $x'\beta + \beta_0 = 0$ as $x_\perp$ (i.e. $x_\perp'\beta + \beta_0 = 0$), then the distance of x to boundary is the projection of $x - x_\perp$ on unit normal vector $\dfrac{\beta}{\|\beta\|}$:

$$d = \left|(x - x^*)'\frac{\beta}{\|\beta\|}\right| = \frac{1}{\|\beta\|}|x'\beta + \beta_0|$$

further because y_i varies at different sides of boundary:

$$y_i = 1 : x'\beta + \beta_0 > 0 \tag{9.55}$$

$$y_i = -1 : x'\beta + \beta_0 < 0 \tag{9.56}$$

we can replace the $|\cdot|$ using label:

$$d = \frac{1}{\|\beta\|} y(x'\beta + \beta_0)$$

Primal θ_P:

$$\begin{aligned} \underset{\beta,\beta_0:M=1/\|\beta\|}{\arg\min} \quad & \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i \\ s.t. \quad & y_i(x_i'\beta+\beta_0) \geq 1-\xi_i \quad i=1,2,\dots,N \\ & \xi_i \geq 0 \qquad\qquad\qquad\quad i=1,2,\dots,N \end{aligned}$$

write the generalized lagrange function as defined in equation. 6.20:

$$\mathcal{L}(\beta,\beta_0,\xi_i;\alpha,\mu) = \frac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i + \sum_{i=1}^{N}\alpha_i\left[1-\xi_i-y_i(x_i'\beta+\beta_0)\right] - \sum_{i=1}^{N}\mu_i\xi_i \tag{9.57}$$

$$s.t. \quad \alpha_i \geq 0, \quad \mu_i \geq 0, \qquad i=1,2,\dots,N \tag{9.58}$$

dual problem is given when $\dfrac{\partial\mathcal{L}}{\partial\beta,\beta_0,\xi_i} = 0$:

$$\frac{\partial\mathcal{L}}{\partial\beta} = 0 : \hat{\beta} = \sum_{i=1}^{N}\alpha_i y_i x_i \tag{9.59}$$

$$\frac{\partial\mathcal{L}}{\partial\beta_0} = 0 : \sum_{i=1}^{N}\alpha_i y_i = 0 \tag{9.60}$$

$$\frac{\partial\mathcal{L}}{\partial\xi_i} = 0 : C = \alpha_i + \mu_i, \quad i=1,2,\dots,N \tag{9.61}$$

Dual θ_D:

$$\theta_D(\alpha,\mu) = \min_{\beta,\beta_0,\xi_i}\mathcal{L} = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j x_i' x_j + \sum_{i=1}^{N}\alpha_i \tag{9.62}$$

$$s.t. \quad 0 \leq \alpha_i \leq C \tag{9.63}$$

$$\sum_{i=1}^{N}\alpha_i y_i = 0 \tag{9.64}$$

we can maximize θ_D to obtain $\hat{\alpha}_i$, $\hat{\mu}_i = C - \hat{\alpha}_i$. And $(\hat{\beta},\hat{\beta}_0,\xi_i)$ are given utilizing KKT condition for $d^* = \max_{\alpha,\mu}\theta_D = \min_{\beta,\beta_0,\xi_i}\theta_P = p^*$:

$$\hat{\alpha}_i\left[1-\hat{\xi}_i-y_i(x_i'\hat{\beta}+\hat{\beta}_0)\right] = 0 \tag{9.65}$$

$$(C-\hat{\alpha}_i)\hat{\xi}_i = 0 \tag{9.66}$$

$$1-\hat{\xi}_i-y_i(x_i'\hat{\beta}+\hat{\beta}_0) \leq 0 \tag{9.67}$$

$$0 \leq \hat{\alpha}_i \leq C \tag{9.68}$$

$$\hat{\xi}_i \geq 0 \tag{9.69}$$

$$\hat{\beta} = \sum_{i=1}^{N}\hat{\alpha}_i y_i x_i \tag{9.70}$$

discussion on different cases of α_i,ξ_i:

$$\hat{\alpha}_i = 0 : \hat{\xi}_i = 0 \tag{9.71}$$

$$\hat{\alpha}_i = C : y_i(x_i\hat{\beta}+\hat{\beta}_0) = 1-\hat{\xi}_i \tag{9.72}$$

$$0 < \hat{\alpha}_i < C : \hat{\xi}_0 = 0, \; y_i(x_i\hat{\beta}+\hat{\beta}_0) = 1 \tag{9.73}$$

where all points $\mathcal{I}^{\text{sv}} := \{i^{\text{sv}} \big| 0 < \hat{\alpha}_{i^{\text{sv}}} < C,\, \hat{\xi}_{i^{\text{sv}}} = 0\}$ are called '**support vector**', that can be used to determine β_0:

$$\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i = \sum_{i\in\mathcal{I}^{\text{sv}}} \hat{\alpha}_i y_i x_i \tag{9.74}$$

$$\hat{\beta}_0 = y_{i^{\text{sv}}} - x'_{i^{\text{sv}}}\hat{\beta} \tag{9.75}$$

9.3.2 Support Vector Machine as Loss-Penalization Method

SVM Primal can be express in equivalent form with $f(x_i)$ as prediction function, e.g. $f(x_i) = \beta_0 + x_i'\beta$ for linear SVM:

$$\begin{cases} \xi_i \geq 0 \\ \xi_i \geq 1 - y_i f(x_i) \end{cases} \Rightarrow \xi_i \geq \max\{0, 1 - y_i f(x_i)\} = [1 - y_i f(x_i)]_+ \tag{9.76}$$

in which $[\,\cdot\,]_+ \equiv \max\{0,\,\cdot\,\}$ is hinge loss:

$$\arg\min_{\beta,\beta_0} \sum_{i=1}^{N} [1 - y_i f(x_i)]_+ + \frac{\lambda}{2}\|\beta\|^2, \qquad \lambda = \frac{1}{C}, \quad f(x_i) = \beta_0 + x_i'\beta$$

which is naturally in an $\arg\min_f \sum_{i=1}^{N} \mathcal{L}\left(x_i, y_i, f(x_i)\right) + \frac{\lambda}{2}\mathcal{P}(f(\,\cdot\,))$ Loss+Penalty form.

9.3.3 Kernel Support Vector Machine

Section 9.4 Feature Expansion and Kernel Methods

Motivation: Map the data point $x \in \mathcal{X}(e.g. = \mathbb{R}^p)$ to another feature space $\mathcal{F}(e.g. = \mathbb{R}^M)$ (not necessarily a linear transform, usually $M > p$, or just proper to describe the features). The mapping function lies in a Hilbert space $\mathcal{H}$ of function:

$$h(\,\cdot\,) = (h_1(\,\cdot\,), h_2(\,\cdot\,), \ldots, h_M(\,\cdot\,))' \in \mathcal{H} : \mathcal{X} \to \mathcal{F}$$

and we can construct model in feature space.

9.4.1 Reproducing Kernel Hilbert Space and The Representer Theorem

Based on the idea of feature space, make a step forward: the key focus of model is actually 'measuring space structure by similarity between points' rather than having to define a feature space. i.e. describe similarity by a bi-linear **Kernel Function**

$$K(x, x') \in \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

In intuition for Kernel is an 'inner product kernel'. The Kernel corresponds a kind of inner product structure on $\mathcal{H}$, the kernel should satisfies the following properties:

1. Semi-Positive Definition:

$$\int\int K(x,y) g(x) g(y)\,\mathrm{d}x\mathrm{d}y \geq 0, \quad \forall g(\,\cdot\,) \tag{9.77}$$

or an equivalent form:

$$\sum_{i,j=1}^{n} K(x_i, x_j)a_i a_j \geq 0, \quad \forall \{x_i\}_{i=1}^{m}, \{a_i\}_{i=1}^{n}, \quad \forall n \in \mathbb{Z}^+ \tag{9.78}$$

2. symmetry:

$$K(x, y) = K(y, x) \tag{9.79}$$

Eigenvalue γ_i and eigen function $\phi_i(x)$ of Kernel:

$$\int_x K(x, y)\phi_i(y)\,\mathrm{d}y = \gamma_i \phi_i(x) \tag{9.80}$$

In Hilbert space, the eigen functions are orthonormal:

$$\langle \phi_i, \phi_j \rangle = \int_x \phi_i(x)\phi_j(x)\,\mathrm{d}x = \delta_{ij} \tag{9.81}$$

And Kernel $K(x, y)$ could be represented from its eigen value and eigen function:

$$K(x, y) = \sum_i \gamma_i \phi_i(x)\phi_i(y) \tag{9.82}$$

which is Mercer's Thm.: Semi-positive definite symmetric kernel could be expressed as an inner product form. Such a form is also called the kernel trick because it usually avoid calculating inner product in high dimensional space.

☐ **Reproducing Kernel Hilbert Space (RKHS)**

Now use set $\{\phi_i\}$ as the orthonormal base to form a Hilbert space $\mathcal{H}_K = \mathrm{span}\{\phi_i\}$ i.e. any function $f \in \mathcal{H}_K$ could be expressed as expansion

$$\mu(x) = \sum_i \mu_i \phi_i(x) \tag{9.83}$$

The inner product defined for this Hilbert space is[73]

$$\left\langle \sum_i \mu_i \phi_i(x), \sum_i \nu_i \phi_i(x) \right\rangle_{\mathcal{H}_K} = \sum_i \frac{\mu_i \nu_i}{\gamma_i} \tag{9.84}$$

and norm induced by inner product

$$\|f\|_{\mathcal{H}_K} = \sum_i \frac{f_i^2}{\gamma_i}, \qquad f(x) = \sum_i f_i \phi_i(x) \tag{9.85}$$

Note: when x is fixed, $f_x(y) = K(x, y)$ is a function of y, and vice versa. Use the above expansion and inner product:

$$\begin{aligned}
K(x, y) &= \sum_i \gamma_i \phi_i(x)\phi_i(y) && (9.86)\\
&= \sum_i \sqrt{\gamma_i}\phi_i(x)\sqrt{\gamma_i}\phi_i(y) && (9.87)\\
&= \sum_i \frac{(\gamma_i\phi_i(x))(\gamma_i\phi_i(y))}{\gamma_i} && (9.88)\\
&= \left\langle \sum_i \gamma_i\phi_i(x)\phi_i(\xi), \sum_i \gamma_i\phi_i(y)\phi_i(\xi) \right\rangle_{\mathcal{H}_K} && (9.89)\\
&= \langle K(x, \xi), K(\xi, y)\rangle_{\mathcal{H}_K} && (9.90)
\end{aligned}$$

[73] Hilbert space is complete linear space with inner product defined.

which is the reproducing property of Kernel $K(\cdot,\cdot)$ and its corresponding Hilbert space $\mathcal{H}_K$

☐ **Representer Thm. for RKHS**

With Kernel and its corresponding RKHS defined, we could write a optimization problem as loss+penalty form:

$$\underset{f\in\mathcal{H}_K}{\arg\min} \sum_{i=1}^{N} \mathcal{L}(y_i, f(x_i)) + \frac{\lambda}{2}\|f\|^2_{\mathcal{H}_K} \tag{9.91}$$

Representer Thm.: Solution to above optimization has a **finite** form

$$\hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) \tag{9.92}$$

i.e. we can optimize over $\{\hat{\alpha}_i\}_{i=1}^N$, instead of optimizing over $\{f_i\}_{i=1}^{\infty}$.

norm of $\hat{f}$ is represented as

$$\left\|\hat{f}\right\|^2_{\mathcal{H}_K} = \left\langle \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i), \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) \right\rangle_{\mathcal{H}_K} \tag{9.93}$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N} \hat{\alpha}_i\hat{\alpha}_j K(x_i, x_j) \tag{9.94}$$

Optimization problem equation. 9.91 is parameterized by $\{\hat{\alpha}_i\}_{i=1}^N$:

$$\underset{\{\hat{\alpha}_i\}_{i=1}^N\in\mathbb{R}^N}{\arg\min} \sum_{i=1}^{N} \mathcal{L}(y_i, \sum_{j=1}^{N} \hat{\alpha}_j K(x_i, x_j)) + \frac{\lambda}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \hat{\alpha}_i\hat{\alpha}_j K(x_i, x_j) \tag{9.95}$$

Or written in matrix form $y = (y_1, y_2, \ldots, y_N)$ $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_N)$, $K = \{K(x_i, x_j)\}_{i,j=1}^N$:

$$\underset{\alpha\in\mathbb{R}^N}{\arg\min} \sum_{i=1}^{N} \mathcal{L}(y, K\alpha) + \frac{\lambda}{2}\alpha' K\alpha \tag{9.96}$$

Classification criterion

$$\hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) \tag{9.97}$$

9.4.2 Useful Kernel

Some useful Kernel for numeric vector x:

- Linear Kernel (identity):

$$K(x, y) := \langle x, y\rangle \tag{9.98}$$

- d^{th} Degree Polynomial Kernel

$$K(x, y) := (1 + \langle x, y\rangle)^d \tag{9.99}$$

- Radical Base Function Kernel:

$$K(x, y) := \exp\left[-\frac{\|x-y\|^2}{\sigma^2}\right] \tag{9.100}$$

- Sigmoid Kernel:

$$K(x, y) = \tanh\left(1 + \langle x, y \rangle\right) \tag{9.101}$$

Note that equation. 9.95 includes Kernel $K(\cdot, \cdot)$ only, thus Kernel trick could be applied to various scenarios once we could define a proper Kernel. e.g. Substring Kernel for string sequence.

9.4.3 Kernel Support Vector Machine

Replace the inner produce term in Dual problem of SVM equation. 9.62 into Kernel function to obtain Kernel SVM:

$$\arg\min_{\hat{\alpha}} \sum_{i=1}^{N} \hat{\alpha}_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{\alpha}_i \hat{\alpha}_j y_i y_j K(x_i, x_j) \tag{9.102}$$

$$\hat{f}(x) = \sum_{i \in \mathcal{I}^{\text{sv}}} \hat{\alpha}_i y_i K(x, x_i) + \hat{\beta}_0 \tag{9.103}$$

Or use the loss+penalization primmal form of SVM:

$$\arg\min_{\hat{\alpha}} \sum_{i=1}^{N} \left[1 - y_i \sum_{j=1}^{N} \hat{\alpha}_j K(x_i, x_j)\right]_+ + \frac{\lambda}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{\alpha}_i \hat{\alpha}_j K(x_i, x_j), \quad \lambda = \frac{1}{C} \tag{9.104}$$

$$\hat{y}(x) = \begin{cases} 1 & , \hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) \geq s \\ -1 & , \hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) < s \end{cases} \tag{9.105}$$

Note that the loss function form is $[1 - y_i f(x_i)]_+$

9.4.4 Kernel Regression

□ **Kernel Regression with Squared Error Loss**

Recall linear regression with RS loss

$$\arg\min_{\beta_0, \beta} \sum_{i=1}^{N} \left[y_i - \beta_0 - x_i'\beta\right]^2 + \frac{\lambda}{2} \|\beta\|_2^2 \tag{9.106}$$

replace linear classification $f(x) = \beta_0 + x'\beta$ into Kernel $K\alpha$:

$$\arg\min_{\hat{\alpha}} (y - K\hat{\alpha})'(y - K\hat{\alpha}) + \frac{\lambda}{2} \hat{\alpha}' K \hat{\alpha} \tag{9.107}$$

Solution is similar to ridge regression form:

$$\hat{\alpha} = (K + \lambda I)^{-1} y \tag{9.108}$$

□ **Kernel Logistic Regression**

In logistic regression, the loss function is binomial deviance $\log\left[1 + e^{-yf(x)}\right]$

$$\arg\min_{\hat{\alpha}} \sum_{i=1}^{N} \log\left[1 + e^{y_i \sum_{j=1}^{N} \hat{\alpha}_j K(x_i, x_j)}\right] + \frac{\lambda}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{\alpha}_i \hat{\alpha}_j K(x_i, x_j) \tag{9.109}$$

$$\hat{y}(x) = \begin{cases} 1 & , \hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) \geq s \\ -1 & , \hat{f}(x) = \sum_{i=1}^{N} \hat{\alpha}_i K(x, x_i) < s \end{cases} \tag{9.110}$$

Section 9.5 Clustering

Clustering is an important scenario of unsupervised learning $\mathcal{D} = \{x_i\}_{i=1}^N$, to cluster 'similar' data points into the same group.

9.5.1 Proximity Matrix

For separation concern, we should first define some metric to measure similarity between data

$$d_{ij} = D(x_i, x_j) \tag{9.111}$$

common usage of distance measure see section. 4.7

And form the proximity matrix W:

$$D = \{d_{ij}\}_{i,j=1}^N \tag{9.112}$$

Usually some clustering algorithm would claim some properties:

- Non-negative element and non-zero diagonal:

$$d_{ij} \geq 0, \forall i, j. \qquad d_{ii} = 0, \forall i \tag{9.113}$$

- Symmetry

$$D = D^T \tag{9.114}$$

Overall dissimilarity:

$$\bar{D} = \frac{1}{N^2}\sum_{i=1}^N \sum_{j=1}^N D(x_i, x_j) \tag{9.115}$$

☐ **Optimizing Goal of Clustering**

With similarity/dissimilarity defined, clustering target could be expressed as maximizing within cluster scatter/ minimizing between cluster scatter, with respect to clustering group $C(\cdot)$

$$\underset{C(\cdot)}{\arg\max} \frac{1}{2}\sum_{k=1}^K \sum_{i:C(x_i)=k} \sum_{j:C(x_j)=k} D(x_i, x_j) \tag{9.116}$$

$$\underset{C(\cdot)}{\arg\min} \frac{1}{2}\sum_{k=1}^K \sum_{i:C(x_i)=k} \sum_{j:C(x_j)\neq k} D(x_i, x_j) \tag{9.117}$$

The two forms are equivalent due to a fixed sum:

$$\frac{1}{2}\sum_{k=1}^K \sum_{i:C(x_i)=k} \sum_{j:C(x_j)=k} D(x_i, x_j) + \frac{1}{2}\sum_{k=1}^K \sum_{i:C(x_i)=k} \sum_{j:C(x_j)\neq k} D(x_i, x_j) = \frac{1}{2}\sum_{i=1}^N \sum_{j=1}^N D(x_i, x_j) := T = \text{const} \tag{9.118}$$

Usually search for cluster assignment is based on iterative greedy descent search.

Some frequently used clustering methods are included in section. 4.7

- Hierarchical Method

- K-Means
- EM-Gaussian Mixture Model
- DBSCAN & OPTICS Density Method

In this section, an extra model based on spectrum is introduced

9.5.2 Spectrum Clustering

Express the dataset as a Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$, where $\mathcal{V} = \{v_i\}_{i=1}^N$ for vertex, $\mathcal{E} = \{e_{ij}\}_{i,j=1}^N$, $\mathcal{W} = \{w_{ij}\}_{i,j=1}^N$ for edges and weights. In this case cluster is a graph partition problem.

□ **Graph Laplacian**

Some definition:

- Degree of vertex:

$$d_i = \sum_{j=1}^N w_{ij} \tag{9.119}$$

- Degree matrix

$$D = \text{diag}\{d_1, d_2, \ldots, d_N\} \tag{9.120}$$

- Unnormalized graph Laplacian:

$$L := D - W \tag{9.121}$$

  is symmetric and semi-positive definite

$$\xi' L \xi = \sum_{i,j=1}^N w_{ij}(\xi_i - \xi_j)^2 \geq 0, \quad \forall \xi \in \mathbb{R}^N \tag{9.122}$$

Spectrum is based on studying the eigen vector and eigen value of L.

- For any graph Laplacian $\underset{m\times m}{L}$, $\mathbf{1}_m$ is a eigen vector with eigen value 0
- In the case that $\mathcal{G}$ is **not** fully connected, with K subgraph $\mathcal{G} = \{\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_K\}$, i.e. W and L could be written in diagonal form (usually need some row/column transformation)

$$L = \begin{bmatrix} L_1 & 0 & \ldots & 0 \\ 0 & L_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & L_K \end{bmatrix} \tag{9.123}$$

  the multiplicity of eigen value 0 is K, with each eigen vector as

$$\mathbf{1}_{\mathcal{G}_k} = [\mathbb{I}(v_1 \in \mathcal{G}_k), \ldots, \mathbb{I}(v_N) \in \mathcal{G}_k], \quad k = 1, 2, \ldots, K \tag{9.124}$$

- In real world case, the graph could probably expressed as a small deviance from a graph with subgraph:

$$L = \begin{bmatrix} L_1 & 0 & \dots & 0 \\ 0 & L_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & L_K \end{bmatrix} + N \underset{\delta}{\times} N \tag{9.125}$$

  where we would expect the smallest K eigen value $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_K$ corresponds to the K cluster we want.

Algorithm *Spectral Clustering*

---

1. Compute $\underset{N\times N}{L}$
2. Determine the K smallest eigen values $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_K$ with eigen vector $u_i, i = 1, 2, \dots, K$

$$U = [u_1, u_2, \dots, u_K] = \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1K} \\ u_{21} & u_{22} & \dots & u_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N1} & u_{N2} & \dots & u_{NK} \end{bmatrix} = [z_1, z_2, \dots, z_N]^T \tag{9.126}$$

$$z_i = [u_{i1}, u_{i2}, \dots, u_{iK}]^T, \quad i = 1, 2, \dots, N \tag{9.127}$$

3. Cluster $\{z_i\}_{i=1}^N$ with e.g. K-Means.

Choice of normalized graph Laplacian, would cause different cluster results:

- Ratio Cut $L = I - D^{-1}W$

$$\underset{\{\mathcal{G}_1,\dots,\mathcal{G}_K\}}{\arg\min} \frac{1}{2} \sum_{i=1}^K \frac{\text{Bet}(\mathcal{G}_i, \mathcal{G}_i^\complement)}{|\mathcal{G}_i|} \tag{9.128}$$

- Normalized Cut $L = I - D^{-1/2}WD^{-1/2}$

$$\underset{\{\mathcal{G}_1,\dots,\mathcal{G}_K\}}{\arg\min} \frac{1}{2} \sum_{i=1}^K \frac{\text{Bet}(\mathcal{G}_i, \mathcal{G}_i^\complement)}{\sum_{i\in\mathcal{G}_i}\sum_{j\in\mathcal{G}} d_{ij}} \tag{9.129}$$

Section 9.6 Tree-Based Classification Model

Idea of tree: divide the space $\mathcal{X}$ into grids R_m and assign prediction into the most frequent class

$$\hat{f}(x \in R_m) = \arg\max_k \sum_{x_i \in R_m} \mathbb{I}(y_i = k) \tag{9.130}$$

But such method is not practical in high dimensional due to curse of dimensionality. Nore practical method would be a greedy search, each step along one variable.

9.6.1 Tree-Based Classification

☐ **Branch Growing Process**

Grow branch on a node

Algorithm *Classification Tree*

In each branck growing on a node:

1. Look for a splitting variable x_j and split value s:

$$\arg\min_{j,s}\left[N_{\text{left}}\text{ImPu}(x_i \in R_{\text{left}}(j,s)) + N_{\text{right}}\text{ImPu}(x_i \in R_{\text{right}}(j,s))\right] \tag{9.131}$$

$$R_{\text{left}}(j,s) = \{x : x_j \le s\}, \quad R_{\text{right}}(j,x) = \{x : x_j > s\} \tag{9.132}$$

useful impurity measure $\text{ImPu}(\{x\})$ with $p_k(X = \{x\})$ defined

$$p_k(X) = \frac{\sum_{x\in X}\mathbb{I}(C(x)=k)}{|X|} \tag{9.133}$$

- Misclassification rate

$$1 - \max_k p_k \tag{9.134}$$

- Gini impurity

$$\sum_{k=1}^{K} p_k(1-p_k) = \sum_{k=1}^{K}\sum_{k'\neq k} p_k p_{k'} \tag{9.135}$$

Gini impurity with category weight $\underset{K\times K}{W_K} = \{w_{kk'}\}_{k,k'=1}^{K}$

$$\sum_{k=1}^{K}\sum_{k'\neq k} w_{kk'}p_k p_{k'} \tag{9.136}$$

- Entropy

$$-\sum_{k=1}^{K} p_k \log p_k \tag{9.137}$$

2. usually the process ends when

$$|\text{node}| \le \text{const}, \quad \forall\text{node} \tag{9.138}$$

3. Apply cost complexity pruning strategy

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m \text{ImPu}(R_m) + \alpha|T| \tag{9.139}$$

where T is tree, $|T|$ for number of nodes in the tree.

Comment:

- Tree methods is well-interpreted, especially similar to a natural desicion making process

- Handle non-linear classification pattern
- Unstable to data.

Performance of tree classification could be largely improved with bagging method and boosting method.

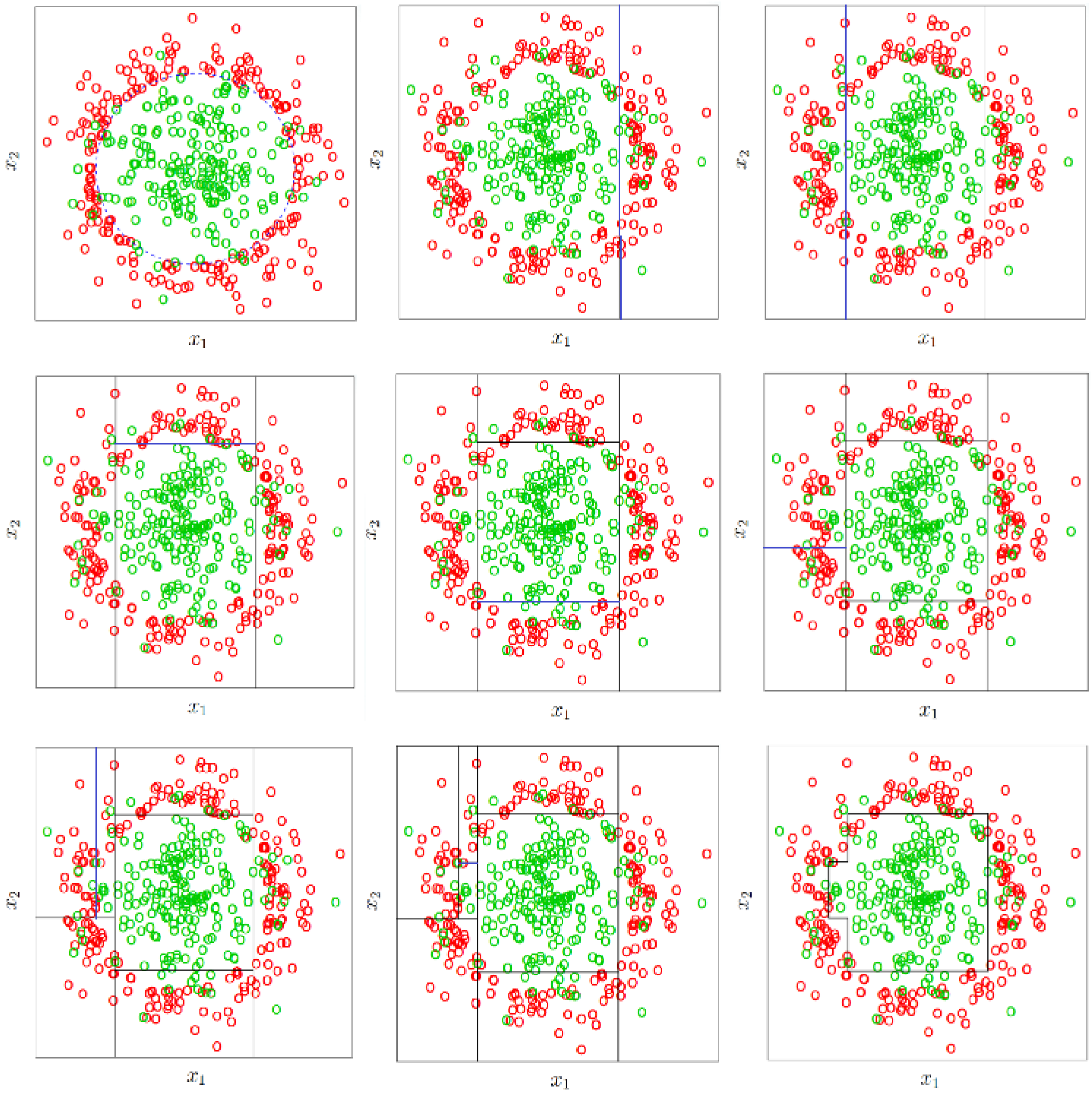


图 7:

9.6.2 Bagging and Boosting

□ **Bagging**

Bagging is short for **B**ootstrap **Agg**regation. Idea: for B boostrapped training data, the boostrapping result

$$\hat{f}_{\text{boot}}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}_b(x) \text{ or } = \arg\max_k \sum_{b=1}^{B}\mathbb{I}(\hat{f}_b(x) = k) \tag{9.140}$$

□ **Random Forest**

Random Forest aims at decorrelating trees to reduce variance when averaging trees.

Algorithm *Random Forest Bagging*

---

1. Generate B different boostrapped training data. (*random 1* by bootstrap sampling)

2. For each sample, grow a tree. In each split of tree (i.e. a branch growth), $q \approx \sqrt{p}$ variable components are randomly selected for classification. (*random 2* by randomizing components)

3. Take average or vote of all B trees as the final result

Comment: A prune is usually needed, cause variance is reduced by averaging.

☐ **Boosting**

Idea: Fitting result of previous trees could be used to modify following trees. The error rate of each tree would influence the vote weight when bagging the results.

Algorithm *Adaboost*

---

1. Each observant is given weights $w_i^{(0)} = \dfrac{1}{N}$, $i = 1, 2, \ldots, N$

2. For $m = 1 : M$, M for loops of boosting:

   (a) Grow a tree $T^{(m)}(x)$ with weight $w_i^{(m)}$

   (b) Compute **error rate**

$$\text{err}^{(t)} := \frac{\sum_{i=1}^N w_i^{(m)} \mathbb{I}(y_i \neq T^{(m)}(x_i))}{\sum_{i=1}^N w_i^{(m)}} \tag{9.141}$$

   and define

$$\alpha^{(m)} = \log\left[(1 - \text{err}^{(m)})/\text{err}^{(m)}\right] \tag{9.142}$$

   (c) Reset weights by

$$w_i^{(m+1)} = w^{(m)} \cdot \exp\left[\alpha^{(m)} \mathbb{I}(y_i \neq T^{(m)}(x_i))\right] \tag{9.143}$$

3. Output

$$\hat{f}(x) = \text{sgn}\left[\sum_{m=1}^M \alpha^{(m)} T^{(m)}(x)\right] \tag{9.144}$$

Section 9.7 Neural Network

☐ **Linear Perceptron with Activate Function**

Usually linear perceptron is used as a neuron in neutral network:

$$y = g(w_0 + w_1 x_1 + \ldots + w_p x_p) = g(x'w), \quad x_0 \equiv 1 \tag{9.145}$$

where $g(\cdot)$ is activate function. Such Perceptron could be optimized by gradient

Some useful activate function:

- Linear Threshold Unit (LTU)

$$g(\xi) = \begin{cases} 0, & \xi < 0 \\ 1, & \xi \geq 0 \end{cases} = \eta(\xi) \tag{9.146}$$

- Logistic Function

$$g(\xi) = \frac{1}{1 + e^{-\xi}} \tag{9.147}$$

- Hyperbolic Tangent Function

$$g(\xi) = \tanh \xi = \frac{e^{2\xi} - 1}{e^{2\xi} + 1} \tag{9.148}$$

- Rectified Linear Unit (ReLU)

$$g(\xi) = \begin{cases} 0, & \xi < 0 \\ \xi, & \xi \geq 0 \end{cases} \tag{9.149}$$

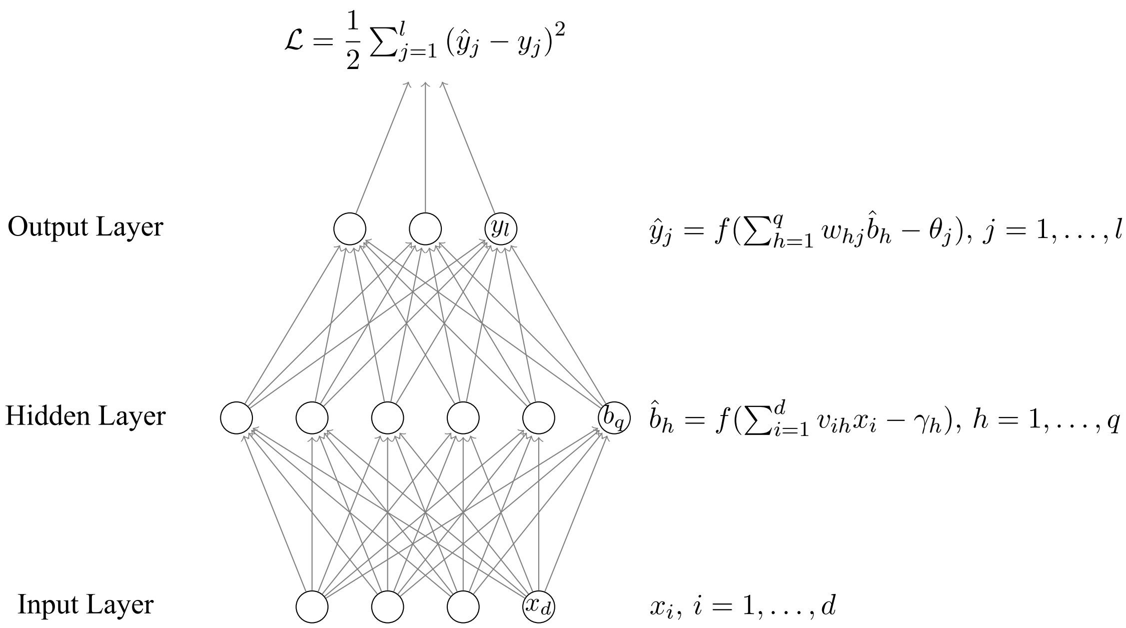


图 8: Structure of Feed-Forward Neural Network (1 Layer)

A MonoLayer perceptron with enough neurons (hidden units) could represent any coutinuous function. MultiLayer Perceptron (MLP) could even represent discontinuous functions.

9.7.1 Back Propagation

Perceptron system is usually optimized by back propagation (of gradient).

An example to optimize v_{ih}, γ_h in figure. 8:

$$\frac{\partial \mathcal{L}}{\partial v_{ih}} = \sum_{j=1}^{l} \frac{\partial \mathcal{L}}{\partial \hat{y}_j} \frac{\partial \hat{y}_j}{\partial \hat{b}_h} \frac{\partial \hat{b}_h}{\partial v_{ih}} \tag{9.150}$$

$$= \sum_{j=1}^{l} \hat{y}_j(\hat{y}_j - y_j) \cdot \frac{\partial f(u)}{\partial u}\Big|_{u=\sum w_{hj}\hat{b}_h-\theta_j} w_{hj} \cdot \frac{\partial f(v)}{\partial v}\Big|_{v=\sum_{i=1}^{d} v_{ih}x_i-\gamma_h} x_i \tag{9.151}$$

$$\frac{\partial \mathcal{L}}{\partial \gamma_h} = \sum_{j=1}^{l} \frac{\partial \mathcal{L}}{\partial \hat{y}_j} \frac{\partial \hat{y}_j}{\partial \hat{b}_h} \frac{\partial \hat{b}_h}{\partial \gamma_h} \tag{9.152}$$

$$= \sum_{j=1}^{l} \hat{y}_j(\hat{y}_j - y_j) \cdot \frac{\partial f(u)}{\partial u}\Big|_{u=\sum w_{hj}\hat{b}_h-\theta_j} w_{hj} \cdot \frac{\partial f(v)}{\partial v}\Big|_{v=\sum_{i=1}^{d} v_{ih}x_i-\gamma_h} \cdot (-1) \tag{9.153}$$

Chapter. X 应用时间序列部分

Instructor: Dong Li

Section 10.1 Time Series Data and Model

10.1.1 Time Series Data and Tasks

Time Series : a sequential r.v. indexed in time order.

$$\{Y_t\},\ t \in \mathcal{T} \quad \mathcal{T} \text{ is index set} \tag{10.1}$$

and actual data of time series, i.e. times series data is called a **Realization** of time series, denoted[74]

$$\{y_t\},\ t \in T \subset \mathcal{T}$$

e.g. in forecasting task, T encodes history. In this chapter we usually focus on easier case of arithmetic progression $T = \{1, 2, \dots, N\}$, or at least numeric orderal sequence.

Time Series Analysis (TSA): Analysis on time series data to extract meaningful statistics/other characteristics. Task of TSA includes:

- Describing and Explanaing the machanism of time series
- Forecasting
- Guiding the intervention of Time Series

In this section several modelling/forecasting methods would be included.

10.1.2 Time Series Model

There are plenty of useful modelling methods:

- Regression Model: View y as function of t, regression on some model $y = f(t)$ with loss $\mathcal{L}$. e.g. linear regression

  $$y = \beta_0 + \beta_1 t + \varepsilon, \quad \mathcal{L} = \sum_{t \in T} (y_t - \hat{y}_t)^2$$

  Modelling strategy is similar to that introduced in linear regression, see Chapter. 3
- STL Method: Seasonal and Trend decomposition using Loess. A decomposition of time series into 'TS = Trend + Season + Random', i.e.

  $$Y_\tau = T_\tau + S_\tau + X_\tau \tag{10.2}$$

  and we could model T_τ, S_τ, X_τ separately. The focus is the modelling of random term X_t, which we expect to be 'stationarily random' through time. (Usually we model this part also by ARMA model)
- Exponential Smoothing Model: Use weighted average over history to predict future.
- ARIMA Model: The main focus of this chapter.

[74] A note on $T \subset \mathcal{T}$: actually T has to be discrete beacuse it is a sample of $\mathcal{T}$. while $\mathcal{T}$ is not necessarily defined as discrete.

Section 10.2 Stochastic Process and Statistics

10.2.1 Basic Knowledge of Stochastic Process

A stochastic process can be denoted:

$$\{X_t : t \in \mathcal{T}\} : \Omega \times \mathcal{T} \to \mathcal{E} \tag{10.3}$$

☐ **Some important cases of stochastic process:**

- i.i.d. sequence: ε_t i.i.d. $\sim \varepsilon$
- White Noise: uncorrelated for different subscript t in the sense of 2nd moment, $\varepsilon_t \sim \mathrm{WN}(\mu, \sigma^2)$. where

$$\begin{aligned}\mathbb{E}\left(\varepsilon_t\right) =& \mu \\ cov(\varepsilon_t, \varepsilon_s) =& \sigma^2 \delta_{t,s}\end{aligned}$$

  Further we can append more constraints on WN:

  + $\{\varepsilon_t\}$ independent: independent white noise $\varepsilon_t \sim \mathrm{IWN}(\mu, \sigma^2)$
  + $\mu = 0$: zero-mean white noise $\varepsilon_t \sim \mathrm{WN}(0, \sigma^2)$
  + $\mu = 0$, $\sigma^2 = 1$: standard white noise $\varepsilon_t \sim \mathrm{WN}(0, 1)$
  + $\varepsilon \sim N(\mu, \sigma^2)$: normal white noise.

- Martingale difference sequence (MDS): zero expectation given history information: $\varepsilon_t \sim$ MDS, where

$$\begin{aligned}\mathbb{E}\left(|\varepsilon_t|\right) <& \infty \\ \mathbb{E}\left(\varepsilon_t | \mathcal{F}_{t-1}\right) =& 0\end{aligned}$$

  where $\mathcal{F}_\tau$ denotes the history until time τ:

$$\mathcal{F}_\tau \equiv \sigma\left(\varepsilon_s,\, s \le \tau\right) \{\varepsilon_s, \varepsilon_{s-1}, \varepsilon_{s-2}, \ldots\} \tag{10.4}$$

Relation: i.i.d. $>$ MDS $>$ WN $>$ Stationary

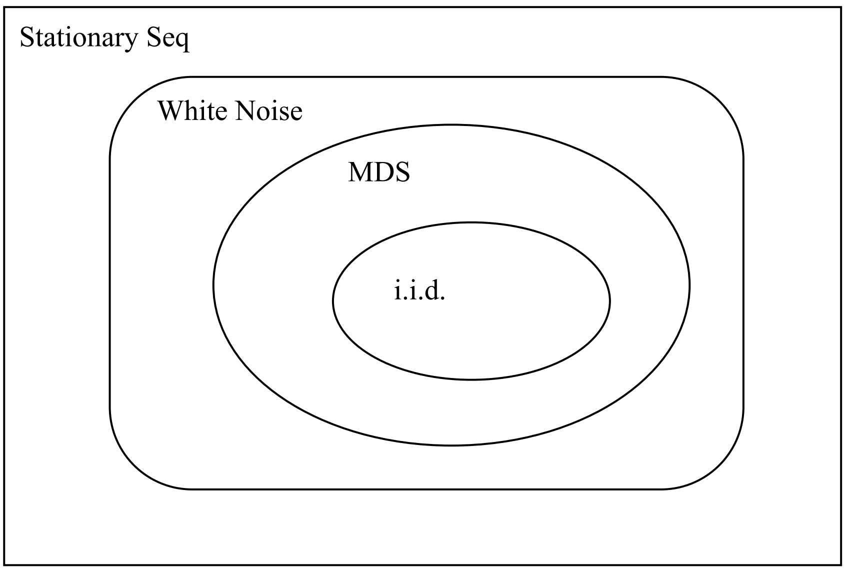


图 9: Relation bet. Sequences

☐ **Measure of dependence within stochastic process**

Given a stochastic process $\{X_t : t \in \mathcal{T}\}$

- Mean Function

$$\mu_t = \mathbb{E}(X_t) \tag{10.5}$$

- AutoCovariance Function (ACVF) and AutoCorrelation Function (ACF):

$$\begin{aligned}\text{ACVF: } \gamma_{t,s} \equiv& cov(X_t, X_s), & \mathcal{T}\times\mathcal{T} \to& \mathbb{R}\\ \text{ACF: } \rho_{t,s} \equiv& corr(X_t, X_s) = \frac{\gamma_{t,s}}{\sqrt{\gamma_{t,t}\gamma_{s,s}}}, & \mathcal{T}\times\mathcal{T} \to& [-1,1]\end{aligned}$$

- Stationarity: Stationarity is a measure that the 'correlation structure of stochastic process looks the same' at any time t, i.e. is stationary through time.
  - Weakly Stationary (WS): given $\mathbb{E}\left(X_t^2\right) < \infty$, has const mean and cov independent of time

$$\begin{aligned}\mathbb{E}(X_t) =& \mu_t = \mu\\ cov(X_t, X_t + k) =& \gamma_{t,t+k} = \gamma_k \perp\!\!\!\perp t\end{aligned}$$

  - Strictly Stationary (SS): joint distribution invariant through time. For any given $\{t_1, t_2, \ldots, t_n\} \subset \mathcal{T}$

$$f_{X_{t_1}, X_{t_2}, \ldots, X_{t_n}} = f_{X_{t_1+h}, X_{t_2+h}, \ldots, X_{t_n+h}}, \quad \forall h \tag{10.6}$$

  Some note on WS and SS:

  - Generally speaking, WS and SS are not equivalant, WS $\not\Leftrightarrow$ SS (note that SS does not put constraint on $\mathbb{E}\left(X_t^2\right)$)
  - equivalent for gaussian stochastic process.
  - ACF and ACVF of WS:

$$\begin{aligned}\gamma_{t,t+k} =& \gamma_k = \gamma_{-k}, \quad \forall t \in \mathcal{T}\\ \rho_{t,t+k} =& \rho_k = \frac{\gamma_k}{\gamma_0}, \quad \forall t \in \mathcal{T}\end{aligned}$$

  Notation of ACVF matrix:

$$\Gamma_k = \{\gamma_{i-j}\}_{i,j=1}^k = \begin{bmatrix}\gamma_0 & \gamma_1 & \gamma_2 & \cdots & \gamma_{k-2} & \gamma_{k-1}\\ \gamma_1 & \gamma_0 & \gamma_1 & \cdots & \gamma_{k-3} & \gamma_{k-2}\\ \gamma_2 & \gamma_1 & \gamma_0 & \cdots & \gamma_{k-4} & \gamma_{k-3}\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ \gamma_{k-2} & \gamma_{k-3} & \gamma_{k-4} & \cdots & \gamma_0 & \gamma_1\\ \gamma_{k-1} & \gamma_{k-2} & \gamma_{k-3} & \cdots & \gamma_1 & \gamma_0\end{bmatrix}_{k\times k} \tag{10.7}$$

  Γ_k is semi-positive definite.

$$\sum_{i=1}^k \sum_{j=1}^k \alpha_i \alpha_j \gamma_{|t_i - t_j|} \geq 0, \quad \forall k, \{t_1, \ldots, t_k\}, \vec{\alpha} \tag{10.8}$$

- Partial Autocorrelation (PACF): correlation given information between two time points, orginal definition

$$\phi_{11} = \phi_1 \tag{10.9}$$

$$\phi_{kk} = corr\big(X_t - L(X_t|X_{t+1},\dots,X_{t+k-1}), X_{t+k} - L(X_{t+k}|X_{t+1},\dots,X_{t+k-1})\big), \quad k \geq 2 \tag{10.10}$$

where $L(X_\tau|X_{t+1},\dots,X_{t+k-1})$ is the **Best Linear Estimation** of linear model

$$X_\tau = \beta_0 + \beta_1 X_{t+1} + \ldots + \beta_{k-1} X_{t+k-1} + \epsilon$$

deduction:

  - Best linear estimation $\hat{X}_\tau \equiv L(X_\tau|X_{t+1},\dots,X_{t+k-1})$ satisfies

$$\{\beta_0, \beta\} = \arg\min_{\beta_0,\beta} \mathbb{E}\left(\hat{X}_\tau - \beta_0 - \sum_{j=1}^{k-1} \beta_j X_{t+j}\right)^2 \tag{10.11}$$

  solution: denote $X = (X_{t+1},\dots,X_{t+k-1})$, $\beta = (\beta_1,\dots,\beta_{k-1})$

$$\begin{aligned}\hat{\beta} =& \Sigma_X^{-1}\Sigma_{X,X_\tau} \\ \hat{\beta}_0 =& \mathbb{E}\left(X_\tau\right) - \mathbb{E}\left(X\right)'\hat{\beta}\end{aligned}$$

  i.e.

$$L(X_\tau|X_{t+1},\dots,X_{t+k-1}) = \mathbb{E}\left(X_\tau\right) + \Sigma_{X_\tau,X}\Sigma_X^{-1}(X - \mathbb{E}\left(X\right)) \tag{10.12}$$

  Simplified case for zero-mean Weakly Stationary $\mathbb{E}(X_t) = \mu$; γ_k, Γ_k

$$L(X_{t+k}|X_{t+1},\dots,X_{t+k-1}) = \mathbb{E}\big(X_{t+k}\big) + \Sigma_{X_{t+k},X}\Sigma_X^{-1}(X - \mathbb{E}\left(X\right)) \tag{10.13}$$

$$= \gamma_{k-1}'\Gamma_{k-1}^{-1}X_{t+k-1:t+1} \tag{10.14}$$

Calculation formula for zero-mean Weakly Stationary:

  - using determinant form

$$\begin{aligned}\phi_{11} =& \rho_1 \\ \phi_{kk} =& \frac{\begin{vmatrix} 1 & \rho_1 & \rho_2 & \cdots & \rho_{k-2} & \color{red}{\rho_1} \\ \rho_1 & 1 & \rho_1 & \cdots & \rho_{k-3} & \color{red}{\rho_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \color{red}{\vdots} \\ \rho_{k-1} & \rho_{k-2} & \rho_{k-3} & \cdots & \rho_1 & \color{red}{\rho_k} \end{vmatrix}_{k\times k}}{\begin{vmatrix} 1 & \rho_1 & \rho_2 & \cdots & \rho_{k-2} & \color{blue}{\rho_{k-1}} \\ \rho_1 & 1 & \rho_1 & \cdots & \rho_{k-3} & \color{blue}{\rho_{k-2}} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \color{blue}{\vdots} \\ \rho_{k-1} & \rho_{k-2} & \rho_{k-3} & \cdots & \rho_1 & \color{blue}{1} \end{vmatrix}_{k\times k}}\end{aligned}$$

– Levinson-Durbin's recursive formula

$$\phi_{11} = \rho_1 \tag{10.15}$$

$$\phi_{k+1,k+1} = \frac{\rho_{k+1} - \sum_{j=1}^{k} \phi_{k,j}\rho_{k+1-j}}{1 - \sum_{j=1}^{k} \phi_{k,j}\rho_j}, \quad k \geq 1 \tag{10.16}$$

$$\phi_{k+1,j} = \phi_{k,j} - \phi_{k+1,k+1}\phi_{k,k+1-j}, \quad j = 1, 2, \ldots, k \tag{10.17}$$

where $\phi_{k+1,j}$ here is a formal notation for recursion. But we will see its meaning in AR(p) model (equation. 10.37)

- Wold Decomposition: zero-mean weakly stationary time series can be decomposed as :

$$X_t = \sum_{j=-\infty}^{\infty} \phi_j \varepsilon_{t-j} + V_t \tag{10.18}$$

where

$$\phi_0 = 1$$
$$\varepsilon_t \sim \mathrm{WN}(0, \sigma^2)$$

- Spectrum of zero-mean weak stationary time series $\{X_t\}$:

$$X_t = \int_\lambda \xi(\lambda) e^{i\lambda t} \,\mathrm{d}\lambda \tag{10.19}$$

We can use this form to construct ACF, ACVF, etc.

– ACVF:

$$\begin{aligned}
\gamma_k =& cov(X_t, X_{t+k}) \\
=& \mathbb{E}\left(X_t^* X_{t+k}\right) \\
=& \int_t \int_{\lambda_1} \int_{\lambda_2} \xi^*(\lambda_1)\xi \,\mathrm{d}\lambda_2 e^{i(\lambda_2-\lambda_1)t + i\lambda_2 k} f(t) \,\mathrm{d}\lambda_1 \,\mathrm{d}t \\
=& \int_{\lambda_1} \int_{\lambda_2} \xi^*(\lambda_1)\xi \,\mathrm{d}\lambda_2 \,\mathrm{d}\lambda_1 \\
=& \int_{\lambda_2} e^{-\lambda_2 k} \int_t \int_{\lambda_1} \xi^*(\lambda_1)\xi \,\mathrm{d}\lambda_2 e^{i(\lambda_2-\lambda_1)t} f(t) \,\mathrm{d}\lambda_1 \,\mathrm{d}t \,\mathrm{d}\lambda_2 \\
\equiv& \int_\lambda e^{-\lambda k} \nu(\lambda) \,\mathrm{d}\lambda
\end{aligned}$$

here function $F(\lambda) = \int \nu(\lambda) \,\mathrm{d}\lambda$ is the **spectrum** of γ_k

For $k = 0, 1, 2, \ldots$:

$$\gamma_k = \int_{-\pi}^{\pi} \nu(\lambda) e^{i\lambda k} \,\mathrm{d}\lambda \tag{10.20}$$

and also use inverse fourier transform: for weak stationary TS $X_t = \sum_{j=-\infty}^{\infty} \phi_j \varepsilon_{t-j}$, $\varepsilon_t \sim \mathrm{WN}(0, \sigma^2)$

$$\nu(\lambda) = \frac{\sigma^2}{2\pi} \left| \sum_{j=-\infty}^{\infty} \phi_j e^{i\lambda j} \right|^2 \tag{10.21}$$

□ **Statistics**

To estimate the above $\mu_t = \mu$, γ_k, ρ_k, ϕ_{kk} given a realization of $\{X_t\}$, say we have $\{x_t\}_{t=1}^n$, we can construct:

- Sample mean μ:

$$\hat{\mu} = \hat{x}_n = \frac{1}{n}\sum_{t=1}^{n} x_t \tag{10.22}$$

  $\hat{\mu}$ is the unbiased, consistent estimator, with

$$\sqrt{n}(\hat{\mu} - \mu) \xrightarrow{\mathscr{L}} N(0, \sigma^2)$$

  an estimator using spectrum:

$$\sqrt{n}(\hat{\mu} - \mu) \xrightarrow{\mathscr{L}} N(0, 2\pi\nu(0)) \tag{10.23}$$

$$2\pi\nu(0) = \gamma_0 + 2\sum_{j=1}^{\infty}\gamma_j = \sum_{j=-\infty}^{\infty}\gamma_j \tag{10.24}$$

- ACVF γ_k:

$$\begin{aligned}\hat{\gamma}_k =& \frac{1}{n}\sum_{t=1}^{n-k}(x_t - \hat{\mu})(x_{t+k} - \hat{\mu}) \\ \hat{\hat{\gamma}}_k =& \frac{1}{n-k}\sum_{t=1}^{n-k}(x_t - \hat{\mu})(x_{t+k} - \hat{\mu})\end{aligned}$$

  Note for actual usage:

  - We usually avoid estimation for $k \to n$ due to large error when $n - k$ is small
  - In most cases we use $\hat{\gamma}_k$ rather than $\hat{\hat{\gamma}}_k$, for two reasons:
    * We often estimate γ_k for small k, which means $\hat{\gamma}_k \approx \hat{\hat{\gamma}}_k$
    * $\hat{\gamma}_k$ could guarantee the semi-positive-definition of $\hat{\Gamma}_k$:

$$\hat{\Gamma}_k = \{\hat{\gamma}_{i-j}\}_{i,j=1}^k$$

  asymptotic distribution: denote i.i.d. standard normal time series $W_t \sim$ i.i.d. $N(0,1)$

$$\sqrt{n}(\hat{\gamma}_0 - \gamma_0, \hat{\gamma}_1 - \gamma_1, \ldots, \hat{\gamma}_h - \gamma_h) \xrightarrow{\mathscr{L}} (\xi_0, \xi_1, \ldots, \xi_h) \tag{10.25}$$

$$\xi_j = (\frac{\sqrt{\mathbb{E}\,(\varepsilon^4) - \sigma^4}}{\sigma^2}\gamma_j)W_0 + \sum_{t=1}^{\infty}(\gamma_{t+j} + \gamma_{t-j})W_t, \quad j \geq 0 \tag{10.26}$$

- ACF ρ_k:

$$\hat{\rho}_k = \frac{\hat{\gamma}_k}{\hat{\gamma}_0} = \frac{\sum_{t=1}^{n-k}(x_t - \hat{\mu})(x_{t+k} - \hat{\mu})}{\sum_{t=1}^{n-k}(x_t - \hat{\mu})^2}$$

  asymptotic distribution: denote i.i.d. standard normal time series $W_t \sim$ i.i.d. $N(0,1)$

$$\sqrt{n}(\hat{\gamma}_0 - \gamma_0, \hat{\gamma}_1 - \gamma_1, \ldots, \hat{\gamma}_h - \gamma_h) \xrightarrow{\mathscr{L}} (R_0, R_1, \ldots, R_h) \tag{10.27}$$

$$R_j = \sum_{t=1}^{\infty}(\phi_{t+j}\rho_{t-j} - 2\rho_t\rho_j)W(t), \quad j \geq 1 \tag{10.28}$$

- PACF ϕ_{kk}: take $\hat{\rho}_k$ in the calculation equation of ϕ_{kk}.

Section 10.3 ARMA Model

Two of the basic modeling methods for time series: Auto-Regression (AR) and Moving-Average (MA)

10.3.1 Backshift Operator and Difference Equation

□ Backshift Operator $\mathscr{B}$

For clearer notation of ARMA and induce the solution, we first introduce backshift operator $\mathscr{B}$ of time series: given time series $\{X_t\}$[75]

$$\mathscr{B}X_t = X_{t-1}, \quad \forall t \tag{10.30}$$

further it can be used as variable of function by Laurant function series expansion:

$$\begin{aligned}\psi(z) &= \sum_{j=-\infty}^{\infty} \psi_j z^j \\ \psi(\mathscr{B}) &= \sum_{j=-\infty}^{\infty} \psi_j \mathscr{B}^j \\ \psi(\mathscr{B})X_t &= \sum_{j=-\infty}^{\infty} \psi_j \mathscr{B}^j X_t = \sum_{j=-\infty}^{\infty} \psi_j X_{t-j}\end{aligned}$$

for time series $\{X_t\}$, $\{Y_t\}$. r.v. U, V, W:

$$\phi(\mathscr{B})(UX_t + VY_t + W) = U\psi(\mathscr{B})X_t + V\psi(\mathscr{B})Y_t + W\psi(1) \tag{10.31}$$

□ Difference Equation

p^{th} order ordinary difference equation:

$$X_t - [a_1X_{t-1} + a_2X_{t-2} + \ldots + a_pX_{t-p}] = 0 \tag{10.32}$$

can be solved using backshift operator: define characteristic equation which would have p roots ζ_j

$$\begin{aligned}A(z) =&1 - \left[a_1 z + a_2 z^2 + \ldots + a_p z^p\right] \\ =&1 - \sum_{j=1}^{p} a_j z^j \\ =&\prod_{j=1}^{p}(1 - \zeta_j z)\end{aligned}$$

[75] Backshift operator could be used to construct difference operator $\Delta = (1 - \mathscr{B})$, e.g.

$$\begin{aligned}\Delta X_t &= (1 - \mathscr{B})X_t = X_t - X_{t-1} \\ \Delta^2 X_t =&(1 - \mathscr{B})^2 X_t = X_t - 2X_{t-1} + X_{t-2} \\ &\ldots\end{aligned}$$

or seasonal difference operator $\Delta_k = (1 - \mathscr{B}^k)$, e.g.

$$\Delta_4 X_t = (1 - \mathscr{B}^4) = X_t - X_{t-4} \tag{10.29}$$

$$
\begin{aligned}
A(\mathscr{B}) =& 1-\sum_{j=1}^{p} a_j \mathscr{B}^j \\
=& \prod_{j=1}^{p}(1-\zeta_j \mathscr{B})
\end{aligned}
$$

similar to ODE, we can construct general solution from ζ_j, and particular solution.[76]

10.3.2 AR Model

Auto-Regression model (of order p) contains (p^{th} order) backshift on X_t:

$$
X_t = \phi_1 X_{t-1} + \phi_2 X_{t-2} + \ldots + \phi_p X_{t-p} + \varepsilon_t, \quad \varepsilon_t \sim \text{WN}(\mu_\varepsilon, \sigma^2) \tag{10.33}
$$

or expressed in backshift operator with $\phi(z) = 1 - \sum_{j=1}^{p} \phi_j z^j$, where the root of $\phi(z) = 0$ denoted α_j

$$
\begin{aligned}
&\phi(\mathscr{B}) X_t = \varepsilon_t, \quad \varepsilon_t \sim \text{WN}(\mu_\varepsilon, \sigma^2) \\
&\phi(z) = 1 - \sum_{j=1}^{p} \phi_j z^j = \prod_{j=1}^{p}(1-\alpha_j z)
\end{aligned}
$$

☐ **Properties and Solution: (here we consider stationary case $\mu_\varepsilon = 0$)**

- (Weak) Stationarity condition:

$$
|\alpha_j| > 1, \, \forall j \tag{10.34}
$$

- Solution of X_t: using the expansion of ϕ^{-1}

$$
\begin{aligned}
\phi(z) =& 1 - \sum_{j=1}^{p} \phi_j z^j \\
\phi^{-1}(z) =& \sum_{j=0}^{\infty} \psi_j z^j, \quad \psi_0 = 1
\end{aligned}
$$

  naturally expressed in the form of Wold Decomposition:

$$
\phi(\mathscr{B}) X_t = \varepsilon_t \Rightarrow X_t = \phi^{-1}(\mathscr{B}) \varepsilon_t = \sum_{j=0}^{\infty} \psi_j \varepsilon_{t-j}, \quad \psi_0 = 1
$$

- ACF and ACVF:

$$
\begin{aligned}
\gamma_k =& \sigma^2 \sum_{j=0}^{\infty} \psi_j \psi_{j+k} \\
\rho_k =& \frac{\sum_{j=0}^{\infty} \psi_j \psi_{j+k}}{\sum_{j=0}^{\infty} \psi_j^2}
\end{aligned}
$$

- Spectrum density $\nu(\lambda)$:

$$
\begin{aligned}
\nu(\lambda) =& \frac{\sigma^2}{2\pi} \left| \sum_{j=0}^{\infty} \psi_j e^{i\lambda j} \right|^2 \\
=& \frac{\sigma^2}{2\pi} \left| \phi^{-1}(e^{i\lambda}) \right|^2
\end{aligned}
$$

[76] Cases for multiple root see https://www.math.pku.edu.cn/teachers/lidf/course/atsa/atsanotes/html/_atsanotes/atsa-lagdiff.html

- Yule-Walker Equation: we have

$$
\begin{aligned}
\mathbb{E}\left(X_t X_{t-k}\right) =& \phi_1 \mathbb{E}\left(X_{t-1} X_{t-k}\right)+\ldots+\phi_p \mathbb{E}\left(X_{t-p} X_{t-k}\right)+\mathbb{E}\left(\varepsilon_t X_{t-k}\right), \quad \forall k=1,2, \ldots, p \\
\Rightarrow \gamma_k =& \phi_1 \gamma_{k-1}+\ldots+\phi_p \gamma_{k-p}, \quad \forall k=1,2, \ldots, p
\end{aligned}
$$

and for $k=0$:

$$
\gamma_0=\phi_1 \gamma_1+\ldots+\phi_p \gamma_p+\sigma^2
$$

write in matrix form to get Yule-Walker Equation:

$$
\begin{aligned}
\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_p \end{bmatrix} &= \begin{bmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{p-1} \\ \gamma_1 & \gamma_0 & \cdots & \gamma_{p-2} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_{p-1} & \gamma_{p-2} & \cdots & \gamma_0 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_p \end{bmatrix} \\
\sigma^2 &= \gamma_0-\phi_1 \gamma_1-\ldots-\phi_p \gamma_p
\end{aligned}
$$

or in dense matrix form (1):

$$
\begin{aligned}
\gamma &= \Gamma \phi \\
\sigma^2 &= \gamma_0-\phi^{\prime} \gamma
\end{aligned}
$$

dense form (2):

$$
\begin{bmatrix} -\sigma^2 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} \gamma_0 & \gamma_1 & \gamma_2 & \cdots & \gamma_p \\ \gamma_1 & \gamma_0 & \gamma_1 & \cdots & \gamma_{p-1} \\ \gamma_2 & \gamma_1 & \gamma_0 & \cdots & \gamma_{p-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_p & \gamma_{p-1} & \gamma_{p-2} & \cdots & \gamma_0 \end{bmatrix} \begin{bmatrix} -1 \\ \phi_1 \\ \phi_2 \\ \vdots \\ \phi_p \end{bmatrix} \tag{10.35}
$$

- PACF: the coefficient of AR(p) has straight relation with $\phi_{k,j}$: for all given $k \geq p$

$$
\left(\phi_1, \ldots, \phi_p, 0, \ldots, 0\right)=\left(\phi_{k, 1}, \ldots, \phi_{k, p}, \phi_{k, p+1}, \ldots, \phi_{k, k}\right)
$$

(Note that $\phi_{p, j}=\phi_{p+1, j}=\phi_{p+2, j}=\ldots$ using Levinson-Durbin' recursion equation. 10.15).

☐ **Estimation: Key focus is the estimation of ϕ_i, $i=1,2, \ldots, p$ and σ^2 (assume a TS of $\mu_{\varepsilon}=0$)**

Y-W Estimation and OLS Estimation are moment methods, asymptotically the same. MLE Estimation is usually more precise, but hard to calculate.

- Yule-Walker Estimation: use $\gamma=\Gamma \phi$. First estimate $\hat{\gamma}$, as well as $\hat{\Gamma}$, and get estimation for ϕ, σ^2

$$
\begin{aligned}
\hat{\phi} &= \hat{\Gamma}^{-1} \hat{\gamma} \\
\hat{\sigma}^2 &= \hat{\gamma}_0-\hat{\gamma}^{\prime} \hat{\Gamma}^{-1} \hat{\gamma}
\end{aligned}
$$

Asymptotic distribution:

$$
\sqrt{n}(\hat{\phi}-\phi) \xrightarrow{\mathscr{L}} N_p\left(0, \sigma^2 \Gamma^{-1}\right) \tag{10.36}
$$

- Levinson-Durbin's recursion for Yule-Walker Estimation: since PACF are the same as coefficients $\phi_{k,j} = \phi_j$, we can use Durbin's recursion to avoid calculation of $\hat{\Gamma}^{-1}$

$$\begin{aligned}
\hat{\phi}_{11} =& \hat{\rho}_1 && (10.37)\\
\hat{\phi}_{k+1,k+1} =& \frac{\hat{\rho}_{k+1} - \sum_{j=1}^{k} \hat{\phi}_{k,j}\hat{\rho}_{k+1-j}}{1 - \sum_{j=1}^{k} \hat{\phi}_{k,j}\hat{\rho}_j}, \quad k \geq 1 && (10.38)\\
\hat{\phi}_{k+1,j} =& \hat{\phi}_{k,j} - \hat{\phi}_{k+1,k+1}\hat{\phi}_{k,k+1-j}, \quad j = 1, 2, \ldots, k && (10.39)\\
\hat{\sigma}_0^2 =& \hat{\gamma}_0 && (10.40)\\
\hat{\sigma}_k^2 =& \hat{\sigma}_{k-1}^2(1 - \hat{\phi}_{k,k}^2) && (10.41)
\end{aligned}$$

estimator:

$$\hat{\phi}_j = \hat{\phi}_{p,j} \tag{10.42}$$

- OLS Estimation: using the linear combination form of AR model:

$$\hat{\phi} = \arg\min_{\phi} \sum_{t=p+1}^{n} \left[x_t - \sum_{j=1}^{p} \phi_j x_{t-j} \right]^2 \tag{10.43}$$

the solution is in the form of OLS estimator $(X'X)^{-1}XY$, with X, Y properly defined

- MLE Estimation: under normal assumption

$$\phi(\mathscr{B})X_t = \varepsilon_t, \quad \varepsilon_t \sim N(0, \sigma^2) \tag{10.44}$$

Likelihood: define $\theta = \{\phi_1, \ldots, \phi_p, \sigma^2\}$

$$\begin{aligned}
L(\theta; x_1, \ldots, x_n) =& f(x_1, \ldots, x_p|\theta) \prod_{t=p+1}^{n} f(x_t|x_{t-1}, \ldots, x_1; \theta)\\
\approx\propto& \prod_{t=p+1}^{n} f(x_t|x_{t-1}, \ldots, x_1; \theta)\\
=& \prod_{t=p+1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{ -\frac{1}{2\sigma^2}(x_t - \sum_{j=1}^{p} \phi_j x_{t-j})^2 \right\}\\
=& (2\pi\sigma^2)^{-(n-p)/2} \exp\left\{ -\frac{1}{2\sigma^2} \sum_{t=p+1}^{n} (x_t - \sum_{j=1}^{p} \phi_j x_{t-j})^2 \right\}
\end{aligned}$$

- Estimation to spectrum density:

$$\hat{\nu}(\lambda) = \frac{\hat{\sigma}^2}{2\pi} \left| 1 - \sum_{j=1}^{\hat{p}} \hat{\phi}_j e^{i\lambda j} \right|^{-2} \tag{10.45}$$

10.3.3 MA Model

Moving-Average model (of order$q$) contains (q^{th} order) backshift on ε_t:

$$X_t = \varepsilon_t + \theta_1\varepsilon_{t-1} + \ldots + \theta_q\varepsilon_{t-q}, \quad \varepsilon_t \sim \mathrm{WN}(\mu_\varepsilon, \sigma^2) \tag{10.46}$$

or expressed in backshift operator with $\theta(z) = 1 + \sum_{j=1}^{q} \theta_j z^j$, where the root of $\theta(z) = 0$ denoted κ_j

$$X_t = \theta(\mathscr{B})\varepsilon_t, \quad \varepsilon_t \sim \text{WN}(\mu_\varepsilon, \sigma^2) \tag{10.47}$$

$$\theta(z) = 1 + \sum_{j=1}^{q} \theta_j z^j = \prod_{j=1}^{q}(1 - \kappa_j z) \tag{10.48}$$

$$= \sum_{j=0}^{q} \theta_j z^j, \quad \theta_j = 1 \tag{10.49}$$

here we could note that AR(p) model has solution in the form of MA(∞):

$$\text{AR}(p) : X_t = \sum_{j=0}^{\infty} \psi_j \varepsilon_{t-j}, \quad \psi_0 = 1 \tag{10.50}$$

☐ **Properties and Solution: (here we consider stationary case $\mu_\varepsilon = 0$)**

- Invertibility: if and only if

$$|\kappa_j| > 1, \forall j \tag{10.51}$$

- ACF and ACVF:

$$\gamma_k = \begin{cases} \sigma^2 \sum_{j=0}^{q-k} \theta_j \theta_{j+k}, & 0 \le k \le q \\ 0, & k > q \end{cases} \tag{10.52}$$

$$\rho_k = \begin{cases} \dfrac{\sum_{j=0}^{q-k} \theta_j \theta_{j+k}}{\sum_{j=0}^{q} \theta_j^2}, & 0 \le k \le q \\ 0, & k > q \end{cases} \tag{10.53}$$

- Solution: $\hat{\theta}_j$ could solved from $\{\gamma_k\}$

10.3.4 ARMA Model

Auto-Regerssion-Moving-Average model ARMA(p, q) in the form of

$$\phi(\mathscr{B})X_t = \theta(\mathscr{B})\varepsilon_t \tag{10.54}$$

$$\phi(z) = 1 - \sum_{j=1}^{p} \phi_j z^j = \prod_{j=1}^{p}(1 - \alpha_j z) \tag{10.55}$$

$$\theta(z) = 1 + \sum_{j=1}^{q} \theta_j z^j = \prod_{j=1}^{q}(1 - \kappa_j z) \tag{10.56}$$

☐ **Properties and Solution: (here we consider stationary case $\mu_\varepsilon = 0$)**

- Solution:

$$X_t = \phi^{-1}(\mathscr{B})\theta(\mathscr{B})\varepsilon_t =\equiv \Psi(\mathscr{B})\varepsilon_t \tag{10.57}$$

- Weak Stationarity: if and only if AR part is WS, i.e.

$$|\alpha_j| > 1, \forall j \tag{10.58}$$

- Invertibility: if and only if MA part is invertible, i.e.

$$|\kappa_j| > 1, \forall j \tag{10.59}$$

10.3.5 ARIMA Model

ARIMA(p, d, q) model adds an difference term $\Delta^d = (1 - \mathscr{B})^d$ in ARMA(p, q):

$$\phi(\mathscr{B})(1 - \mathscr{B})^d X_t = \theta(\mathscr{B}) \tag{10.60}$$

Section 10.4 Seasonal Model for Time Series

This part includes some ideas for modelling seasonal term (usually as well as trend term) in $Y_t = \mathbf{T}_t + \mathbf{S}_t + X_t$.

Usually we describe the trend term as the 'mean' of time series over time, and sensonal term with zero-mean and period $P > 1$.

表 10: Buys-Ballot Table of seasonal period s

	Season (j)					
Period (i)	1	2	$\ldots$	s	$\bar{y}_{i\cdot}$	$\hat{\sigma}^2_{i\cdot}$
1	y_1	y_2	$\ldots$	y_s	$\bar{y}_{1\cdot}$	$\hat{\sigma}_{1\cdot}$
2	y_{s+1}	y_{s+2}	$\ldots$	y_{2s}	$\bar{y}_{2\cdot}$	$\hat{\sigma}_{2\cdot}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$
m	$y_{(m-1)s+1}$	$y_{(m-1)s+2}$	$\ldots$	y_{ms}	$\bar{y}_{m\cdot}$	$\hat{\sigma}^2_{m\cdot}$
$\bar{y}_{\cdot j}$	$\bar{y}_{\cdot 1}$	$\bar{y}_{\cdot 2}$	$\ldots$	$\bar{y}_{\cdot s}$	$\bar{y}_{\cdot\cdot}$	-
$\hat{\sigma}^2_{\cdot i}$	$\hat{\sigma}^2_{\cdot 1}$	$\hat{\sigma}^2_{\cdot 2}$	$\ldots$	$\hat{\sigma}^2_{\cdot s}$	-	$\hat{\sigma}^2_{\cdot\cdot}$

10.4.1 Regression Model

A common functional description is polynomial trend + Fourier expansion senson, i.e.

$$\begin{aligned} Y_t =& T_t + S_t + X_t & (10.61) \\ =& \alpha_0 + \sum_{j=1}^{m} \alpha_j t^j + \sum_{j=1}^{[s/2]} \left[\beta_j \sin(\frac{2\pi}{s} jt) + \gamma_j \cos(\frac{2\pi}{s} jt) \right] & (10.62) \end{aligned}$$

Note: for regression model, T_t and S_t are treated as invariant term.

Estimation of paramters $\{\alpha_0, \alpha_j, \beta_j, \gamma_j\}$ use e.g. MSE estimator:

$$\{\hat{\alpha}_0, \hat{\alpha}_j, \hat{\beta}_j, \hat{\gamma}_j\} = \underset{\{\alpha_0, \alpha_j, \beta_j, \gamma_j\}}{\arg\min} \sum_{t \in T} [y_t - (T_t + S_t)]^2 \tag{10.63}$$

10.4.2 Moving Average Model

First estimate Trend term, then Seasonal term

Trend term is estimated by a symmetric moving average window $\{\omega_j\}_{j=-w}^{w}$ with band width w

$$\hat{T}_t = \sum_{j=-w}^{w} \omega_j y_{t-j} \tag{10.64}$$

$$\omega_j = \omega_{-j}, \quad j = -w, -w+1, \dots, w-1, w \tag{10.65}$$

$$\sum_{j=-w}^{w} \omega_j = 1 \tag{10.66}$$

then seasonal term is naturally estimated by

$$\hat{S}_t = y_t - \hat{T}_t$$

10.4.3 Seasonal ARIMA Model

Multiplicative seasonal ARIMA model with period s of Y_t: ARIMA$(p,d,q) \times (P,D,Q)_s$

$$\Phi_P(\mathscr{B}^s)\phi_p(\mathscr{B})(1-\mathscr{B})^d(1-\mathscr{B}^s)^D Y_t = \Theta_Q(\mathscr{B}^s)\theta_q(\mathscr{B}^s)\varepsilon_t, \quad \varepsilon_t \sim \mathrm{WN}(0,\sigma^2) \tag{10.67}$$

On the ACF plot of SARIMA, you should see peak at $t_{\text{lag}} \propto s$

Section 10.5 Model Selection and Diagnostics

10.5.1 Model Building of ARIMA

☐ **Box-Jenkins Approach for ARIMA Model:**

1. Data Transformation: Note that in the general model $Y_t = T_t + S_t + X_t$ we would expect a ‘stationary’ random term, thus a transform for stable variance is needed, see section. 3.5.1 for detailed methods. Then we could preliminarily detect the Stationarity of sequence, e.g. by plotting.
2. Seaonal Term Detection: usually by plotting ACF plot & ACVF plot, further we could also use spectrum plot, seasonal subseries plot.
3. Stationarity Detection: Detect stationarity e.g. by unit-root test.
4.

10.5.2 Order Determination of ARIMA Model

☐ **Order Determination of AR**(p)

- PACF test: use the proper of $\phi_{k,k}$ for $k \geq p$ where

$$\phi_{kk} = \begin{cases} \phi_p, & k \leq p \\ 0, & k > p \end{cases} \tag{10.68}$$

for all given $k > p$: Asymptotic distribution:

$$\sqrt{n}(\hat{\phi}_{k,1} - \phi_{k,1}, \dots, \hat{\phi}_{k,k} - \phi_{k,k}) \xrightarrow{\mathscr{L}} N(0, \sigma^2\Gamma_k^{-1}) \tag{10.69}$$

specially it could be proved that $\left(\sigma^2\Gamma_k^{-1}\right)_{k,k} = \left(\sigma^2\Gamma_k^{-1}\right)_{1,1} = 1, \quad k > p$.

i.e. test statistics for AR(p):

$$\hat{\phi}_{k,k} \xrightarrow{\mathscr{L}} N(0,1), \quad w.r.t.\ H_0 : \phi_{k,k} = 0, \quad k > p \tag{10.70}$$

Plot $\hat{\phi}_{k,k}$-k to determine the proper k as $\hat{p}$.

- AIC/BIC method: use $\hat{p} = \arg\min \mathrm{AIC}(k)$ or $\arg\min \mathrm{BIC}(k)$:

$$\mathrm{AIC}(k) = \ln \hat{\sigma}_k^2 + \frac{2k}{n}$$
$$\mathrm{BIC}(k) = \ln \hat{\sigma}_k^2 + \frac{k\ln n}{n}$$

☐ **Order Determination of MA**(q)

- ACF test: use the cut off property of ρ_k of MA(q):

$$\rho_k = \begin{cases} \dfrac{\sum_{j=0}^{q-k}\theta_j\theta_{j+k}}{\sum_{j=0}^{q}\theta_j^2}, & 0 \le k \le q \\ 0, & k > q \end{cases} \tag{10.71}$$

use the asymptotic distribution of $\hat{\rho}_m$ in equation. 10.27, for $m > q$:

$$\sqrt{n}\hat{\rho}_m \xrightarrow{\mathscr{L}} R_m \tag{10.72}$$
$$= \sum_{t=1}^{\infty}(\rho_{t+m} + \rho_{t-m} - \rho_t\rho_m)W_t \tag{10.73}$$
$$= \sum_{l=-q}^{q}\rho_l W_{l+m}, \quad m > q \tag{10.74}$$
$$\sim N(0, 1 + 2\sum_{j=1}^{q}\rho_j^2) \tag{10.75}$$

i.e. test statistics for MA(q):

$$T_q(m) = \frac{\sqrt{n}\hat{\rho}_m}{\sqrt{1 + 2\sum_{j=1}^{q}\hat{\rho}_j^2}} \xrightarrow{\mathscr{L}} N(0,1), \quad H_0 : \rho_m = 0, \quad m > q$$

- AIC/BIC method: use $\hat{q} = \arg\min \mathrm{AIC}(m)$ or $\arg\min \mathrm{BIC}(m)$:

$$\mathrm{AIC}(m) = \ln \hat{\sigma}_m^2 + \frac{2m}{n}$$
$$\mathrm{BIC}(m) = \ln \hat{\sigma}_m^2 + \frac{m\ln n}{n}$$

☐ **Order Determination of ARMA**(p, q)

- AIC/BIC method:

$$\hat{p}, \hat{q} = \arg\min_{k,m} \mathrm{AIC}(k, m) = \arg\min_{k,m} \ln \hat{\sigma}_{k,m}^2 + \frac{2(k+m)}{n}$$
$$\hat{p}, \hat{q} = \arg\min_{k,m} \mathrm{BIC}(k, m) = \arg\min_{k,m} \ln \hat{\sigma}_{k,m}^2 + \frac{(k+m)\ln n}{n}$$

- EACF for ARIMA(p, d, q): Extended ACF forms a matrix for determining (p, d, q) using extended Yule-Walker Equation

10.5.3 Outlier Detection

Here we introduce two kinds of outlier in time series: Additive Outlier (AO) and Innovative Outlier (IO).

☐ **Notation for Outlier**

- Step function in time series: a rise of value 1 at time τ:

$$S_t^{(\tau)} = \begin{cases} 0, & t < \tau \\ 1, & t \geq \tau \end{cases}$$

- Pulse function in time series: a pulse of value 1 at time τ:

$$P_t^{(\tau)} = (1-\mathscr{B})S_t^{(\tau)} = \begin{cases} 0, & t \neq \tau \\ 1, & t = \tau \end{cases}$$

☐ **Additive Outlier**

A pulse outlier of y at τ:

$$\tilde{y}_t = y_t + \omega_A P_t^{(\tau)}$$

the outlier would not influence $t \neq \tau$, thus is additive.

☐ **Innovative Outlier**

A pulse outlier of ε at τ:

$$\varepsilon_\tau = \varepsilon_t + \omega_I$$

$t \neq \tau$ would also be influenced by this outlier.

Section 10.6 Forecast of Time Series

10.6.1 MSE Forecast Criterion

The criterion for forecasting is to minimizing some loss function, usually taken as MSE loss:

$$\hat{X}_{\tau|t} = \operatorname*{arg\,min}_{X_\tau} \mathbb{E}[\left(X_\tau - X_{\tau|t}\right)^2] = \mathbb{E}\left(X_{\tau|t}\right) \tag{10.76}$$

our mission is to construct a function $g(\cdot)$ so that $\hat{X}_{\tau|t} = g(\mathscr{F}_t)$ can act as the estimator. $\mathscr{F}_t = \{X_t, X_{t-1}, X_{t-2}, \ldots\}$ denotes the history until t.

10.6.2 Best Linear Estimator

A simple and straightforward method is a linear combination form of $\mathscr{F}_t$:

$$\hat{X}_{\tau|t} = \sum_{j=0}^{\infty} \beta_j X_{t-j} \tag{10.77}$$

$$\beta_j = \operatorname*{arg\,min}_{\{\beta_j\}} \mathbb{E}\left[\left(X_\tau - \sum_{j=0}^{\infty} \beta_j X_{t-j}\right)^2\right] \tag{10.78}$$

i.e.

$$\hat{X}_{\tau|t} = L(X_\tau|\mathscr{F}_t) \tag{10.79}$$

Solution was given in equation. 10.13:

$$\beta = \Sigma^{-1}_{X_{\mathscr{F}_t}} \Sigma_{\mathscr{F}_t, X_\tau} \tag{10.80}$$

- e.g. ont-step forecast for zero-mean weakly stationary sequence:

$$\hat{X}_{t+1|t} = \sum_{j=0}^{\infty} \beta_j X_{t-j} \tag{10.81}$$

$$\vec{\beta} = \Gamma^{-1}\gamma \tag{10.82}$$

(For actual case, calculate for a proper truncation p for $\hat{X}_{t+1|t} = \sum_{j=0}^{p} \beta_j X_{t-j}$ would be fine)

Best linear estimator is the best estimator for ARMA(p, q) with WN noise.

10.6.3 Forecast of AR(p)

AR(p):

$$X_{t+1} = \sum_{j=1}^{p} \phi_j X_{t+1-j} + \varepsilon_{t+1} \tag{10.83}$$

1. First estimate coefficients, e.g. using Yule-Walker estimator $\hat{\phi}_j$, $j = 1, 2, \ldots, p$
2. Esitmate of $X_{t+1|t}$

$$\hat{X}_{t+1|t} = \sum_{j=1}^{p} \hat{\phi}_1 X_{t+1-j} \tag{10.84}$$

$$\hat{\sigma}^2_{t+1|t} = \hat{\sigma}^2 = \hat{\gamma}_0 \tag{10.85}$$

3. Estimate of $X_{t+h|t}$: estimation conduct sequentially for $h = 1, 2, \ldots$:

$$\hat{X}_{t+1|t} = \hat{\phi}_1 X_t + \hat{\phi}_2 X_{t-1} + \ldots + \hat{\phi}_p X_{t+1-p} \tag{10.86}$$

$$\hat{X}_{t+2|t} = \hat{\phi}_1 \hat{X}_{t+1|t} + \hat{\phi}_2 X_t + \hat{\phi}_3 X_{t-1} + \ldots + \hat{\phi}_p X_{t+2-p} \tag{10.87}$$

$$\hat{X}_{t+3|t} = \hat{\phi}_1 \hat{X}_{t+2|t} + \hat{\phi}_2 \hat{X}_{t+1|t} + \hat{\phi}_3 X_t + \hat{\phi}_4 X_{t-1} + \ldots + \hat{\phi}_p X_{t+3-p} \tag{10.88}$$

$$\ldots \tag{10.89}$$

10.6.4 Forecast of MA(q)

MA(q):

$$X_{t+1} = \varepsilon_{t+1} + \sum_{j=1}^{q} \theta_j \varepsilon_{t+1-j} \tag{10.90}$$

1. First estimate coefficients $\hat{\theta}_j$, $j = 1, 2, \ldots, q$
2. Estimate of $X_{t+h|t}$: first for each $k = 1, 2, \ldots, t$, calculate residual estimator:

$$\hat{\varepsilon}_k = X_k - L(X_k|\mathscr{F}_{k-1}) = X_k - L(X_k|X_{k-1}, \ldots, X_1) \tag{10.91}$$

then calculate forecast:

$$\hat{X}_{t+h|t} = \begin{cases} \sum_{j=h}^{q} \hat{\theta}_j \hat{\varepsilon}_{t+1-j}, & h = 1, 2, \dots, q \\ 0, & h > q \end{cases} \tag{10.92}$$

10.6.5 Forecast of ARMA(p, q)

ARMA(p, q):

$$\phi(\mathscr{B}) X_t = \theta(\mathscr{B}) \varepsilon_t \Rightarrow X_t = \phi^{-1}(\mathscr{B}) \theta(\mathscr{B}) \varepsilon_t \equiv \psi(\mathscr{B}) \varepsilon_t \tag{10.93}$$

similarly estimate ψ_j and ε_j and forecast as MA(∞)

10.6.6 Forecast of ARIMA(p, d, q)

Chapter. XI 因果推断导论部分

Instructor: Wanlu Deng

Section 11.1 Neyman-Rubin Framework

Neyman-Rubin Framework (Donald B.Rubin, 1978), also called Potential Outcome Framework is based on **counterfactual outcome** inference to judge causal effect. Main problem is to deal with **Confounder**.

☐ **Motivation of N-R Model: Difference Between 'Correlation' and 'Causality'**

Assume we now has a set of $\{(W_i, Y_i)\}$ where W_i happens before Y_i and i for i^{th} object.

- **Correlation** describes the relation between W_i and Y_i;
- while **Causality** describes the relation between Y_i and some **unseen** $\tilde{Y}_i$ corresponding to **What If** W_i takes another value.

Their difference is significant, correlation is mostly based on objective data, while causality contains a lot about how we **'imagine'** what did not happen, and compare to reality. The $Y_i - \tilde{Y}_i$ is causal effect (Note that they both has $_i$, acting on the same object, the different causal effect on different unit also make it not so useful to increase sample size).

11.1.1 Key Elements and Notations

In this part we first introduce a simple model: Two choice for causes and two (potential) outcomes.

e.g. Take medicine or not $\longrightarrow$ Headache level.

- **Unit**: The atomic object in causal inference, e.g. one headache person at certain time. We infer 'what would happen to unit i if . . .'.[77]
- **Treatment** W_i: (when 'cause' event had not happen), what we could had done, expressed as W_i, $W_i \in \{0, 1, \dots, N_{\text{NUMBER\_OF\_TREATMENT}}\}$, in simple model $W_i \in \{0, 1\}$, 1 for treated and 0 for controlled.
  - Treatment Group: Set of $\{\text{Unit}_i | W_i = 1\}$;
  - Controlled Group: Set of $\{\text{Unit}_i | W_i = 0\}$.
- **Potential Outcome** Y_i(PO): For each unit operating each treatment(or control), the potential outcome $Y(W = w)$.[78] In simple model, use $Y_i(1)$ for treatment and $Y_i(0)$ for control.
- **Observed Outcome** Y_i^F: The actually happened outcome, $Y_i^F = Y_i(W = w_{\text{REAL\_CASE}}) := Y_i(W = w_i^F)$
- **CounterFactual Outcome** Y_i^{CF}: The potential outcome when the $!w_i^F$ would have been operated (does exist but we did not observed the 'world line' where w_i^{CF} was operated, thus unknown to us), $Y_i^{CF} = Y_i(W = 1 -$

[77] Same object at different time should be considered as different unit. We may join some **hypothesis** that time doesnot matter, but not for the **definition** of unit.

[78] The 'EigenOutcome' of the model, despite of what really happens.

Maybe can be seen as what would happen when the operation had not been done.

$w_{\text{REAL\_CASE}}) := Y_i(W = w_i^{CF})$

$$Y_i^F = Y_i(W_i^F) = \begin{cases} Y_i(1) & W_i = 1 \\ Y_i(0) & W_i = 0 \end{cases}$$

$$Y_i^{CF} = Y_i(1 - W_i^F) = \begin{cases} Y_i(0) & W_i = 1 \\ Y_i(1) & W_i = 0 \end{cases}$$

- **Causal Effect** τ_i: Difference between potential outcome, $\tau = Y_i(W=1) - Y_i(W=0) = Y_i(1) - Y_i(0)$
- **Pre-Treatment Variables/Covariates** X_i: Some background elements that might attribute to treatment selection/potential outcome. Anyway may cause confusion to causal inference.
- **Subgroup**:

☐ **Treatment Effect**

- **ATE**: Average Treatment Effect (ATE) of the whole population:

$$\text{ATE} = E(Y(1) - Y(0))$$

Estimand:

$$\hat{\text{ATE}} = \frac{1}{N}\sum_{i=1}^{N}(Y_i(1) - Y_i(0))$$

- **ATT/ATC**: Average Treatment Effect of Treated/Controlled Group (ATT/ATC):

$$\text{ATT} = E(Y(1)|w=1) - E(Y(0)|w=1) \qquad \text{ATC} = E(Y(1)|w=0) - E(Y(0)|w=0)$$

Estimand:

$$\hat{\text{ATT}} = \frac{1}{N_t}\sum_{i:w_i=1}(Y_i(1) - Y_i(0)) \qquad \hat{\text{ATC}} = \frac{1}{N_c}\sum_{i:w_i=0}(Y_i(1) - Y_i(0))$$

- **CATE**: Conditional Average Treatment Effect (CATE): 'Conditional' for 'given covariant X'

$$\text{CATE}_x = E(Y(1)|X=x) - E(Y(0)|X=x)$$

Estimand: (Denote # $X_i = x$ as $N(x)$)

$$\hat{\text{CATE}} = \frac{1}{N(x)}\sum_{i:X_i=x}(Y_i(1) - Y_i(0))$$

- **ITE**: Individual Treatment Effect:

$$\text{ITE}_i = Y_i(W=1) - Y_i(W=0)$$

Where in Estimands, we only know one of $Y_i(1)/Y_i(0)$ as Y^F, the Y^{CF} needs to be **predicted**.

11.1.2 Assignment Mechanism

- **Assignment Mechanism**: is a function $\{X_i, Y_i(0), Y_i(1)\} \to P(W_i)$: The probability that how a unit would have been given treatment/control.

$$\sum_{\vec{W}\in\{0,1\}^N} P(\vec{W}|X, Y(1), Y(0)) = 1$$

- **Finite Population Propensity Score**: The average unit assignment probability for all unit with $X_i = x$:

$$e(x) = \frac{1}{N(x)} \sum_{i:X_i=x} P(W_i = 1|X, Y(1), Y(0))$$

For $N(x) = 0$, define $e(x) = 0$

11.1.3 Difficulty and Goal of Causal Inference

☐ **Difficulty:**

- **Inadequate Observation Points**: The **Causal Effect** we want to study is ATE $= E(Y(1)-Y(0))$. Note that each unit has **two** potential outcomes $Y(1)$ and $Y(0)$ for treated/controlled respectively. However we can only observed one of them $Y^C = Y(W = w_{\text{REAL\_CASE}})$, i.e. at least **half of potential outcomes are unobserved**, we need to 'predict' the missing point using covariants.
- **Biased Assignment Mechanism**: Covariants may cause biased treatment/control assignment, from which we can never estimate an unbiased causal effect.

☐ **Goal:**

The goal of causal inference is to estimate the treatment effects with $\{X, W, Y^F\}$ given.

11.1.4 Assumptions

- **SUTVA** (Stable Unit Treatment Value Assumption): A usually reasonable assumption to simplify causal model:
  - No interference between units;
  - No hidden variations of treatment.
- **Individualistic Assignment**: Assignment probability of each unit does **not** depends on the covariants and PO of other units:

$$P_i(W = w|X, Y(1), Y(0)) = P_i(W|X_i, Y_i(1), Y_i(0))^w (1 - P_i(W|X_i, Y_i(1), Y_i(0)))^{1-w}, \ \forall i = 1, 2, \ldots, N$$

For simplification, denote

$$P_i(W = 1|X, Y(1), Y(0)) = q(X, Y(1), Y(0))$$

Under individualistic assignment assumption, propensity score is simplified:

$$e(x) = \frac{1}{N(x)} \sum_{i:X_i=x} P(W = 1|X, Y(1), Y(0)) = \frac{1}{N(x)} \sum_{i:X_i=x} P(W = 1|X_i, Y_i(1), Y_i(0))$$

- **Probabilistic Assignment**: Probility for both $W_i = 1$ and $W_i = 0$ are non-zero (to ensure a reasonable causal model)

$$0 < P(W|X, Y(1)Y(0)) < 1, \forall X, Y(1), Y(0)$$

- **Unconfounded Assignment**: Assignment mechanism is independent of PO

$$P(W|X, Y(1), Y(0)) = P(W|X)$$

□ **With above assumption, assignment mechanism and propemnsity score can be simplified:**

$$\text{Assignment Mechanism:} P(\vec{W}|X, Y(1), Y(0)) = \frac{1}{Z}\prod_{i=1}^{N} q(X_i)_i^W (1 - q(X_i))^{1-W_i}$$

Section 11.2 Pearl Framework

(Judea Pearl, 1995)

Chapter. XII 应用随机过程部分

Instructor: Pengkun Yang

参考文献

[1] 清华大学统计学研究中心辅修课程课件与讲义. W. Deng, J. Wang, Z. Zhou, D. Li, T. Wang, S. Yu.

[2] Springer Series in Statistics (SSS). https://www.springer.com/series/692

[3] RStudio Cheatsheets https://www.rstudio.com/resources/cheatsheets

[4] 概率导论 (第二版・修订版). Dimitri P. Bertsekas, John N. Tsitsiklis. 人民邮电出版社.

[5] 北京大学《概率统计 A》课程讲义. 李东风. https://www.math.pku.edu.cn/teachers/lidf/course/probstathsy/probstathsy.pdf

[6] 数理统计（第二版）. 韦来生. 科学出版社.

[7] Statistical Inference(2nd Edition). George Casella, Roger L. Berger. Duxbury Press.

[8] Applied Linear Statistical Models(5th Edition). Michael H. Kutner, Christopher J. Nachtsheim, John Neter, William Li. McGraw-Hill Compaines, Inc.

[9] 线性模型引论. 王松桂 et. al. 科学出版社.

[10] Linear Models with R(2nd Edition). Julian J. Faraway. CRC Press.

[11] Generalized Linear Model Lecture Note. Germán Rodríguez. https://data.princeton.edu/wws509/notes

[12] 实用多元统计分析（第六版）. Richard A. Johnson, Dean W. Wichern. 清华大学出版社.

[13] R In Action: Data Analysis and Graphics with R(2nd Edition). Robert I. Kabacoff. Manning Publications Co.

[14] R Programming For Data Science. Roger D. Peng. Lean Publishing.

[15] Numerical Linear Algebra. I Lloyd N. Trefethen, David Bau Ill. Society for Industrial and Applied Mathematics

[16] Numerical Optimization(2nd Edition). J. Nocedal, Stephen J. Wright. Springer Science+Business Media, LLC.

[17] 北京大学《统计计算》课程讲义. 李东风. https://www.math.pku.edu.cn/teachers/lidf/docs/statcomp/html/_statcompbook/statcomp2ndv.pdf

[18] 生存分析与可靠性. 陈家鼎. 北京大学出版社.

[19] 机器学习. 周志华. 清华大学出版社.

[20] 机器学习公式详解. 谢文睿, 秦州. 人民邮电出版社.

[21] 神经网络与深度学习. 邱锡鹏. https://nndl.github.io/

[22] Time Series Analysis With Applications in R(2nd Edition). Jonathan D. Cryer, Kung-Sik Chan. Springer Science+Business Media, LLC.

[23] 北京大学《应用时间序列分析》课程讲义. 李东风. https://www.math.pku.edu.cn/teachers/lidf/course/atsa/atsanotes/html/_atsanotes/atsanotes.pdf

[24] Forecasting: Principles and Practice (2nd Edition). Hyndman, R.J., Athanasopoulos, G. https://otexts.com/fppcn

[25] Causal Inference for Statistics, Social, and Biomedical Sciences: An Introduction. Guido W. Imbens & Donald B. Rubin. Cambridge University Press.

[26] Causal Inference in Statistics - A Primer. Judea Pearl. Wiley.

索引