

Simple Linear Regression

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Assumption

1. Uncorrelated/independent
2. Common variance σ^2 , $\text{Var}(Y_i) = \sigma^2$
3. Linear, $\mathbb{E}(Y_i|x_i) = \beta_0 + \beta_1 x_i$

Least Squares Estimation

$$Q = \sum_{i=1}^n \{y_i - E(Y_i|x_i)\}^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

$$\frac{\partial Q}{\partial \beta_0} = 0 \Rightarrow \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\frac{\partial Q}{\partial \beta_1} = 0 \Rightarrow \hat{\beta}_1 = \frac{S_{XY}}{S_{XX}}$$

$$S_{XX} = \sum_{i=1}^n (x_i - \bar{x})^2$$

$$S_{XY} = \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) = \sum_{i=1}^n (x_i - \bar{x})\bar{y}$$

$$S_{YY} = \sum_{i=1}^n (y_i - \bar{y})^2$$

$\hat{\beta}_0$ and $\hat{\beta}_1$ are expressed as a function of the random variables Y_i instead of the observed data y_i

Properties

$\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased and consistent estimators of β_0 and β_1 , respectively

$$\mathbb{E}(\hat{Y}_i) = \beta_0 + \beta_1 \bar{x}$$

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

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

$$\text{Var}(\hat{\beta}_1) = \frac{\sigma^2}{S_{XX}}$$

$$\text{Var}(\hat{\beta}_0) = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{XX}} \right)$$

$$\begin{aligned} \text{cov}(\hat{\beta}_0, \hat{\beta}_1) &= \text{cov} \left(\sum \left(\frac{1}{n} - \frac{\bar{x}(x_i - \bar{x})}{S_{XX}} \right) Y_i, \sum \frac{x_i - \bar{x}}{S_{XX}} Y_i \right) \\ &= \sum \left(\frac{1}{n} - \frac{\bar{x}(x_i - \bar{x})}{S_{XX}} \right) \left(\frac{x_i - \bar{x}}{S_{XX}} \right) \text{Var}(Y_i) = -\frac{\bar{x}}{S_{XX}} \sigma^2 \end{aligned}$$

$$\text{cov}(\bar{Y}, \hat{\beta}_1) = \text{cov} \left(\sum \frac{1}{n} Y_i, \sum \frac{x_i - \bar{x}}{S_{XX}} Y_i \right) = 0$$

$$\text{s.e.}(\hat{\beta}_1) = \sqrt{\text{Var}(\hat{\beta}_1)} = \sqrt{\frac{\hat{\sigma}^2}{S_{XX}}}$$

$$\text{s.e.}(\hat{\beta}_0) = \sqrt{\text{Var}(\hat{\beta}_0)} = \sqrt{\hat{\sigma}^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{XX}} \right)}$$

estimate

Residual and Regression Sums of Squares

$$e_i = y_i - \hat{y}_i = (y_i - \bar{y}) - \hat{\beta}_1(x_i - \bar{x})$$

$$\text{RSS} = \sum e_i^2 = S_{YY} - \frac{S_{XY}^2}{S_{XX}} = S_{YY} - \text{regressionSS} = \text{totalSS} - \text{regressionSS}$$

$$\mathbb{E}(\text{RSS}) = (n-2)\sigma^2$$

$$\hat{\sigma}^2 = s^2 = \frac{1}{n-2} \text{RSS} = \frac{\text{RSS}}{\text{DF}} = \text{residualMeanSquare}$$

$$Q = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 = S_{XX} \left(\beta_1 - \frac{S_{XY}}{S_{XX}} \right)^2 + n(\beta_0 - \bar{y} - \beta_1 \bar{x})^2 + S_{YY} - \frac{S_{XY}^2}{S_{XX}}$$

Coefficient of determination (Multiple R-Squared)

$$R^2 = \frac{\text{regressionSS}}{\text{totalSS}} = \frac{S_{XY}^2/S_{XX}}{S_{YY}} = \frac{S_{XY}^2}{S_{XX}S_{YY}}$$

Alternative Formulation

$$\mathbb{E}(Y_i|x_i) = \gamma + \beta_1(x_i - \bar{x})$$

So that γ is the expected response at $x = \bar{x}$, rather than at $x = 0$.

$$\text{Least Squares Estimation, } \hat{\gamma} = \bar{y}, \hat{\beta}_1 = \frac{S_{XY}}{S_{XX}}$$

$$\text{Var}(\hat{\gamma}) = \frac{\sigma^2}{n}, \text{cov}(\hat{\gamma}, \hat{\beta}_1) = 0$$

$$\text{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_*) = \text{Var}(\hat{\gamma} + \hat{\beta}_1(x_* - \bar{x})) = \sigma^2 \left(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{XX}} \right)$$

Inference: Confidence Interval (Expected Response)

$$\mathbb{E}(Y|x_*) = \beta_0 + \beta_1 x_*$$

$$\hat{\mathbb{E}}(Y|x_*) = \hat{\beta}_0 + \hat{\beta}_1 x_* = \bar{y} + \hat{\beta}_1(x_* - \bar{x})$$

Using $\hat{\beta}_1$ or properties of variance,

$$\text{Var}(\hat{\mathbb{E}}(Y|x_*)) = \sigma^2 \left(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{XX}} \right)$$

$$T \sim t_{n-2}$$

Inference: Prediction Interval (Future Response)

$$Y_* = \beta_0 + \beta_1 x_* + \varepsilon, \text{ where } \varepsilon \sim N(0, \sigma^2)$$

$$\text{Var}(Y_*) = \sigma^2 \left(1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{XX}} \right)$$

$$T \sim t_{n-2}$$

Inference (When Normal Distributed)

$$\hat{\beta}_1 \sim N \left(\beta_1, \frac{\sigma^2}{S_{XX}} \right) \xrightarrow{\frac{\hat{\beta}_1 - \beta_1}{\sqrt{\sigma^2/S_{XX}}}} \frac{\hat{\beta}_1 - \beta_1}{\sqrt{\sigma^2/S_{XX}}} \sim N(0,1)$$

$$\frac{\hat{\beta}_1 - \beta_1}{\sqrt{\hat{\sigma}^2/S_{XX}}} \sim t_{n-2}$$

ANOVA

SOURCE	DF	SS	MS	F	P
Regression	1	$\frac{S_{XY}^2}{S_{XX}}$	$\frac{S_{XY}^2}{S_{XX}}$	$\frac{S_{XY}^2}{S_{XX}\hat{\sigma}^2}$	
Residual	n - 2	$S_{YY} - \frac{S_{XY}^2}{S_{XX}}$	$\hat{\sigma}^2$		
Total	n - 1	S_{YY}			

$$\text{MS} = \frac{\text{SS}}{\text{DF}}$$

$$F = \frac{\text{regressionMS}}{\text{residualMS}} = \frac{\text{regressionSS}}{1} / \frac{\text{residualSS}}{n-2} \sim F_{1,n-2}$$

F can be used to test whether the expected response depends on the explanatory variable.

Inference (when Normal distributed)

$$\begin{aligned}\widehat{\beta}_1 &\sim N\left(\beta_1, \frac{\sigma^2}{S_{XX}}\right) \longrightarrow \frac{\widehat{\beta}_1 - \beta_1}{\sqrt{\sigma^2/S_{XX}}} \sim N(0,1) \longrightarrow \frac{\widehat{\beta}_1 - \beta_1}{\sqrt{\hat{\sigma}^2/S_{XX}}} \sim t_{n-2} \\ \widehat{\beta}_0 &\sim N\left(\beta_0, \sigma^2 \left(\frac{1}{n} + \bar{x}^2\right)\right) \longrightarrow \frac{\widehat{\beta}_0 - \beta_0}{\sqrt{\sigma^2 \left(\frac{1}{n} + \bar{x}^2\right)}} \sim N(0,1) \longrightarrow \frac{\widehat{\beta}_0 - \beta_0}{\sqrt{\hat{\sigma}^2 \left(\frac{1}{n} + \bar{x}^2\right)}} \sim t_{n-2} \\ \bar{Y} &\sim N\left(\beta_0 + \beta_1 \bar{x}, \frac{\sigma^2}{n}\right), \text{ independently of } \widehat{\beta}_1 \\ \frac{RSS}{\sigma^2} &= \frac{(n-2)\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-2}^2, \text{ independently of } \widehat{\beta}_1 \text{ and } \bar{Y}\end{aligned}$$

$$\begin{cases} Z \sim N(0,1) \\ Y \sim \chi_n^2 \end{cases} \rightarrow T = \frac{Z}{\sqrt{Y/n}} \sim t_n$$

$$T = \frac{\widehat{\beta}_1 - \beta_1}{\sqrt{\hat{\sigma}^2/S_{XX}}} = \frac{\frac{\widehat{\beta}_1 - \beta_1}{\sqrt{\sigma^2/S_{XX}}}}{\sqrt{\frac{(n-2)\hat{\sigma}^2}{\sigma^2}/(n-2)}} = \frac{Z}{\sqrt{Y/(n-2)}} \sim t_{n-2}$$

Leverage

$$\begin{aligned}\hat{y}_i &= \widehat{\beta}_0 + \widehat{\beta}_1 x_i = \bar{y} + \widehat{\beta}_1(x_i - \bar{x}) = \bar{y} + (x_i - \bar{x}) \sum_{j=1}^n \frac{(x_j - \bar{x})y_j}{S_{XX}} \\ &= \sum_{j=1}^n \left(\frac{1}{n} + \frac{(x_i - \bar{x})(x_j - \bar{x})}{S_{XX}} \right) y_j = \sum_{j=1}^n a_{ij} y_j\end{aligned}$$

Influence Matrix: $A = \{a_{ij}\}$

Leverage is A_{ii} , a measure of how much that particular data point influences its own fitted value. (*potential*)

Large Residual + High Leverage = Strong Influence

Small Residual + High Leverage = not too great influence (while inconsistent)

Large Residual + Low Leverage = not much effect on the fit

Cook's distance

$$d_i = \frac{1}{3\hat{\sigma}^2} \sum_{j=1}^n (\widehat{y}_{j(i)} - \widehat{y}_j)^2$$

$\widehat{y}_{j(i)}$ is the i 'th fitted value obtained when the j 'th point is excluded when computing the regression model.

$3 = p + 1$, where p is the number of unknown parameters.

Cook's distance measures the influence that each data point is *in fact* exerting on the fit.

Large Cook's Distance = potential outliers

variable.

Analysis of Residuals

$$\varepsilon_i = Y_i - \mathbb{E}(Y_i|x_i) = Y_i - \beta_0 - \beta_1 x_i$$

Assumptions (derive from original assumptions):

1. Uncorrelated/independent, $\text{cov}(\varepsilon_i, \varepsilon_j|x) = 0$
2. Common variance σ^2 , $\text{Var}(\varepsilon_i|x) = \sigma^2$
3. $\mathbb{E}(\varepsilon_i|x) = 0$
4. If Y_i is Normal, $\varepsilon_i \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$

Estimate ε_i ,

$$e_i = y_i - \widehat{\beta}_0 - \widehat{\beta}_1 x_i = y_i - \bar{y} - \widehat{\beta}_1(x_i - \bar{x})$$

$$p_{ij} = \frac{1}{n} + \frac{(x_i - \bar{x})(x_j - \bar{x})}{S_{XX}}$$

Then, (corresponding random variable)

$$\text{cov}(E_j, E_i|x) = -p_{ij}\sigma^2$$

$$\text{Var}(E_i|x) = (1 - p_{ii})\sigma^2 = \left(1 - \frac{1}{n} - \frac{(x_i - \bar{x})^2}{S_{XX}}\right)\sigma^2$$

$$\mathbb{E}(E_i|x) = 0$$

If Y_i are Normal, so are the E_i .

If n is large and none of the quantities $|x_i - \bar{x}|$ is large then the p_{ij} are small.

Standardized Residuals

$$r_i = \frac{e_i}{\text{estimated standard error of } E_i} = \frac{e_i}{\sqrt{\hat{\sigma}^2 \left(1 - \frac{1}{n} - \frac{(x_i - \bar{x})^2}{S_{XX}}\right)}}$$

- i. Plot r_i against x_i , look for sign that $\mathbb{E}(R_i|x_i)$, $\text{Var}(R_i|x_i)$ depends on x_i
- ii. See if any unusually large values, $|r_i| > 2.5, > 3$
- iii. Plot Normal probability of r_i

Multiple Regression

1. $\mathbb{E}(\mathbf{Y}|\mathbf{X}) = \mathbf{X}\beta$, $\text{Var}(\mathbf{Y}|\mathbf{X}) = \sigma^2 \mathbf{I}_n$

Specially, in simple linear regression, $y_i = \beta_0 + \beta_1 x_i$,

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \mathbb{E}(\mathbf{Y}|\mathbf{X}) = \mathbf{1}_n \beta_0 + \mathbf{x} \beta_1, \text{Var}(\mathbf{Y}|\mathbf{X}) = \sigma^2 \mathbf{I}_n$$

2. Least squares estimation: $Q = \sum_{i=1}^n \{y_i - \mathbb{E}(Y_i|\mathbf{X})\}^2 = \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\beta + \beta^T \mathbf{X}^T \mathbf{X} \beta$

Least squares *unbiased* estimator: $\hat{\beta} = (\mathbf{X}\mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$

$$\mathbb{E}(\hat{\beta}|\mathbf{X}) = \beta, \text{Var}(\hat{\beta}|\mathbf{X}) = \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}, \text{Var}(\mathbf{c}^T \hat{\beta}|\mathbf{X}) = \sigma^2 \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{c}$$

3. Vector of residuals: $\mathbf{e} = \mathbf{y} - \mathbf{X}\hat{\beta} = (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbf{y}$,

where $\mathbf{P}_\mathbf{X} = \mathbf{X}(\mathbf{X}\mathbf{X})^{-1} \mathbf{X}^T$ is $n \times n$, symmetric, idempotent, rank p ,

$$(\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbf{X} = \mathbf{0}, (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbf{P}_\mathbf{X} = \mathbf{0}$$

$$\mathbb{E}(\mathbf{e}|\mathbf{X}) = (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbb{E}(\mathbf{Y}|\mathbf{X}) = (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\mathbf{X}\beta = \mathbf{0}$$

$$\text{Var}(\mathbf{e}|\mathbf{X}) = (\mathbf{I}_n - \mathbf{P}_\mathbf{X})\sigma^2 \mathbf{I}_n (\mathbf{I}_n - \mathbf{P}_\mathbf{X}) = \sigma^2 (\mathbf{I}_n - \mathbf{P}_\mathbf{X})$$

$$\text{RSS} = \mathbf{e}^T \mathbf{e} = \mathbf{y}^T \mathbf{y} - \hat{\beta}^T \mathbf{X}^T \mathbf{y}, \hat{\sigma}^2 = \frac{\text{RSS}}{n-p} = \frac{\mathbf{y}^T \mathbf{y} - \hat{\beta}^T \mathbf{X}^T \mathbf{y}}{n-p}$$

4. Alternative formulation (for models with an intercept)

$$\mathbb{E}(Y_i|\mathbf{X}) = \gamma + \beta_1(x_{i1} - \bar{x}_1) + \beta_2(x_{i2} - \bar{x}_2) + \cdots + \beta_q(x_{iq} - \bar{x}_q)$$

$$\mathbb{E}(\mathbf{Y}|\mathbf{X}) = \gamma \mathbf{1}_n + \dot{\mathbf{X}} \dot{\beta}, \text{ where } \dot{\mathbf{X}}_{ij} = x_{ij} - \bar{x}_j, \dot{\beta} = (\beta_1 \cdots \beta_q)^T, \gamma = \beta_0 + \beta_1 \bar{x}_1 + \cdots + \beta_q \bar{x}_q$$

Least squares *unbiased* estimators: $\hat{\gamma} = \bar{y}$, $\hat{\beta} = (\dot{\mathbf{X}}^T \dot{\mathbf{X}})^{-1} \dot{\mathbf{X}}^T \mathbf{y}$

$$\text{Var}(\hat{\beta}|\mathbf{X}) = \sigma^2 (\dot{\mathbf{X}}^T \dot{\mathbf{X}})^{-1}, \text{Var}(\hat{\gamma}|\mathbf{X}) = n^{-1} \sigma^2, \text{cov}(\hat{\beta}, \hat{\gamma}|\mathbf{X}) = \mathbf{0}$$

5. Distributional results:

- $\hat{\beta} \sim N(\beta, \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1})$
- regression (model) SS $\mathbf{Y}^T \mathbf{P}_\mathbf{X} \mathbf{Y} \sim \sigma^2 \chi^2(q, \sigma^{-2} \dot{\beta}^T \dot{\mathbf{X}}^T \dot{\mathbf{X}} \dot{\beta})$
- RSS $\mathbf{Y}^T (\mathbf{I}_n - \mathbf{P}_\mathbf{X}) \mathbf{Y} \sim \sigma^2 \chi^2(n - q - 1, 0)$
- RSS and regression SS are independent
- $\frac{\mathbf{c}^T \hat{\beta} - \mathbf{c}^T \beta}{\sigma \sqrt{\mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{c}}} \sim N(0, 1)$ and $\frac{\mathbf{c}^T \hat{\beta} - \mathbf{c}^T \beta}{\hat{\sigma} \sqrt{\mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{c}}} \sim t(n-p)$ (test hypotheses about linear funcs of the parameters)

6. 95% Confidence interval: $\mathbf{c}^T \hat{\beta} \pm t_{0.025} \hat{\sigma} \sqrt{\mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{c}}$

$$\text{CI for future response: } \mathbf{x}_*^T \hat{\beta} \pm t_{0.025} \hat{\sigma} \sqrt{\mathbf{x}_*^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_*}$$

$$\text{Prediction interval: } \mathbf{x}_*^T \hat{\beta} \pm t_{0.025} \hat{\sigma} \sqrt{1 + \mathbf{x}_*^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_*}$$

7. To test $\beta = \mathbf{0}$,

$$F = \frac{\text{regression SS}}{\text{RSS}} \sim F(p, n-p) \text{ (chk simple linear regression, but with different SS)}$$

8. To test a more general linear hypothesis about the coefficients of the model, $\mathbf{C}\beta = \mathbf{d}$,

$$\text{Extra SS} = (\mathbf{C}\hat{\beta} - \mathbf{d})^T (\mathbf{C}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{C}^T)^{-1} (\mathbf{C}\hat{\beta} - \mathbf{d})$$

$$F = \frac{(\text{ESS for } H_0)/c}{\text{RMS}} = \frac{(\text{RSS under } H_0 - \text{RSS under full model})/c}{\text{RMS}} \sim F(k, n-p)$$