

多元线性回归分析

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I. 多元线性回归模型

设变量 Y 与 X_1, X_2, \dots, X_p 之间有线性关系

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \varepsilon$$

其中 ε 均值为0, 方差为 σ^2 , $\beta_0, \beta_1, \beta_2, \dots, \beta_p$ 和 σ^2 是未知参数。

当 $p \geq 2$, 称以上公式为**多元线性回归模型**。

- n 次独立观测值记为 $(x_{i1}, x_{i2}, \dots, x_{ip}; y_i)$, $i = 1, 2, \dots, n$.

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} + \varepsilon_i$$

■ 矩阵形式

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \text{均值为0,等方差,不相关(协方差矩阵为}\sigma^2 \mathbf{I}_n)$$

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \cdots & & & & \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \cdots \\ \beta_p \end{bmatrix} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \cdots \\ \varepsilon_n \end{bmatrix}$$

误差的平方和
$$\begin{aligned} Q(\boldsymbol{\beta}) &= \sum_{i=1}^n \varepsilon_i^2 = \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{Y}^T \mathbf{Y} - \mathbf{Y}^T \mathbf{X}\boldsymbol{\beta} - \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{Y} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta} \end{aligned}$$

■ 矩阵的求导公式

列向量 $\alpha_{n \times 1}$, $x_{n \times 1}$ 和矩阵 $A_{n \times n}$, 标量对向量的求导:

$$\frac{\partial \alpha^T x}{\partial x} = \alpha, \quad \frac{\partial x^T \alpha}{\partial x} = \alpha, \quad \frac{\partial x^T A x}{\partial x} = (A^T + A)x.$$

2. 最小二乘估计

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

如果 $(\mathbf{X}^T \mathbf{X})_{(p+1) \times (p+1)}$ 是列满秩的, 那么

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{Y})$$

▪ 估计量的性质

$$E(\hat{\beta}) = ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) E(\mathbf{Y}) = ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) (\mathbf{X}\beta) = \beta$$

$$\text{Cov}(\hat{\beta}) = ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) \text{Cov}(\mathbf{Y}) ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T)^T$$

$$= ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) (\sigma^2 \mathbf{I}_n) ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T)^T$$

$$= \sigma^2 ((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) (\mathbf{X}^T (\mathbf{X}^T \mathbf{X})^{-1})$$

$$= \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}$$

■ 经验回归方程 $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_p X_p$

■ 回代分析 $\hat{Y} = X\hat{\beta} = X(X^T X)^{-1}(X^T Y) = HY.$

- H 是对称幂等矩阵, $H^T = X^{TT}(X^T X)^{-1T} X^T = H.$

$$H^2 = (X(X^T X)^{-1} X^T) (X(X^T X)^{-1} X^T) = (X(X^T X)^{-1} X^T) = H.$$

- $(I_n - H)$ 也是对称幂等矩阵

$$(I_n - H)^T = I_n^T - H^T = I_n - H.$$

$$(I_n - H)^2 = I_n - I_n H - H I_n + H^2 = I_n - H.$$

$$(I_n - H)X = I_n X - (X(X^T X)^{-1} X^T) X = X - X = 0.$$

3. 残差向量

$$\begin{aligned}\hat{\boldsymbol{\varepsilon}} &= \mathbf{Y} - \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}} = (\mathbf{I}_n - \mathbf{H})\mathbf{Y} \\ &= (\mathbf{I}_n - \mathbf{H})(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}) = (\mathbf{I}_n - \mathbf{H})\mathbf{X}\boldsymbol{\beta} + (\mathbf{I}_n - \mathbf{H})\boldsymbol{\varepsilon} \\ &= (\mathbf{I}_n - \mathbf{H})\boldsymbol{\varepsilon}.\end{aligned}$$

- 残差向量的性质 $E(\hat{\boldsymbol{\varepsilon}}) = (\mathbf{I}_n - \mathbf{H})E(\boldsymbol{\varepsilon}) = \mathbf{0}$.

$$\begin{aligned}\text{Cov}(\hat{\boldsymbol{\varepsilon}}) &= E(\hat{\boldsymbol{\varepsilon}}\hat{\boldsymbol{\varepsilon}}^T) = E((\mathbf{I}_n - \mathbf{H})\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T(\mathbf{I}_n - \mathbf{H})^T) \\ &= (\mathbf{I}_n - \mathbf{H})E(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T)(\mathbf{I}_n - \mathbf{H})^T \\ &= (\mathbf{I}_n - \mathbf{H})(\sigma^2\mathbf{I}_n)(\mathbf{I}_n - \mathbf{H}) \\ &= \sigma^2(\mathbf{I}_n - \mathbf{H})^2 = \sigma^2(\mathbf{I}_n - \mathbf{H}).\end{aligned}$$

■ 矩阵的迹的性质

-对于标量 b ,和方阵 $A_{n \times n}$ 及其特征值 $\lambda_1, \dots, \lambda_n$,

$$\text{迹} \quad \text{tr}(A) = \sum_{i=1}^n a_{ii} = \sum_{i=1}^n \lambda_i$$

$$\text{tr}(A) = \text{tr}(A^T), \quad \text{tr}(b) = b.$$

-对于矩阵 $B_{n \times m}$ 和 $C_{m \times n}$,

$$\text{tr}(BC) = \text{tr}(CB).$$

$$\text{tr}(ABC) = \text{tr}(CAB) = \text{tr}(BCA).$$

-对于标量 w_1, w_2 和 n 阶方阵 A_1, A_2 ,

$$\text{tr}(w_1 A_1 + w_2 A_2) = w_1 \text{tr}(A_1) + w_2 \text{tr}(A_2).$$

-对于列满秩矩阵 $B_{m \times q}$, $(B^T B)$ 是可逆的, 且

$$\text{tr}((B^T B)^{-1}(B^T B)) = q = \text{tr}(B(B^T B)^{-1}B^T).$$

-对于行满秩矩阵 $C_{k \times n}$, (CC^T) 是可逆的, 且

$$\text{tr}((CC^T)^{-1}(CC^T)) = k = \text{tr}(C^T(CC^T)^{-1}C).$$

■ 残差平方和(SSE)

$$Q(\hat{\beta}) = \sum_{i=1}^n \hat{\varepsilon}_i^2 = \hat{\varepsilon}^T \hat{\varepsilon} = (Y - X\hat{\beta})^T (Y - X\hat{\beta})$$

$$\begin{aligned} &= ((I_n - H)\varepsilon)^T ((I_n - H)\varepsilon) = \varepsilon^T (I_n - H)\varepsilon \\ &= tr(\varepsilon^T (I_n - H)\varepsilon) = tr((I_n - H)\varepsilon\varepsilon^T) \end{aligned}$$

$$E(Q(\hat{\beta})) = tr((I_n - H)E(\varepsilon\varepsilon^T)) = tr((I_n - H)Cov(\varepsilon))$$

$$= tr((I_n - H)\sigma^2 I_n) = \sigma^2 tr(I_n - H)$$

$$= \sigma^2 (tr(I_n) - tr(X(X^T X)^{-1} X^T))$$

$$= \sigma^2 (n - tr(X^T X(X^T X)^{-1})) = \sigma^2 (n - (p + 1))$$

- 误差项的方差估计

$$\hat{\sigma}^2 = \frac{SSE}{n - (p + 1)} = \frac{\hat{\boldsymbol{\varepsilon}}^T \hat{\boldsymbol{\varepsilon}}}{n - (p + 1)} = \frac{\mathbf{Y}^T (\mathbf{I}_n - \mathbf{H}) \mathbf{Y}}{n - (p + 1)}.$$

- 估计量的性质

$$E(\hat{\boldsymbol{\beta}}) = \boldsymbol{\beta}, \quad E(\hat{\boldsymbol{\varepsilon}}) = \mathbf{0}, \quad E(\hat{\sigma}^2) = \sigma^2, \quad \text{无偏估计}$$

$$Cov(\hat{\boldsymbol{\beta}}) = E((\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T) = \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}$$

$$Cov(\hat{\boldsymbol{\varepsilon}}) = E(\hat{\boldsymbol{\varepsilon}} \hat{\boldsymbol{\varepsilon}}^T) = \sigma^2 (\mathbf{I}_n - \mathbf{H}).$$

4. 多元正态线性回归模型

$$Y = X\beta + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I_n)$$

■ 估计量的性质

$$\hat{\beta} = (X^T X)^{-1} (X^T Y) \sim N(\beta, \sigma^2 (X^T X)^{-1});$$

$$\hat{\varepsilon} = (I_n - H)Y \sim N(0, \sigma^2 (I_n - H))$$

$$\frac{SSE}{\sigma^2} = (n - p - 1) \frac{\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-p-1}^2;$$

$\hat{\beta}$ 和 $\hat{\sigma}^2$ 相互独立;

5. 单个回归系数的显著性检验 (t检验)

$$H_0 : \beta_j = 0 \quad \text{vs.} \quad H_1 : \beta_j \neq 0.$$

- 检验统计量 $T = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{C_{jj}}} \stackrel{H_0 \text{真}}{\sim} t(n-p-1),$

$$\text{其中 } \hat{\sigma} = \sqrt{\frac{SSE}{n-p-1}}, \quad C = (\mathbf{X}^T \mathbf{X})^{-1}.$$

- 拒绝域 $|T| > t_{\alpha/2}(n-p-1)$

6. 回归方程的显著性检验 (F检验)

$H_0 : \beta_0 = \beta_1 = \dots = \beta_p = 0$ vs. $H_1 : \text{至少有一个系数不为0.}$

- 检验统计量 $F = \frac{SSR/p}{SSE/(n-p-1)} \stackrel{H_0 \text{真}}{\sim} F(p, n-p-1)$
- 拒绝域 $F > F_\alpha(p, (n-p-1))$
- 方差分析表 $SST = SSR + SSE$

$SST = \sum (y_i - \bar{y})^2$, 反映了数据 y_i 's 波动性的大小;

$SSR = \sum (\hat{y}_i - \bar{y})^2$, 反映了由于 X_1, \dots, X_p 的变化引起的数据 y_i 's 的波动;

$SSE = \sum (y_i - \hat{y}_i)^2$, 反映了除去 X_i 's 的影响外, 其他因素引起的 y_i 's 的波动

7. 拟合程度 (R^2)

- 决定系数 $R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$
- 修正的决定系数 $R^{2*} = \frac{SSR/p}{SST/(n-1)}$

8. 预测及统计推断

- 点估计, 新的观测值 $\mathbf{x} = (1, x_1, x_2, \dots, x_p)$,

$$\hat{y} = \mathbf{x}\hat{\boldsymbol{\beta}} \sim N(\mathbf{x}\boldsymbol{\beta}, \mathbf{x}\text{Cov}(\hat{\boldsymbol{\beta}})\mathbf{x}^T) = N(\mathbf{x}\boldsymbol{\beta}, \sigma^2 \mathbf{x}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}^T).$$

- 区间估计, $\hat{y} \pm t_{\alpha/2}(n - p - 1)\hat{\sigma} \sqrt{\mathbf{x}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}^T}$

例：使用datarium包中的marketing数据集，我们将建立一个多元回归模型。根据在三种广告媒体（youtube, facebook和newspaper）上投入的预算来预测sales。计算公式如下：

$$sales = b_0 + b_1 * youtube + b_2 * facebook + b_3 * newspaper.$$

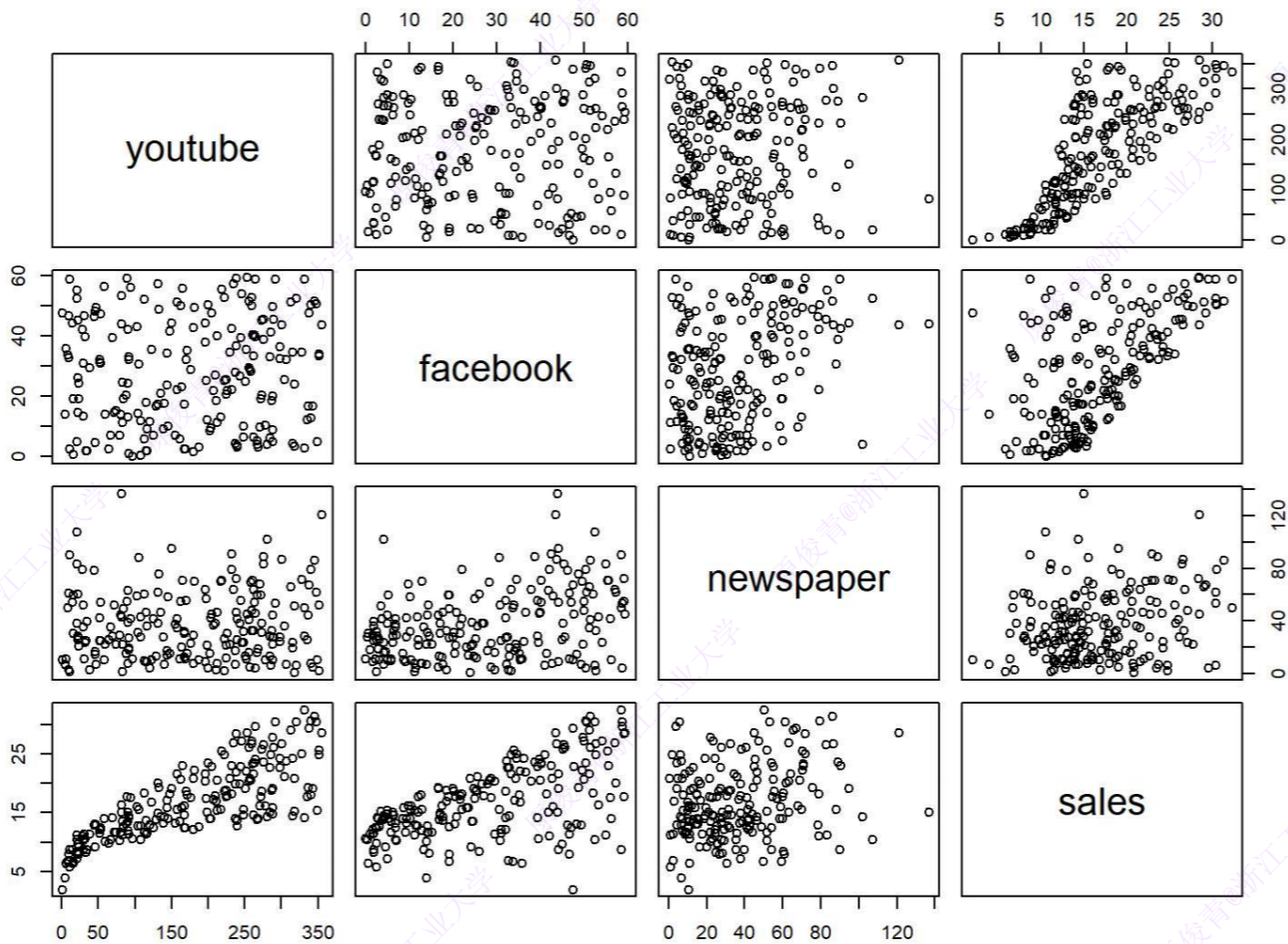
```
data("marketing", package = "datarium")  
dim(marketing)
```

```
## [1] 200  4
```

```
head(marketing)
```

```
##  youtube facebook newspaper sales  
## 1  276.12    45.36    83.04  26.52  
## 2   53.40    47.16    54.12  12.48  
## 3   20.64    55.08    83.16  11.16  
## 4  181.80    49.56    70.20  22.20  
## 5  216.96    12.96    70.08  15.48  
## 6   10.44    58.68    90.00   8.64
```

```
plot(marketing)
```



- 检查二变量相关关系

```
cor(marketing)
```

```
##           youtube  facebook  newspaper    sales
## youtube  1.00000000 0.05480866 0.05664787 0.7822244
## facebook 0.05480866 1.00000000 0.35410375 0.5762226
## newspaper 0.05664787 0.35410375 1.00000000 0.2282990
## sales    0.78222442 0.57622257 0.22829903 1.0000000
```

- 将数据分为训练组和测试组，按 8:2 的比例

```
set.seed(2022) # 设置随机种子使结果可重复
idx = sample(nrow(marketing), 0.8 * nrow(marketing))
trainData <- marketing[idx, ]
testData  <- marketing[-idx, ]
```

```
model_1 <- lm(sales ~ youtube + facebook + newspaper, data = trainData)
summary(model_1) #summary(model_1)$coef
```

```
##
## Call:
## lm(formula = sales ~ youtube + facebook + newspaper, data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.1666  -1.1738   0.3923   1.5835   3.4380
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.369249   0.437066   7.709 1.39e-12 ***
## youtube      0.046567   0.001595  29.203 < 2e-16 ***
## facebook     0.182270   0.010363  17.588 < 2e-16 ***
## newspaper    0.001606   0.007048   0.228   0.82
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.137 on 156 degrees of freedom
## Multiple R-squared:  0.8902, Adjusted R-squared:  0.8881
## F-statistic: 421.7 on 3 and 156 DF,  p-value: < 2.2e-16
```



```
model_2 <- lm(sales ~ youtube + facebook, data = trainData)
summary(model_2) #summary(model_1)$coef
```

```
##
## Call:
## lm(formula = sales ~ youtube + facebook, data = trainData)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.2223  -1.2030   0.3522   1.5695   3.4318
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.400910   0.413150   8.232 6.69e-14 ***
## youtube      0.046591   0.001586  29.370 < 2e-16 ***
## facebook     0.183128   0.009627  19.022 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.13 on 157 degrees of freedom
## Multiple R-squared:  0.8902, Adjusted R-squared:  0.8888
## F-statistic: 636.3 on 2 and 157 DF,  p-value: < 2.2e-16
```

- 回归模型 $sales = 3.4 + 0.047 * youtube + 0.183 * facebook$
- 预测, 点估计和区间估计

```
newdata <- data.frame(youtube = 2000, facebook = 1000, newspaper = 1000) # New advertising budgets
predict(model_2, newdata, interval="prediction", level=0.95) # Predict sales values
```

```
##          fit      lwr      upr
## 1 279.7107 260.1261 299.2953
```

```
test<-data.frame(trainData, predict(model_2, trainData))
y_true<-as.vector(test[,4])
SST <- crossprod(y_true-mean(y_true)); SST
```

```
##          [,1]
## [1,] 6488.245
```

```
y_hat<-as.vector(test[,5]); SSR <- crossprod(y_hat - mean(y_true)); SSR
```

```
##           [,1]  
## [1,] 5775.737
```

```
err<- y_true - y_hat; SSE <- t(err) %*% err; SSE
```

```
##           [,1]  
## [1,] 712.5088
```

```
sig_hat <- sqrt(SSE/(nrow(test)-length(model_2$coef)-1)); sig_hat
```

```
##           [,1]  
## [1,] 2.137139
```

```
R_sq <- SSR/SST; R_sq
```

```
##           [,1]  
## [1,] 0.8901847
```

9. 回归模型诊断

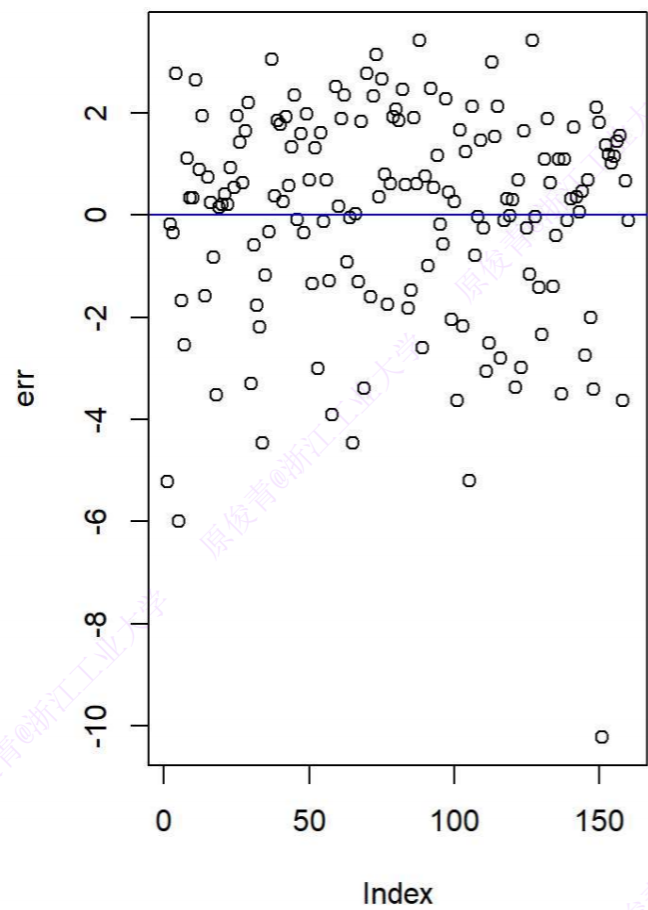
$$Y = X\beta + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I_n)$$

- 借助残差探测样本中的异常值, 等方差

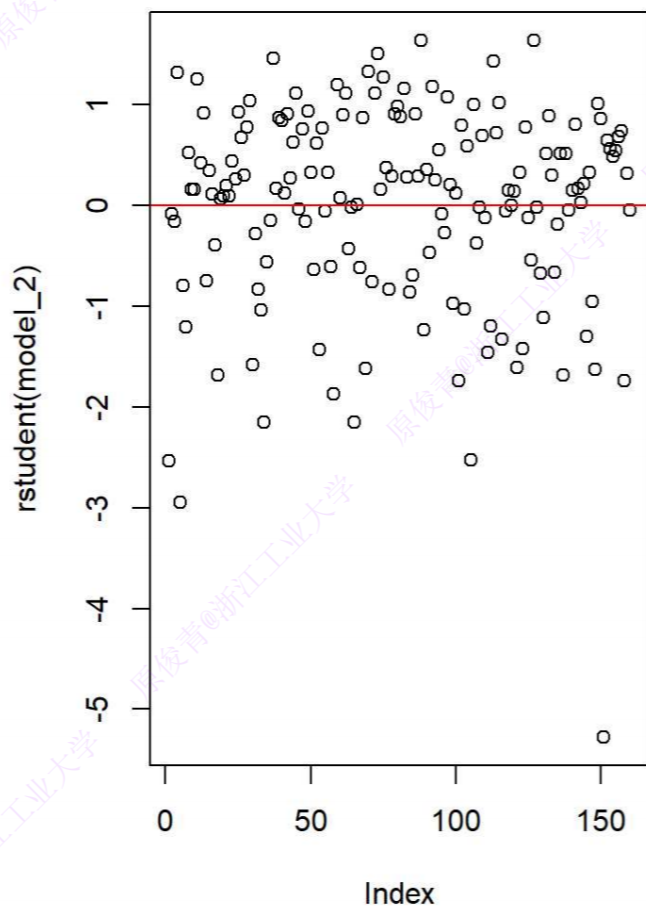
-①. 绘制残差的散点图, 检验等方差, 异常值;

```
opar=par(mfrow=c(1,2))
plot(err, main='残差'); abline(h=mean(err), col='blue')
plot(rstudent(model_2), main='标准化残差'); abline(h=0, col='red')
```

残差



标准化残差



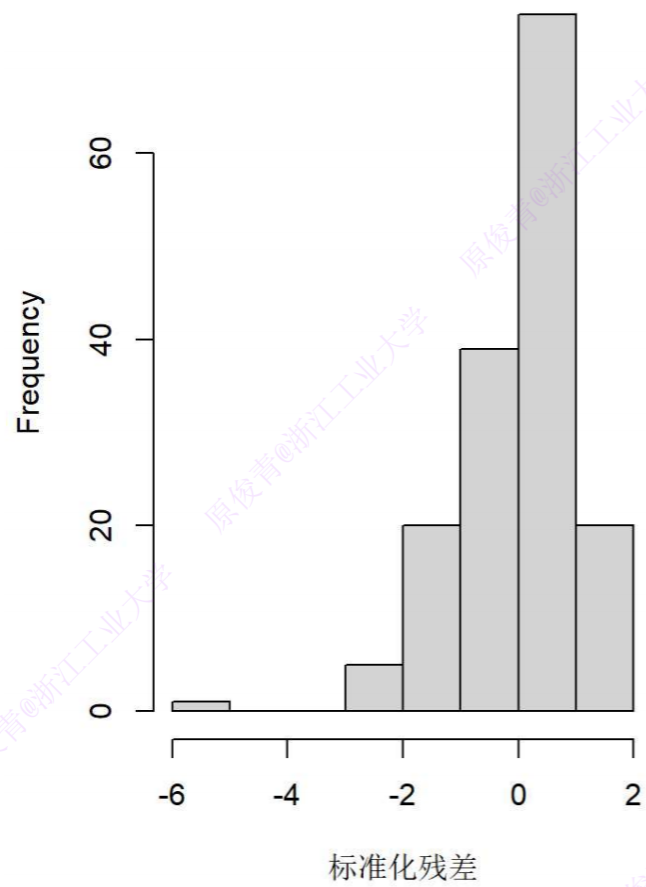
```
par(opar)
```

- 残差是否服从均值为零, 等方差的正态分布

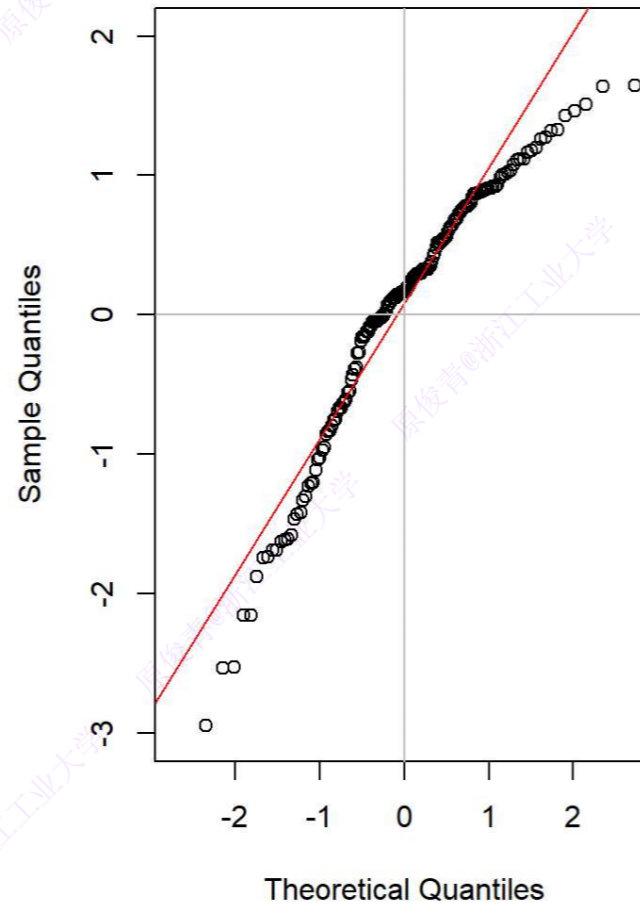
-①. 绘制残差的直方图, QQ图, 看分布, 检验正态性;

```
opar=par(mfrow=c(1,2))
hist(rstudent(model_2), xlab='标准化残差', main='直方图')
qqnorm(rstudent(model_2), ylim=c(-3,2), main='QQ plot')
qqline(rstudent(model_2), col='red')
abline(h=0, pch=3, col='gray'); abline(v=0, pch=3, col='gray')
```

直方图



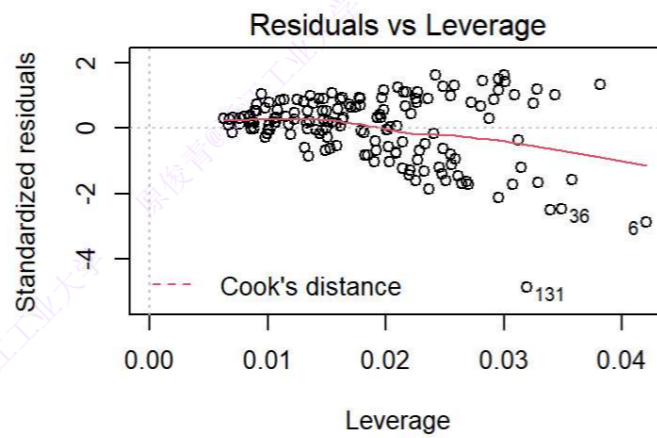
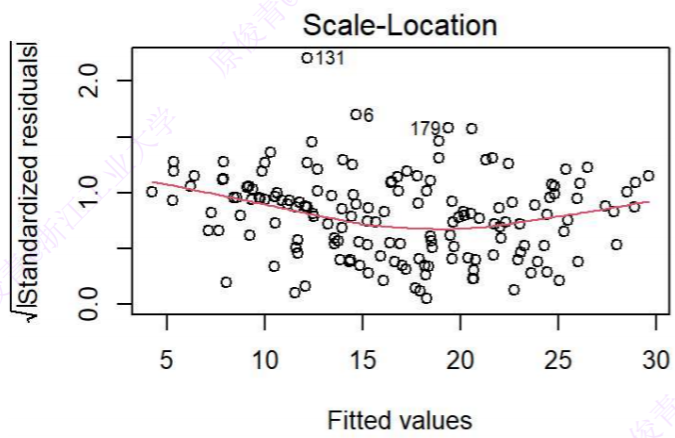
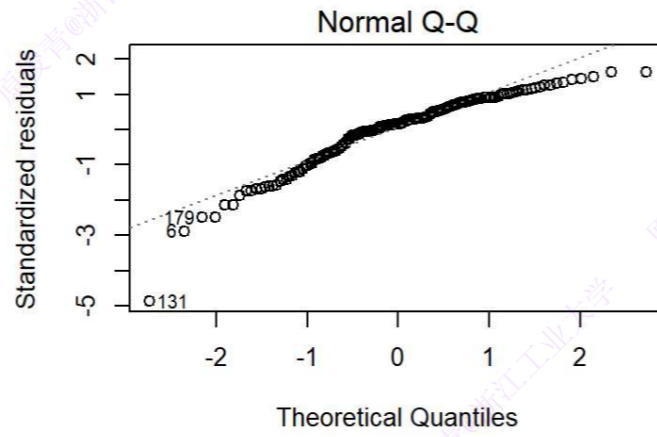
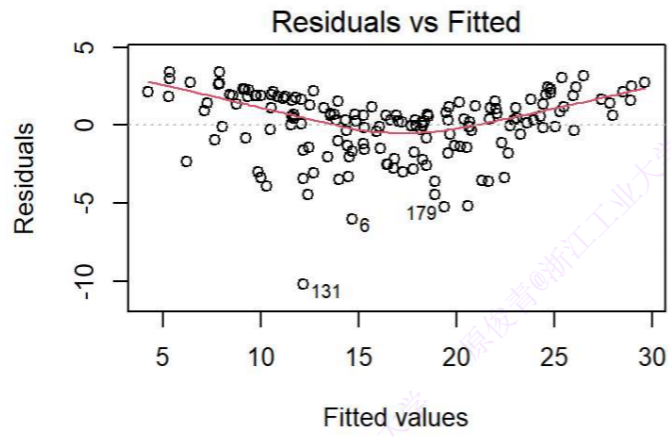
QQ plot



```
par(opar)
```

- 基础绘图系统的plot函数输入对象为回归模型时，返回对象是四幅模型诊断图。
- 四幅图依次为残差-拟合图、正态Q-Q图、尺度-位置图、残差-杠杆图；
- 除残差-杠杆图用于检验异常点外，其余三幅图均用于检验模型结果是否符合假设。

```
opar=par(mfrow=c(2,2))  
plot(model_2)
```

```
par(opar)
```

$$\hat{\boldsymbol{\varepsilon}} = (\mathbf{I}_n - \mathbf{H})\mathbf{Y} \sim N(0, \sigma^2(\mathbf{I}_n - \mathbf{H}))$$

-②. 零均值t检验, $H_0 : E(\hat{\boldsymbol{\varepsilon}}) = 0$;

```
t.test(err)      ##H_0: E(err)=0
```

```
##  
## One Sample t-test  
##  
## data:  err  
## t = -5.4399e-14, df = 159, p-value = 1  
## alternative hypothesis: true mean is not equal to 0  
## 95 percent confidence interval:  
## -0.3305239  0.3305239  
## sample estimates:  
## mean of x  
## -9.103829e-15
```

-③. Shapiro-Wilk正态性检验, H_0 : 正态分布;

$$\text{检验统计量: } W = \frac{(\sum_{i=1}^n a_i X_{(i)})^2}{\sum_{i=1}^n (X_i - \bar{X})^2}$$

其中, $(a_1, a_2, \dots, a_n) = \frac{M^T V^{-1}}{C}$, $M = (m_1, m_2, \dots, m_n)^T$, $m_i = E(Y_{(i)})$,

$$V = \text{Cov}(\mathbf{Y}, \mathbf{Y}), \quad \mathbf{Y} = (Y_1, Y_2, \dots, Y_n)^T, \quad Y_i \sim N(0, 1).$$

$$C = \|\mathbf{V}^{-1} \mathbf{M}\| = (\mathbf{M}^T \mathbf{V}^{-1} \mathbf{V}^{-1} \mathbf{M})^{1/2}.$$

H_0 为真时, W 接近 1。

```
shapiro.test(err) ##H_0: 正态分布
```

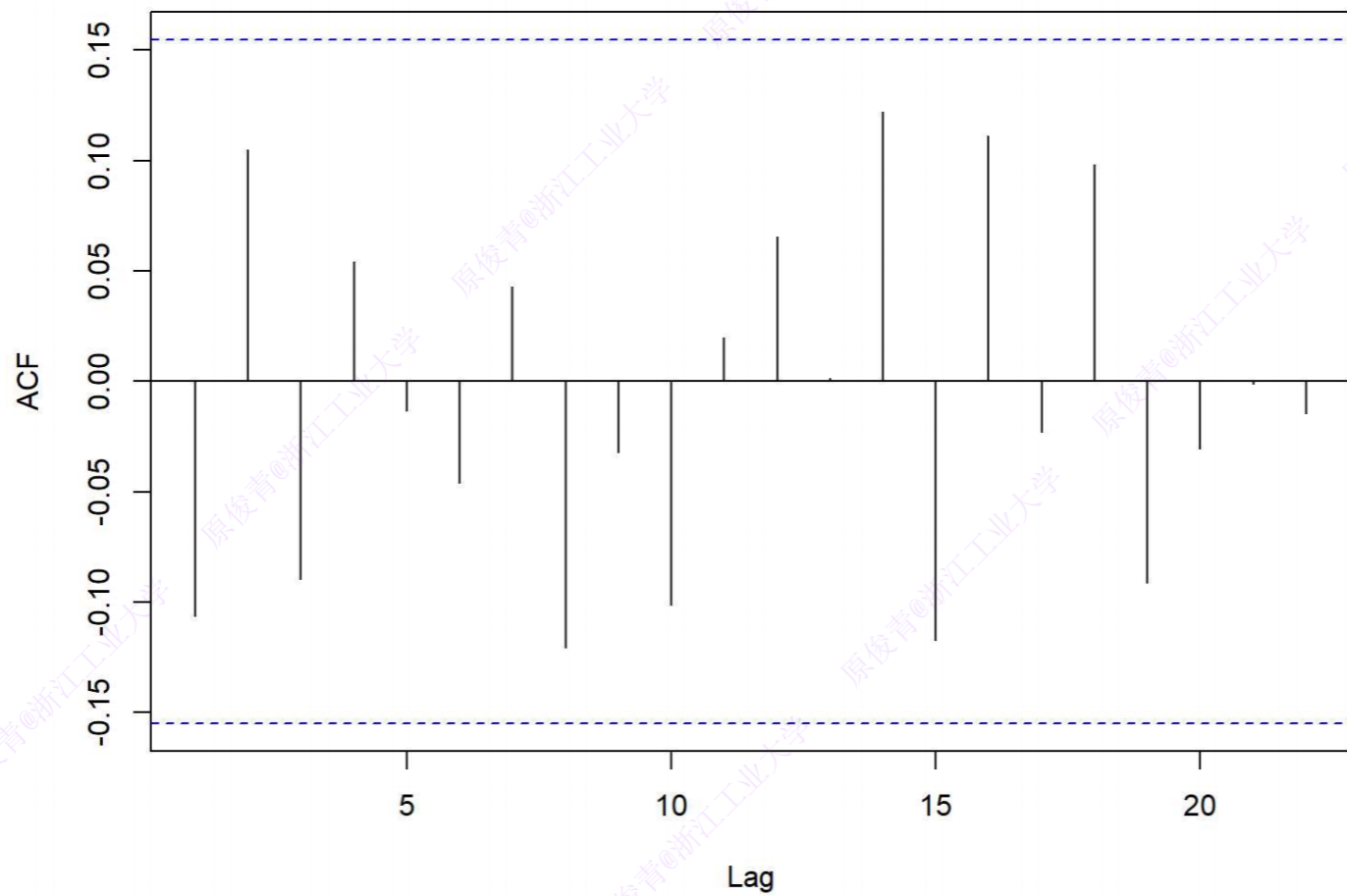
```
##  
## Shapiro-Wilk normality test  
##  
## data:  err  
## W = 0.92185, p-value = 1.321e-07
```

- 残差序列是否独立

-④. 绘制时间序列的自相关函数图ACF, 检验相关性;

```
acf(err) ##自相关函数图
```

Series err



-⑤. Durbin-Watson独立性检验, H_0 : 不相关 $\rho = 0$;

$$DW = \frac{\sum_{i=2}^n (e_i - e_{i-1})^2}{\sum_{i=2}^n (e_i)^2}$$

若残差项间是正相关, 则其差异必小; 若残差项间是负相关, 则其差异必大。

- 当DW值愈接近2时, 残差项间愈无相关
- 当DW值愈接近0时, 残差项间正相关愈强
- 当DW值愈接近4时, 残差项间负相关愈强

```
##DW检验, H_0: 不相关
DW.test<-function(tserr){
  Z_err <- zlag(tserr)
  D_err <- tserr[-1]-Z_err[-1]
  crossprod(D_err,D_err)/crossprod(tserr[-1], tserr[-1])
}

tserr <- residuals(model_2);
DW.test(tserr)
```

```
##           [, 1]
## [1, ] 2.261129
```


-⑥. 游程检验, H_0 : 独立性;

<https://baike.baidu.com/item/%E6%B8%B8%E7%A8%8B%E6%A3%80%E9%AA%8C/9163984?fr=aladdin>

```
runs(err) ##游程检验, H_0: 独立
```

```
## $pvalue
## [1] 0.962
##
## $observed.runs
## [1] 79
##
## $expected.runs
## [1] 78.1875
##
## $n1
## [1] 65
##
## $n2
## [1] 95
##
## $k
## [1] 0
```