最小二乘法应用在一元线性回归任务中时，最优化问题为

$$\min \sum_{i=1}^{n}(y_i - \hat{y})^2$$

又 $\hat{y} = b_0 + b_1 x_i$ ，即问题为

$$\min \sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2$$

记 $f = \sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2$，则

$$\begin{aligned}\frac{\partial f}{\partial b_0} &= \sum_{i=1}^{n} -2(y_i - b_0 - b_1 x_i) \\ &= -2(\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} b_0 - \sum_{i=1}^{n} b_1 x_i) \\ &= 2(nb_0 - \sum_{i=1}^{n} y_i + \sum_{i=1}^{n} b_1 x_i)\end{aligned}$$

令 $\frac{\partial f}{\partial b_0} = 0$得

$$b_0 = \frac{\sum_{i=1}^{n} y_i - b_1 x_i}{n} = \bar{y} - b_1 \bar{x}$$

将其代入f得

$$\begin{aligned}f &= \sum_{i=1}^{n}(y_i - \bar{y} + b_1 \bar{x} - b_1 x_i)^2 \\ &= \sum_{i=1}^{n}(y_i - \bar{y} + b_1(\bar{x} - x_i))^2\end{aligned}$$

则得

$$\begin{aligned}\frac{\partial f}{\partial b_1} &= \sum_{i=1}^{n} 2(y_i - \bar{y} + b_1(\bar{x} - x_i))(\bar{x} - x_i) \\ &= 2\sum_{i=1}^{n}(y_i - \bar{y})(\bar{x} - x_i) + b_1(\bar{x} - x_i)^2\end{aligned}$$

令 $\frac{\partial f}{\partial b_1} = 0$ 得

$$\begin{aligned}\sum_{i=1}^{n} b_1(\bar{x} - x_i)^2 &= \sum_{i=1}^{n}(y_i - \bar{y})(x_i - \bar{x}) \\ b_1 &= \frac{\sum_{i=1}^{n}(y_i - \bar{y})(x_i - \bar{x})}{\sum_{i=1}^{n}(\bar{x} - x_i)^2}\end{aligned}$$