

Simple Linear Regression

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1 Recall

- MLE (Maximum Likelihood Estimation): Given independent and identically distributed (i.i.d.) samples X_1, X_2, \dots, X_n from a distribution with parameter θ , the MLE of θ is $\hat{\theta}_n = \arg \max_{\theta} \prod_{i=1}^n f_{\theta}(X_i)$. Under regular conditions, $\hat{\theta}_n$ converges in probability to θ^* (WLLN) and converges in distribution to $N(\theta^*, I^{-1}(\theta^*))$ (CLT).
- Score function: $s_{\theta}(x) = \nabla \log f_{\theta}(x)$.
- Fisher Information:
 1. $I(\theta) = \mathbb{V}(s_{\theta}(X))$.
 2. $I_n(\theta) = \mathbb{V}(\nabla \ell_n(\theta))$.
- Properties:
 1. $I_n(\theta) = \sum_{i=1}^n \mathbb{V}(s_{\theta}(X_i)) = nI(\theta)$.
 2. $\mathbb{E}[s_{\theta}(X)] = 0$.
 3. $I(\theta) = -\mathbb{E}[\nabla^2 \log f_{\theta}(X)]$.
 4. Combining 1 and 3, $I_n(\theta) = -\mathbb{E}[\nabla^2 \ell_n(\theta)]$.
- Theorem: $\frac{\hat{\theta}_n - \theta^*}{\hat{s}e} \xrightarrow{d} N(0, 1)$, where $\hat{s}e = \frac{1}{\sqrt{I_n(\hat{\theta}_n)}}$.
- Example: Bernoulli distribution $Ber(p)$.
 - $\hat{p}_n = \bar{X}_n$.
 - $f_p(x) = p^x(1-p)^{1-x}$.
 - $s_p(x) = \nabla \log f_p(x) = \frac{x}{p} - \frac{1-x}{1-p}$.
 - $I(p) = -\mathbb{E}[s'_p(X)] = \frac{1}{p(1-p)}$.
 - $\frac{\hat{p}_n - p}{\hat{s}e} \xrightarrow{d} N(0, 1)$, where $\hat{s}e = \frac{1}{\sqrt{nI(\hat{p}_n)}} = \sqrt{\frac{\hat{p}_n(1-\hat{p}_n)}{n}}$.

2 Hypothesis Testing

- Example: A/B Testing
 - CTR (Click-Through Rate): $R_A = 7.3\%$, $R_B = 7.29\%$.
 - Hypotheses:
 - * $H_0 : R_A = R_B$.
 - * $H_1 : R_A \neq R_B$.
 - Test Statistic: $T(X) = |R_A - R_B|$.
 - Rejection Region: $T(X) \in C_n = \{T(X) > c\}$.
 - Confidence Interval: $C_n = [\hat{\theta}_n - z_{\frac{\alpha}{2}} \hat{se}, \hat{\theta}_n + z_{\frac{\alpha}{2}} \hat{se}]$ is an approximate $1 - \alpha$ confidence interval.
 - $P(\theta^* \in C_n) \rightarrow 1 - \alpha$.

3 Simple Linear Regression

Regression is a method for studying the relationship between a response variable Y and a covariate X . One way to summarize the relationship between X and Y is through the regression function.

The simplest version of regression is Simple Linear Regression when X_i is simple (one-dimensional) and $r(x)$ is assumed to be linear.

Data: $\{(x_i, y_i)\}_{i=1}^n$ i.i.d. from $F_{X,Y}$.

Model: $Y = r(X) + \varepsilon$ (prediction).

Variables:

- X : covariance, feature, independent variable.
- Y : response, dependent variable.

MSE (Mean Squared Error): $\min_r \mathbb{E}[(Y - r(X))^2]$.

$$\mathbb{E}[(Y - r(X))^2] = \mathbb{E}[(Y - \mathbb{E}[Y|X])^2 + \mathbb{E}[Y|X]^2 - r(X)]^2 \quad (1)$$

$$= \mathbb{E}[(Y - \mathbb{E}[Y|X])^2] + \mathbb{E}[\mathbb{E}[Y|X] - r(X)]^2 + 2\mathbb{E}[(Y - \mathbb{E}[Y|X])^2 \mathbb{E}[Y|X] - r(X)]^2 \quad (2)$$

$$= \mathbb{E}[(Y - \mathbb{E}[Y|X])^2] + \mathbb{E}[\mathbb{E}[Y|X] - r(X)]^2, \quad (3)$$

where $2\mathbb{E}[(Y - \mathbb{E}[Y|X])^2 \mathbb{E}[Y|X] - r(X)]^2 = 0$. (the process of proof is omitted.)

Since the quantity $\mathbb{E}[(Y - \mathbb{E}[Y|X])^2]$ is independent of the regression function $r(x)$, the minimum value of the expected squared loss $\mathbb{E}[(Y - r(X))^2]$ is attained *if and only if* $r(X) = \mathbb{E}[Y|X]$.

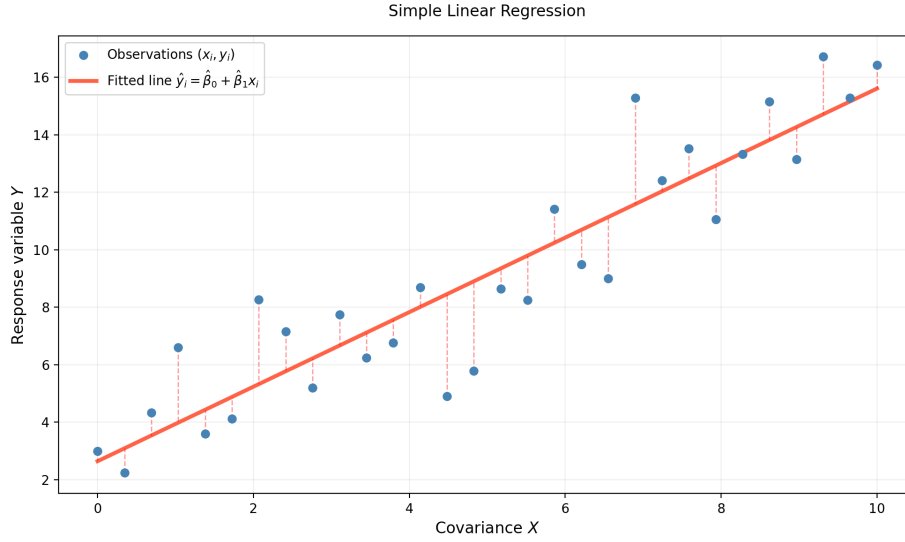


图 1: an Example of SLR

Consequently, the optimal regression function reduces to $r^*(x) = \mathbb{E}[Y|X = x]$, indicating that the functional relationship is fully characterized by the conditional expectation.

Regression Function: $r^*(x) = \mathbb{E}[Y|X = x]$.

Simple Linear Regression:

def: $r(x) \triangleq \beta_0 + \beta_1 x$,

$$Y = r(x) + \epsilon = \beta_0 + \beta_1 X + \epsilon.$$

where $\mathbb{E}[\epsilon_i|X_i] = 0$, $\mathbb{V}(\epsilon_i|X_i) = \sigma^2$.

I'd like to show a figure to make it clear:

Data Generating Process: $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$, $\epsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$.

Estimated Regression Function: $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$.

To find the $\hat{\beta}_0$ and $\hat{\beta}_1$, we need the method OLS.

OLS(Ordinary Least Squares):

$$\hat{\beta}_{\text{OLS}} = \arg \min_{\beta} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2.$$

LAD(the Least Absolute Deviations):

$$\hat{\beta}_{\text{LAD}} = \arg \min_{\beta} \sum_{i=1}^n |y_i - \beta_0 - \beta_1 x_i|.$$

we always prefer LS to LAD because LS is more convenient.

Derivation of Ordinary Least Squares Estimators

First-Order Conditions

$$\begin{aligned}\frac{\partial S}{\partial \beta_0} &= -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i) = 0 \quad \Rightarrow \quad \sum_{i=1}^n y_i = n\beta_0 + \beta_1 \sum_{i=1}^n x_i, \\ \frac{\partial S}{\partial \beta_1} &= -2 \sum_{i=1}^n x_i (y_i - \beta_0 - \beta_1 x_i) = 0 \quad \Rightarrow \quad \sum_{i=1}^n x_i y_i = \beta_0 \sum_{i=1}^n x_i + \beta_1 \sum_{i=1}^n x_i^2.\end{aligned}$$

Solving the Normal Equations:

From the first equation:

$$\bar{y} = \beta_0 + \beta_1 \bar{x}_n \quad \Rightarrow \quad \beta_0 = \bar{y} - \beta_1 \bar{x}_n.$$

Substitute β_0 into the second equation and simplify:

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

The ordinary least squares (OLS) slope estimator is derived from the following sample moments:

$$S_{xx} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x}_n)^2 \quad (\text{Sample variance of } X).$$

$$S_{xy} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x}_n)(y_i - \bar{y}_n) \quad (\text{Sample covariance}).$$

Consequently, the OLS estimator for the slope parameter is:

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}}.$$

Final Estimators:

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}}, \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}_n.$$

Theorem 1 *We have:*

$$\mathbb{E}(\hat{\beta}_0) = \beta_0,$$

$$\mathbb{E}(\hat{\beta}_1) = \beta_1,$$

$$\mathbb{V}(\hat{\beta}_0) = \left(\frac{1}{n} + \frac{\bar{x}_n^2}{nS_{xx}} \right) \sigma^2,$$

$$\mathbb{V}(\hat{\beta}_1) = \frac{\sigma^2}{nS_{xx}}.$$

Proof 1 •

$$\mathbb{E}(\hat{\beta}_0) = \mathbb{E}\left[\frac{S_{xy}}{S_{xx}}\right] = \frac{\mathbb{E}[S_{xy}]}{S_{xx}}.$$

$$\begin{aligned}\mathbb{E}[S_{xy}] &= \frac{1}{n}\mathbb{E}\left[\sum_i (x_i - \bar{x}_n)(y_i - \bar{y}_n)\right] \\ &= \frac{1}{n}\mathbb{E}\left[\sum_i (x_i - \bar{x}_n)y_i\right] \text{ (where } \sum_i (x_i - \bar{x}_n)\bar{y}_n = 0) \\ &= \frac{1}{n}\sum_i (x_i - \bar{x}_n)\mathbb{E}(y_i) \\ &= \frac{1}{n}\sum_i (x_i - \bar{x}_n)(\beta_0 + \beta_1 x_i) \\ &= \frac{\beta_1}{n}\sum_i (x_i - \bar{x}_n)x_i \text{ (where } \sum_i (x_i - \bar{x}_n)\beta_0 = 0) \\ &= \frac{\beta_1}{n}\sum_i (x_i - \bar{x}_n)(x_i - \bar{x}_n) \text{ (where } \sum_i (x_i - \bar{x}_n)\bar{x}_n = 0) \\ &= \beta_1 S_{xx}.\end{aligned}$$

Consequently,

$$\mathbb{E}(\hat{\beta}_1) = \frac{\mathbb{E}[S_{xy}]}{S_{xx}} = \frac{\beta_1 S_{xx}}{S_{xx}} = \beta_1.$$

•

$$\begin{aligned}\mathbb{V}(\hat{\beta}_1) &= \frac{\mathbb{V}(S_{xy})}{S_{xx}^2} \\ &= \frac{\sum_i (x_i - \bar{x}_n)^2 \mathbb{V}(y_i)}{n^2 S_{xx}^2} \\ &= \frac{\sigma^2 \sum_i (x_i - \bar{x}_n)^2}{n^2 S_{xx}^2} \\ &= \frac{\sigma^2}{n S_{xx}}.\end{aligned}$$

•

$$\begin{aligned}\mathbb{E}(\hat{\beta}_0) &= \mathbb{E}[\bar{y}_n - \hat{\beta}_1 \bar{x}_n] = \mathbb{E}[\bar{y}_n] - \bar{x}_n \mathbb{E}(\hat{\beta}_1) \\ &= \beta_1 \bar{x}_n + \beta_0 - \beta_1 \bar{x}_n \\ &= \beta_0.\end{aligned}$$

•

$$\begin{aligned}\mathbb{V}(\hat{\beta}_0) &= \mathbb{V}(\bar{y}_n - \beta_1 \bar{x}_n) \\ &= \mathbb{V}(\bar{y}_n) + \bar{x}_n^2 \mathbb{V}(\hat{\beta}_1) \text{ (where } 2\text{Cov}(\bar{y}_n, \beta_1 \bar{x}_n) = 0) \\ &= \frac{\sigma^2}{n} + \bar{x}_n^2 \frac{\sigma^2}{n S_{xx}}.\end{aligned}$$

The Proof process of $Cov(\bar{y}_n, \beta_1 \bar{x}_n) = 0$:

$$\begin{aligned}
Cov(\bar{y}_n, \beta_1 \bar{x}_n) &= Cov\left(\frac{1}{n} \sum_i y_i, \frac{1}{n} \sum_i (x_i - \bar{x}_n) y_i\right) \\
&= \frac{1}{n^2} Cov\left(\sum_i y_i, \sum_i (x_i - \bar{x}_n) y_i\right) \\
&= \sum_i \sum_j (x_i - \bar{x}_n) Cov(y_i, y_j) \\
&= \frac{1}{n^2} \sum_i (x_i - \bar{x}_n) \sigma^2 \\
&= 0.
\end{aligned}$$

Supplement: Inference of the noise $\hat{\sigma}^2$

$$\hat{\epsilon}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i (i = 1, 2, \dots, n).$$

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (\hat{\epsilon}_i - \bar{\epsilon}_n)^2.$$

Theorem 2 $\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{y}_i)^2$, $\mathbb{E}(\hat{\sigma}^2) = \sigma^2$.