

一元线性回归(一)

I. 引言

1. 期望与中位数的另一种定义:

$$\min_b E(X - b)^2 \Rightarrow E(X) = b$$

$$\min_b E|X - b| \Rightarrow med(X) = b$$

proof.

$$E(X - b)^2 = E(X^2 - 2bX + b^2) = E(X^2) - 2bE(X) + b^2 \quad (1)$$

可将 (1) 式看为 b 的一个一元二次函数, 现求 b 的最小值. 可由公式得: $b = E(X)$.

对于中位数, 我们只考虑连续的情况, 离散时类似可证. 令随机变量 X 的概率密度为 $p(x)$, 概率分布为 $F(X)$, 则有等式成立:

$$E|X - b| = \int_{-\infty}^{\infty} |x - b| p(x) dx = \int_{-\infty}^b (b - x) p(x) dx + \int_b^{\infty} (x - b) p(x) dx$$

现要求 b 的最小值, 两边对 b 求导, 并令导数为 0.

$$\int_{-\infty}^b p(x) dx - \int_b^{\infty} p(x) dx = 0$$

$$\Rightarrow F(b) - (1 - F(b)) = 0, \text{ 即 } F(b) = \frac{1}{2}, b = med(X).$$

2. Conditional Expectation :

i.) Law of Total Expectation :

$$E[E(X|Y)] = E(X)$$

ii.) Law of Total Variance

$$Var(X) = Var[E(X|Y)] + E[Var(X|Y)]$$

proof.

设随机变量 X, Y 的联合密度为 $f(x, y)$, 边缘密度分别为 $f_X(x), f_Y(y)$, 则成立等式:

$$\begin{aligned} \text{i.) } E(X) &= \int x f_X(x) dx = \iint x f(x, y) dx dy \\ &= \iint x [f(x|y) \cdot f_Y(y)] dx dy \\ &= \int [\int x \cdot f(x|y) dx] f_Y(y) dy \end{aligned}$$

$$= \int E(X|y) \cdot f_Y(y) dy = E[E(X|Y)].$$

$$\begin{aligned} \text{ii.) } \text{Var}(X) &= E(X - E(X))^2 = E[X - E(X|Y) + E(X|Y) - E(X)]^2 \\ &= E[X - E(X|Y)]^2 + E[E(X|Y) - E(X)]^2 + 2E[(X - E(X|Y))(E(X|Y) - E(X))] \end{aligned} \quad (1)$$

$$\begin{aligned} \text{而 } E[X - E(X|Y)]^2 &= E \{ E[(X - E(X|Y))^2 | Y] \} \\ &= E \{ E[X^2 + (E(X|Y))^2 - 2XE(X|Y) | Y] \} \\ &= E \{ E(X^2 | Y) + (E(X|Y))^2 - 2(E(X|Y))^2 \} \\ &= E \{ E(X^2 | Y) - (E(X|Y))^2 \} \\ &= E[\text{Var}(X|Y)] \end{aligned}$$

$$\begin{aligned} E[E(X|Y) - E(X)]^2 &= E \{ E(X|Y) - E[E(X|Y)] \}^2 \\ &= \text{Var}[E(X|Y)] \end{aligned}$$

$$\begin{aligned} E[(X - E(X|Y))(E(X|Y) - E(X))] &= E \{ [(X - E(X|Y))(E(X|Y) - E(X))] | Y \} \\ &= (E(X|Y))^2 - E(X)E(X|Y) - (E(X|Y))^2 + E(X|Y)E(X) = 0 \end{aligned}$$

所以 (1) = $\text{Var}(E(X|Y)) + E(\text{Var}(X|Y))$.

II. 一元回归模型

1. OLSE下的参数估计

OLSE的主要思想是寻找参数 β_0, β_1 的估计值使离差平方和达到最小。从而可转化为如下问题：

$$\min_{\beta_0, \beta_1} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

分别对 β_0, β_1 求偏导，并令偏导为 0，结果如下：

$$\begin{cases} -2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0 \\ -2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) x_i = 0 \end{cases}$$

整理后可得：

$$\begin{cases} n\hat{\beta}_0 + (\sum_{i=1}^n x_i)\hat{\beta}_1 = \sum_{i=1}^n y_i & (1) \\ (\sum_{i=1}^n x_i)\hat{\beta}_0 + (\sum_{i=1}^n x_i^2)\hat{\beta}_1 = \sum_{i=1}^n x_i y_i & (2) \end{cases}$$

对 (1) 两边同时除以 n ，整理后可得：

$$\hat{\beta}_0 = \bar{y} - \bar{x}\hat{\beta}_1$$

对于 (2) 注意到有如下两个等式：

$$\begin{aligned} \text{i.) } \sum_{i=1}^n (x_i - \bar{x})^2 &= \sum_{i=1}^n (x_i^2 - 2x_i \cdot \bar{x} + \bar{x}^2) \\ &= \sum_{i=1}^n x_i^2 + n\bar{x}^2 - 2\bar{x} \sum_{i=1}^n x_i \\ &= \sum_{i=1}^n x_i^2 - n\bar{x}^2. \end{aligned}$$

$$\begin{aligned} \text{ii.) } \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) &= \sum_{i=1}^n (x_i y_i + \bar{x}\bar{y} - \bar{x}y_i - \bar{y}x_i) \\ &= \sum_{i=1}^n x_i y_i + n\bar{x}\bar{y} - \bar{x} \sum_{i=1}^n y_i - \bar{y} \sum_{i=1}^n x_i \\ &= \sum_{i=1}^n x_i y_i + n\bar{x}\bar{y} - n\bar{x}\bar{y} - n\bar{x}\bar{y} \\ &= \sum_{i=1}^n x_i y_i - n\bar{x}\bar{y} \end{aligned}$$

由上述公式，(2) 变为：

$$n\bar{x}\hat{\beta}_0 + \left(\sum_{i=1}^n (x_i - \bar{x})^2 + n\bar{x}^2 \right) \hat{\beta}_1 = \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) + n\bar{x}\bar{y}$$

再由 (1) 整理后可得：

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

2. MLE下的参数估计

MLE的主要思想是利用总体的概率密度及其样本提供的信息构造似然函数，通过似然函数取值最大得到对应参数的估计。

对于一元线性回归模型参数的MLE，我们假设 $\varepsilon_i \sim N(0, \sigma^2)$ 时， y_i 服从如下正态分布：

$$y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$$

则 y_i 的概率密度为

$$f_i(y_i) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}}$$

构造似然函数:

$$\begin{aligned} L(\beta_0, \beta_1, \sigma) &= \prod_{i=1}^n f_i(y_i) \\ &= \frac{1}{(\sqrt{2\pi}\sigma)^n} e^{-\frac{\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}} \end{aligned}$$

对似然函数取对数:

$$\ln(L) = -n \ln(\sqrt{2\pi}\sigma) - \frac{\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}$$

为了使似然函数 L 取得最大值, 等价的我们只需使 $\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$ 取得最小值, 即

$$\min_{\beta_0, \beta_1} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

至此与 **OLSE** 一致。

3. **OLSE** 估计的性质

i.) 线性

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} y_i - \bar{y} \sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

注意到:

$$\sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{n\bar{x} - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} = 0$$

所以

$$\hat{\beta}_1 = \sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} y_j$$

是关于 y_j 的线性组合。

由于 $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$ 且 \bar{x} 是常数, 结合上式可得:

$$\beta_0 = \sum_{j=1}^n \left(\frac{1}{n} - \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) y_j$$

也是关于 y_j 的线性组合。

ii.) 无偏性

注意到由 $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$ 可得:

$$E(y_i) = \beta_0 + \beta_1 x_i \quad (\text{Markov - Gauss Condition})$$

所以

$$\begin{aligned} E(\hat{\beta}_1) &= \sum_{j=1}^n \frac{x_j - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} E(y_j) \\ &= \sum_{j=1}^n \frac{x_j - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} (\beta_0 + \beta_1 x_j) \\ &= \beta_0 \cdot \sum_{j=1}^n \frac{x_j - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} + \beta_1 \cdot \sum_{j=1}^n \frac{x_j^2 - x_j \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (1) \end{aligned}$$

注意到

$$\sum_{j=1}^n \frac{x_j - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{n\bar{x} - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} = 0$$

$$\begin{aligned} \sum_{j=1}^n \frac{x_j^2 - x_j \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} &= \frac{\sum_{j=1}^n x_j^2 - n\bar{x}^2}{\sum_{i=1}^n x_i^2 + n\bar{x}^2 - 2\bar{x} \sum_{i=1}^n x_i} \\ &= \frac{\sum_{j=1}^n x_j^2 - n\bar{x}^2}{\sum_{i=1}^n x_i^2 - n\bar{x}^2} = 1 \end{aligned}$$

所以

$$E(\hat{\beta}_1) = (1) = \beta_1.$$

$$\begin{aligned}
E(\hat{\beta}_0) &= \sum_{j=1}^n \left(\frac{1}{n} - \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) E(y_j) \\
&= \sum_{j=1}^n \left(\frac{1}{n} - \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) (\beta_0 + \beta_1 x_j) \\
&= \beta_0 - \beta_0 \bar{x} \cdot \sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} + \beta_1 \bar{x} - \beta_1 \bar{x} \sum_{j=1}^n \frac{x_j^2 - x_j \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

由上述两个已证公式,可得:

$$E(\hat{\beta}_0) = \beta_0 - \beta_0 \bar{x} \cdot 0 + \beta_1 \bar{x} - \beta_1 \bar{x} \cdot 1 = \beta_0.$$

iii.) $\hat{\beta}_0, \hat{\beta}_1$ 的方差:

$$\begin{aligned}
Var(\hat{\beta}_1) &= Var\left(\sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} y_j\right) \\
&= \sum_{j=1}^n \left(\frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 Var(y_j) \quad (\text{Markov - Gauss Condition}) \\
&= \frac{\sum_{j=1}^n (x_j - \bar{x})^2}{\left(\sum_{i=1}^n (x_i - \bar{x})^2 \right)^2} \sigma^2 \\
&= \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{aligned}$$

$$\begin{aligned}
Var(\hat{\beta}_0) &= Var\left(\sum_{j=1}^n \left(\frac{1}{n} - \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) y_j\right) \\
&= \sum_{j=1}^n \left(\frac{1}{n} - \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 Var(y_i) \quad (\text{Markov - Gauss Condition}) \\
&= \sum_{j=1}^n \left(\frac{1}{n^2} + \left(\frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 - \frac{2}{n} \frac{(x_j - \bar{x})\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \sigma^2 \\
&= \sigma^2 \left(\sum_{j=1}^n \frac{1}{n^2} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{2\bar{x}}{n} \sum_{j=1}^n \frac{(x_j - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)
\end{aligned}$$

$$= \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right).$$

协方差：

由于 $y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$, 故对于统计量 \bar{y} 有：

$$Var(\bar{y}) = Var(\hat{\beta}_0 + \hat{\beta}_1 \bar{x}) = Var(\hat{\beta}_0) + \bar{x}^2 Var(\hat{\beta}_1) + 2\bar{x}Cov(\hat{\beta}_1, \hat{\beta}_0)$$

$$\Rightarrow \frac{\sigma^2}{n} = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) + \frac{\bar{x}^2 \sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2} + 2\bar{x}Cov(\hat{\beta}_1, \hat{\beta}_0)$$

$$\Rightarrow Cov(\hat{\beta}_1, \hat{\beta}_0) = - \frac{\bar{x} \sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

$$\Rightarrow Cov(\hat{\beta}_1, \hat{\beta}_0) = - \frac{\bar{x} \sigma^2}{L_{xx}}$$

由于 $\hat{\beta}_0$ 和 $\hat{\beta}_1$ 都是 y_i 的线性组合，且 y_i 间独立同分布，故 $\hat{\beta}_0$ 和 $\hat{\beta}_1$ 也服从正态分布，即：

$$\hat{\beta}_0 \sim N\left(\beta_0, \left(\frac{1}{n} + \frac{\bar{x}^2}{L_{xx}}\right)\sigma^2\right)$$

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{L_{xx}}\right)$$