第九章、回归分析

§9.1 引言

- 自变量/解释变量: x, 因变量/响应变量: y.
- 回归函数: f, 未知.
- 回归模型/方程/关系: $y = f(x) + e$. 其中, e 是误差.
- 例: $x =$ 路程(可设定), $y =$ 耗油量.

  $x =$ 父亲身高(不可设定, 只可测量), $y =$ 儿子身高.

  关心f, 不关心自变量如何变化.

  将x 视为已知参数, 将y, e 视为随机变量或其取值.

- 一元线性回归(正态)模型:

$$y = b_0 + b_1 x + e, \quad e \sim N(0, \sigma^2),$$

其中 b_0, b_1, σ^2 为未知参数.

- 数据(x_i, y_i), $i = 1, \cdots, n$.

$$y_i = b_0 + b_1 x_i + e_i, \quad i = 1, \cdots, n.$$

- x_i 是已知参数,
  y_i 是随机变量(或其取值), 可观测.
  $e_1, \cdots, e_n$ 是i.i.d. 随机变量(或其取值), 不可观测(因为b_0, b_1 是未知参数).

例1.1. x 与y 分别代表某个体的两个特征. 数据: (x_i, y_i), $i = 1, \cdots, n = 50$.

问: x 与y 之间什么依赖关系?

- 散点图:

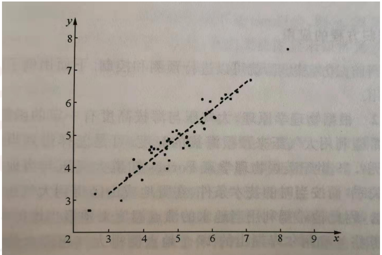


图 9.1.1 数据(x_i, y_i)的散点图

- 初步判断:

  $y_i = b_0 + b_1 x_i + e_i,$

  $i = 1, \cdots, n.$

回归方程的应用.

- 例1.2 (预测). x =水的沸点, y =大气压.

  由$n=17$ 组数据得到预测公式:

$$y=-43.131+0.895x+e.$$

  某地测得$x=x_0$, 那么, 可预测$Y_0=\hat{b}_0+\hat{b}_1 x_0+e_0$.

- 例1.3 (预测与控制). $x=$ 某小区人口数, $y=$ 冬季用煤量, $z=$ 室温.

  通过数据(x_i,y_i,z_i), $i=1,\cdots,n$ 得到回归关系:

$$y=a+bx+e,\quad z=d+fy+\varepsilon.$$

  预测: 根据某小区人口数x_0, 预测用煤量$Y_0=\hat{a}+\hat{b}x_0+e_0$.

  控制: 为控制$z\in[17,18]$, 应该储备多少煤(反求y)?

§9.2 ~ §9.4 一元线性回归及其参数检验

$$y = b_0 + bx + e, \quad e \sim N(0, \sigma^2),$$

其中, σ^2 未知. 数据: (x_i, y_i), $i = 1, \cdots, n$.

- 回归模型: $y_i = b_0 + bx_i + e_i$, $i = 1, \cdots, n$.

$$p_{Y_i}(y_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(y_i - (b_0 + bx_i))^2},$$

x_i: 已知参数; b_0, b: 待估参数; σ^2: 讨厌参数.

- 似然函数: $L(b_0, b, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}^n} e^{-\frac{1}{2\sigma^2} Q(b_0, b)}$.

  均方误差: $Q(b_0, b) = \sum_{i=1}^n [y_i - (b_0 + bx_i)]^2$.

- 定义2.1. $Q(b_0, b)$ 的最小值点$\hat{b}_0$, $\hat{b}$ 被称为最小二乘拟合系数, 或b_0 与b 的最小二乘估计.

- 最大似然估计: $\hat{b}_0$, $\hat{b}$, $\hat{\sigma}^2 = \frac{1}{n} Q(\hat{b}_0, \hat{b})$.

定理2.1. 假设$x_1, \cdots x_n$ 不完全相同, 则

$$\hat{b}_0 = \bar{y} - \hat{b}\bar{x}, \quad \hat{b} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\ell_{xy}}{\ell_{xx}}.$$

其中, $\ell_{uv} = \sum_{i=1}^n (u_i - \bar{u})(v_i - \bar{v})$.

- 找$Q(a, b) = \sum_{i=1}^n [y_i - (b_0 + bx_i)]^2$ 的最小值点.
- $\bar{w} = \frac{1}{n}(w_1 + \cdots + w_n)$:

$$\sum_{i=1}^n w_i^2 = \sum_{i=1}^n (w_i - \bar{w})^2 + n\bar{w}^2.$$

- $Q(a, b) = \sum_{i=1}^n [(y_i - \bar{y}) - b(x_i - \bar{x})]^2 + n(\bar{y} - (b_0 + b\bar{x})^2$.
- $\star = \ell_{yy} - 2b\ell_{xy} + b^2\ell_{xx}$, 最小值点为$\hat{b}$.

定理2.2 & 定理3.2. 若x_i 不全相等, 则$\hat{b}_0$, $\hat{b}$ 是最优线性无偏估计.

$$\hat{b}_0 = \bar{y} - \hat{b}\bar{x}, \quad \hat{b} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\ell_{xy}}{\ell_{xx}}.$$

- $\hat{b}_0$, $\hat{b}$ 是$(y_1, \cdots, y_n)$ 的线性函数.
- $y_i = b_0 + bx_i + e_i, \quad \bar{y} = b_0 + b\bar{x} + \bar{e},$

$$y_i - \bar{y} = b(x_i - \bar{x}) + (e_i - \bar{e}).$$

- $E\hat{b} = b$: $e_1, \cdots, e_n$ i.i.d., 且$e_1 \sim N(0, \sigma^2)$,

$$\hat{b} = b + \frac{1}{\ell_{xx}} \sum_{i=1}^n (x_i - \bar{x})(e_i - \bar{e}) = b + \frac{1}{\ell_{xx}} \sum_{i=1}^n (x_i - \bar{x}) e_i,$$

- $E\hat{b}_0 = b_0$:

$$\hat{b}_0 = \bar{y} - \hat{b}\bar{x} = (b_0 + b\bar{x} + \bar{e}) - \hat{b}\bar{x} = b_0 + (b - \hat{b})\bar{x} + \bar{e}.$$

参数: $\theta = (b_0, b, \sigma^2)$. 假设检验问题(2.14).

$$H_0 : b = 0 \leftrightarrow H_1 : b \neq 0.$$

- 否定H_0, 则表明y 与x 之间有线性依赖关系.
- $\Theta = \{\theta : b_0, b \in \mathbb{R}, \sigma^2 > 0\}$, $\Theta_0 = \{\theta \in \Theta : b = 0\}$.
- 似然函数: $L(\theta) = \frac{1}{\sqrt{2\pi\sigma^2}^n} e^{-\frac{1}{2\sigma^2} Q(b_0, b)}$.
  $$Q(b_0, b) = \sum_{i=1}^n [y_i - (b_0 + bx_i)]^2.$$
- Θ 上的最大似然估计: $\hat{\theta} = (\hat{b}_0, \hat{b}, \hat{\sigma}^2)$, $\hat{b}_0 = \bar{y} - \hat{b}\bar{x}$, $\hat{b} = \frac{\ell_{xy}}{\ell_{xx}}$,
  $$L(\hat{\theta}) = \left(\sqrt{2\pi\hat{\sigma}^2}\right)^{-n/2} e^{-\frac{n}{2}}, \quad \hat{\sigma}^2 = \frac{1}{n} Q(\hat{b}_0, \hat{b}).$$
- Θ_0 上的最大似然估计: $\check{\theta}_0 = (\check{b}_0, \check{b}, \check{\sigma}^2)$, $\check{b}_0 = \bar{y}$, $\check{b} = 0$,
  $$L(\hat{\theta}_0) = \left(\sqrt{2\pi\check{\sigma}_0^2}\right)^{-n/2} e^{-\frac{n}{2}}, \quad \check{\sigma}_0^2 = \frac{1}{n} Q(\check{b}_0, \check{b}).$$

$$H_0 : b = 0 \leftrightarrow H_1 : b \neq 0.$$

- $Q(b_0, b) = \sum_{i=1}^n [y_i - (b_0 + bx_i)]^2$,

$$L(\hat{\theta}) = \left(\sqrt{2\pi\hat{\sigma}^2}\right)^{-n/2} e^{-\frac{n}{2}}, \quad \hat{\sigma}^2 = \frac{1}{n}Q(\hat{b}_0, \hat{b})$$

$$L(\hat{\theta}_0) = \left(\sqrt{2\pi\check{\sigma}_0^2}\right)^{-n/2} e^{-\frac{n}{2}}, \quad \check{\sigma}_0^2 = \frac{1}{n}Q(\bar{y}, 0).$$

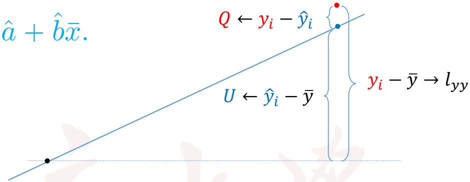
- $Q = Q(\hat{b}_0, \hat{b}) = \sum_{i=1}^n (y_i - \hat{y}_i)^2$, 残差平方和;
  $Q(\bar{y}, 0) = \sum_{i=1}^n (y_i - \bar{y})^2 = \ell_{yy}$,
- 广义似然比: $\lambda(\vec{y}) = L(\hat{\theta})/L(\hat{\theta}_0) = (\ell_{yy}/Q)^{n/2}$.
- 广义似然比否定域:

$$\mathcal{W} = \{\vec{y} : \ell_{yy}/Q > c_1\}.$$

正交分解. $\hat{a} = \bar{y} - \hat{b}\bar{x}$, $\hat{b} = \frac{\ell_{xy}}{\ell_{xx}}$. 产生直线$\hat{f}$: $\hat{y} = \hat{a} + \hat{b}x$,

- $\hat{f}$ 过点$(\bar{x}, \bar{y})$, $\quad \bar{y} = \hat{f}(\bar{x}) = \bar{\hat{y}}$.

$$\bar{y} = \hat{a} + \hat{b}\bar{x}.$$



- 残差平方和Q:

$$Q = \sum_{i=1}^{n}(y_i - (\hat{a} + \hat{b}x_i))^2$$
$$= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2.$$

- 回归平方和U:

$$U = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 = \hat{b}^2 \sum_{i=1}^{n}(x_i - \bar{x})^2.$$

- 引理2.1. $\ell_{yy} = \sum_{i=1}^{n}(y_i - \bar{y})^2 = U + Q$.
- $\sum_{i=1}^{n} \star\star\ {**} = \sum_{i=1}^{n}(y_i - \bar{y})\hat{b}(x_i - \bar{x}) - \sum_{i=1}^{n}(\hat{y}_i - \bar{y})(\hat{y}_i - \bar{y})$

$$= \hat{b}\ell_{xy} - \hat{b}^2\ell_{xx} = 0.$$

- 广义似然比否定域: $\mathcal{W} = \{\vec{y} : U/Q > c_2\}$.

命题4.1. 残差平方和$Q = \sum_{i=1}^n (y_i - \hat{y}_i)^2$ 与回归平方和$U = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 = \hat{b}^2 \ell_{xx}$ 相互独立, 且

$$\frac{1}{\sigma^2} Q \sim \chi^2(n-2); \quad 若b = 0, 则 \frac{U}{\sigma^2} \sim \chi^2(1).$$

- $\hat{b}_0 = b_0 + (b - \hat{b})\bar{x} + \bar{e}, \quad \hat{b} = b + \frac{1}{\ell_{xx}} \sum_i (x_i - \bar{x})(e_i - \bar{e}).$
- $$\begin{aligned} \hat{y}_i - y_i &= (\hat{b}_0 + \hat{b} x_i) - (b_0 + b x_i + e_i) \\ &= (b - \hat{b})\bar{x} + \bar{e} + (\hat{b} - b) x_i - e_i \\ &= (\hat{b} - b)(x_i - \bar{x}) - (e_i - \bar{e}). \end{aligned}$$
- $$(\hat{y}_i - y_i)^2 = (\hat{b} - b)^2 (x_i - \bar{x})^2 + (e_i - \bar{e})^2 \\ -2(\hat{b} - b)(x_i - \bar{x})(e_i - \bar{e}).$$
- $$\begin{aligned} Q &= (\hat{b} - b)^2 \ell_{xx} + \sum_i (e_i - \bar{e})^2 - 2(\hat{b} - b)\ell_{xx}(\hat{b} - b), \\ &= \sum_i (e_i - \bar{e})^2 - \ell_{xx}(\hat{b} - b)^2. \end{aligned}$$

命题4.1(续). $Q=\sum_{i=1}^n(y_i-\hat{y}_i)^2$. 则$\frac{1}{\sigma^2}Q\sim\chi^2(n-2)$.

- $Q=\sum_i(e_i-\bar{e})^2-\ell_{xx}(\hat{b}-b)^2,\quad \hat{b}=b+\sum_i\frac{x_i-\bar{x}}{\ell_{xx}}e_i$.
- $\sum_i(e_i-\bar{e})^2$:

$$\sum_i(e_i-\bar{e})^2=\sum_i e_i^2-n\bar{e}^2$$

$$=\sum_i e_i^2-\left(\sum_i\frac{1}{\sqrt{n}}e_i\right)^2=\sum_i e_i^2-\left(\sum_i a_{1i}e_i\right)^2.$$

- $\ell_{xx}(\hat{b}-b)^2$:

$$\ell_{xx}(\hat{b}-b)^2=\left(\sum_i\frac{x_i-\bar{x}}{\sqrt{\ell_{xx}}}e_i\right)^2=\left(\sum_i a_{2i}e_i\right)^2.$$

- 再补$n-2$ 行, 可得正交矩阵$A=(a_{ki})_{n\times n}$:

$$\sum_i a_{1i}^2=\sum_i a_{2i}^2=1,\quad \sum_i a_{1i}a_{2i}=0.$$

命题4.1(续). $Q=\sum_{i=1}^n(y_i-\hat{y}_i)^2$. 则$\frac{1}{\sigma^2}Q\sim\chi^2(n-2)$.

- $Q=\sum_i e_i^2-(\sum_i a_{1i}e_i)^2-(\sum_i a_{2i}e_i)^2$.

  $A=(a_{ki})_{n\times n}$ 为正交矩阵.

- $W_i=e_i/\sigma$: $W_1,\cdots,W_n$ i.i.d., $W_1\sim N(0,1)$, 则

$$\begin{aligned}EZ_kZ_\ell &= E\sum_i a_{ki}W_i\sum_j a_{\ell j}W_j\\ &= \sum_{i,j}a_{ki}a_{\ell j}EW_iW_j=\sum_i a_{ki}a_{\ell i}=1_{\{k=\ell\}}.\end{aligned}$$

$$(W_1,\cdots,W_n)^T\overset{d}{=}(Z_1,\cdots,Z_n)^T:=A(W_1,\cdots,W_n)^T.$$

- $Q=\sigma^2\left(\sum_i Z_i^2-{Z_1}^2-{Z_2}^2\right)=\sigma^2\sum_{i=3}^n Z_i^2$.

命题4.1(续). 回归平方和$U=\sum_{i=1}^n(\hat{y}_i-\bar{y})^2=\hat{b}^2\ell_{xx}$ 与Q 相互独立, 且若$b=0$, 则

$$\frac{U}{\sigma^2}\sim\chi^2(1).$$

- $\hat{b}$ 与$Q=\sigma^2\sum_{i=3}^n Z_i^2$ 独立:

$$\hat{b}=b+\sum_i\frac{x_i-\bar{x}}{\ell_{xx}}e_i=b+\frac{1}{\sqrt{\ell_{xx}}}\sigma Z_2.$$

- $U=(\sqrt{\ell_{xx}}b+\sigma Z_2)^2$. 若$b=0$, 则

$$\frac{1}{\sigma^2}U=Z_2^2\sim\chi^2(1).$$

- $Q = \sigma^2 \sum_{i=3}^n Z_i^2$, $\quad U = (\sqrt{\ell_{xx}} b + \sigma Z_2)^2$.
- 广义似然比否定域:

$$\mathcal{W} = \left\{ \vec{y} : \frac{U}{Q} > c_2 \right\} = \left\{ \vec{y} : \frac{U}{Q/(n-2)} > \lambda \right\}.$$

- 定理4.3. 在H_0 下, 检验统计量:

$$\xi := \frac{U}{Q/(n-2)} \sim F(1, n-2).$$

因此, $\lambda = F_{1-\alpha}(1, n-2)$.

例2.1. x = 注射后天数,
y = 金残留百分数.

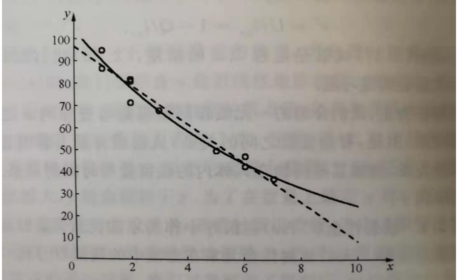


图 9.2.1 示踪放射性金元素残留量衰减图

- 根据散点图建立函数
  $\ln y = b_0 + bx + e$.
- 求$\bar{x}$, $\bar{z}$; $\hat{z}_i = \hat{b}_0 + \hat{b}x_i$:
  $\hat{b} = \ell_{xz}/\ell_{xx}$, $\hat{b}_0 = \bar{z} - \hat{b}\bar{x}$;
- 求残差平方和: $Q = \sum_i (z_i - \hat{z}_i)^2$
  与回归平方和: $U = \sum_i (\hat{z}_i - \bar{z})^2$.
- $n = 10$, 根据$\lambda = F_{0.95}(1, n-2) = F_{0.95}(1, 8) = 5.32$.
  $\frac{U}{Q/(n-2)} = 344.82 > \lambda$ 否定H_0, 强烈认可z 线性依赖于x.