

Simple Linear Regression

Parameters

The simple model is

$$y_i = \beta_0 + \beta_1 x_i$$

with $E(y_i) = \beta_0 + \beta_1 x_i$, $\text{Var}(y_i) = \text{Var}(\beta_0 + \beta_1 x_i + \epsilon) = \sigma^2$

Estimates for β_0, β_1

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x}) y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \sum_{i=1}^n k_i y_i = \frac{S_{xy}}{S_{xx}}$$

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

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

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

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

$$\text{Var}(\hat{\beta}_1) = \sigma^2 \sum_{i=1}^n k_i^2$$

Estimation on σ^2

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

SSE has $n - 2$ degrees of freedom.

$$\hat{\sigma}^2 = \frac{SSE}{n - 2} = MSR$$

Hypothesis Testing on the Parameters

Testing on the slope for a constant β

$$H_0 : \hat{\beta}_1 = \beta, H_1 : \hat{\beta}_1 \neq \beta$$

If σ^2 is known,

$$Z_0 = \frac{\hat{\beta}_1 - \beta}{\sqrt{\sigma^2 / S_{xx}}}$$

If σ^2 is unknown,

$$t_0 = \frac{\hat{\beta}_1 - \beta}{\sqrt{MSE / S_{xx}}}$$

We reject the null hypothesis $|t_0| > t_{\alpha/2, n-2}$. We test the intercept similarly,

$$H_0 : \beta_0 = \beta, H_1 : \beta_0 \neq \beta$$

$$t_0 = \frac{\hat{\beta}_0 - \beta}{se(\hat{\beta}_0)}$$

where $se^2(\hat{\beta}_1) = \frac{MSE}{S_{xx}}$, $se^2(\hat{\beta}_0) = MSE(1/n + \bar{X}^2 / S_{xx})$

Significance of Regression

We test significance with

$$H_0 : \beta_1 = 0, H_1 : \beta_1 \neq 0$$

Using the same statistic, $|t_0| > t_{\alpha/2, n-2}$.

Source	SS	DF
Regression	$SSR = \hat{\beta}_1^2 \sum (X_i - \bar{X})^2$	$p - 1$
Error	$SSE = \sum (Y_i - \hat{Y}_i)^2$	$n - p$
Total	$SSTO = \sum (Y_i - \bar{Y})^2$	$n - 1$

MS=SS/df	E(MS)	F
MSR	$\sigma^2 + \beta_1^2 \sum (X_i - \bar{X})^2$	MSR/MSE
MSE	σ^2	

Confidence Intervals

The confidence interval on the slope β_1 ,

$$\hat{\beta}_1 - t_{\alpha/2, n-2} se(\hat{\beta}_1) \leq \beta_1 \leq \hat{\beta}_1 + t_{\alpha/2, n-2} se(\hat{\beta}_1)$$

For the intercept β_0 ,

$$\hat{\beta}_0 - t_{\alpha/2, n-2} se(\hat{\beta}_0) \leq \beta_0 \leq \hat{\beta}_0 + t_{\alpha/2, n-2} se(\hat{\beta}_0)$$

$$\text{For } \sigma^2, \quad \frac{(n-2)MSE}{\chi_{\alpha/2, n-2}^2} \leq \sigma^2 \leq \frac{(n-2)MSE}{\chi_{1-\alpha/2, n-2}^2}$$

Interval Estimation on Mean Response

An unbiased estimator for $E(y|x_0)$ for a value of regressor $x = x_0$ is

$$E(\hat{y}|x_0) = \hat{\mu}_{y|x_0} = \hat{\beta}_0 + \hat{\beta}_1 x_0$$

The variance is

$$\text{Var}(\hat{\mu}_{y|x_0}) = \frac{\sigma^2}{n} + \frac{\sigma^2(x_0 - \bar{x})^2}{S_{xx}}$$

The sampling distribution for

$$\frac{\hat{\mu}_{y|x_0} - E(y|x_0)}{\sqrt{MSE(1/n + (x_0 - \bar{x})^2 / S_{xx})}} \sim t_{n-2}$$

So the confidence interval is then

$$\left[\hat{\mu}_{y|x_0} \pm t_{\alpha/2, n-2} \sqrt{MSE \left(\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)} \right]$$

Correlation

The coefficient of determination is

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

The adjusted R^2 value is

$$R_{Adj}^2 = 1 - \frac{SSE/(n - k - 1)}{SST/(n - 1)}$$

The pearson correlation coefficient is

$$\rho = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}}$$

When applied to a sample,

$$r = b_1 \left(\frac{S_{xx}}{SST} \right)^{\frac{1}{2}} = \frac{S_{xy}}{(S_{xx} SST)^{1/2}}$$

If we want to test $H_0 : \rho = 0$, $H_1 : \rho \neq 0$, use the t statistic,

$$t = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} \sim t_{n-2}$$

We reject the null hypothesis $H_0 : \rho = 0$ if $|t_0| > t_{\alpha/2, n-2}$. To test $\rho = \rho_0$,

$$H_0 : \rho = \rho_0, H_1 : \rho \neq \rho_0$$

Use the standardized test statistic

$$Z_0 = (\text{arctanh}(r) - \text{arctanh}(\rho_0))\sqrt{n-3}$$

We can obtain our confidence interval with

$$\left[\tanh \left(\text{arctanh}(r) \pm \frac{Z_{\alpha/2}}{\sqrt{n-3}} \right) \right]$$

where $\tanh(u) = (e^u - e^{-u}) / (e^u + e^{-u})$. We reject $H_0 : \rho = \rho_0$ if $|Z_0| > Z_{\alpha/2}$.

Prediction of New Observations

If x_0 is the new value for x , then $\hat{y}_0 = \hat{\beta}_0 + \hat{\beta}_1 x_0$ is the point estimate for the response. The new error is

$$\psi = y_0 - \hat{y}_0 \implies \text{Var}(\psi) = \sigma^2 \left(1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)$$

Then we use the standard error of ψ to construct the prediction interval

$$\left[\hat{y}_0 \pm t_{\alpha/2, n-2} \sqrt{MSE \left(1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)} \right]$$

To hypotheses $H_0 : y_0 = y_{00}$, $H_1 : y_0 \neq y_{00}$, reject null hypothesis when $|t_0| > t_{\alpha/2, n-2}$

$$\frac{y_0 - y_{00}}{\sqrt{MSE \left(1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}} \right)}} \sim t_{n-2}$$

Multiple Linear Regression

Model

We write the multiple linear regression model as

$$Y = X\beta + \epsilon$$

where (Note $p = k + 1$.)

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1k} \\ 1 & x_{21} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nk} \end{bmatrix}$$

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Y is $n \times 1$, X is $n \times p$, β is $p \times 1$, and ϵ is $n \times 1$. In matrix form, we get the fitted line

$$\hat{Y} = X\hat{\beta} = X(X'X)^{-1}X'Y = HY$$

$H = X(X'X)^{-1}X'$ is the **hat matrix**.

Properties of the Hat Matrix

- H is a projection matrix, so it is idempotent and symmetric $HH = H$, $H' = H$.
- The matrix H is orthogonal to the matrix $I - H$, so $(I - H)H = H - HH = 0$. Moreover, $(I - H)$ is idempotent and a project matrix as well.
- The vector of residuals is

$$e = Y - \hat{Y} = Y - HY = (I - H)Y$$

- Y is projected onto a space spanned by the columns of H , and the residuals are in an orthogonal space.

$$Y = HY + (I - H)Y$$

Estimation of σ^2

Residual sum of squares is

$$SSE = \sum_{i=1}^n e_i^2 = e'e = Y'Y - \hat{\beta}'X'Y$$

SSE has $n - p$ degrees of freedom, then MSE is

$$\hat{\sigma}^2 = MSE = \frac{SSE}{n - p}$$

Estimation and Hypothesis Testing

Testing for Significance

We test for significance with

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_k = 0, H_1 : \beta_j \neq 0$$

Rejecting the null hypothesis means at least one regressor contributed significantly. We use an F statistic

$$F_0 = \frac{SSR/k}{SSE/(n - p)} = \frac{MSR}{MSE} \sim F_{k, n-p}$$

We reject the null hypothesis when $F_0 > F_{\alpha, k, n-k-1}$.

The **total sum of squares** is

$$SST = \sum_{i=1}^n Y_i^2 - \frac{1}{n} \left(\sum_{i=1}^n Y_i \right)^2 = Y'Y - \frac{1}{n} \left(\sum_{i=1}^n Y_i \right)^2$$

The **regression sum of squares** is

$$SSR = \hat{\beta}'X'Y - \frac{1}{n} \left(\sum_{i=1}^n Y_i \right)^2$$

The **residual sum of squares** is

$$SSE = Y'Y - \hat{\beta}'X'Y = Y'(I - H)Y$$

We can also write SST and SSR in terms of the J_n , and $n \times n$ matrix with 1's.

$$SST = Y' \left(I - \frac{1}{n} J_n \right) Y$$

$$SSR = Y' \left(H - \frac{1}{n} J_n \right) Y$$

Tests on Individual Coefficients

To test an individual coefficient β_j , we use

$$H_0 : \beta_j = 0, H_1 : \beta_j \neq 0$$

The test statistic is

$$t_0 = \frac{\hat{\beta}_j}{\sqrt{\hat{\sigma}^2 C_{jj}}} = \frac{\hat{\beta}_j}{se(\hat{\beta}_j)}$$

Where C_{jj} is the diagonal entry of $(X'X)^{-1}$. We reject H_0 when $|t_0| > t_{\alpha/2, n-p}$.

If we fail to reject the null hypothesis, we can remove the corresponding regressor x_j from the model.

Extra Sum Of Squares

We want to partition r of the k regressors to test

$$H_0 : \beta_2 = 0, H_1 : \beta_2 \neq 0$$

$Y = X\beta + \epsilon$, where Y is $n \times 1$, X is $n \times p$, β is $p \times 1$, and ϵ is $n \times 1$ with $p = k + 1$.

Full Model

$$Y = X\beta + \epsilon = X_1\beta_1 + X_2\beta_2 + \epsilon$$

X_1 is $n \times (p - r)$, X_2 is $n \times r$.

$$\hat{\beta} = (X'X)^{-1}X'Y, SSR(\beta) = \hat{\beta}'X'Y$$

which has $k = p - 1$ degrees of freedom.

Reduced Model

To test regressors in β_2 , fit the model assuming $H_0 : \beta_2 = 0$ is true.

$$Y = X_1\beta_1 + \epsilon$$

$$\hat{\beta}_1 = (X_1'X_1)^{-1}X_1'Y, SSR(\beta_1) = \hat{\beta}_1'X_1'Y$$

which has $k - r = p - 1 - r$ degrees of freedom. The sum of squares due to β_2 given that β_1 is already in the model is

$$SSR(\beta_2|\beta_1) = SSR(\beta) - SSR(\beta_1)$$

The null hypothesis $\beta_2 = 0$ can be tested with (partial F -test)

$$F_0 = \frac{SSR(\beta_2|\beta_1)/r}{MSE}$$

If $F_0 > F_{\alpha, r, n-p}$, then we reject the null hypothesis and conclude that at least one regressor in X_2 contributes.

Lack of Fit

Pure Error Sum of Squares:

$$SS_{PE} = \sum_{i=1}^m \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2$$

Sum of Squares Due to Lack of Fit:

$$SS_{LOF} = \sum_{i=1}^m n_i (\bar{y} - \hat{y}_i)$$

F -Statistic:

$$F^* = \frac{SS_{LOF}/(m - 2)}{SS_{PE}/(n - m)} = \frac{MS_{LOF}}{MS_{PE}}$$

Testing Lack of Fit

If the regression is linear, then $E(y_i) = \beta_0 + \beta_1 x_i$,

$$H_0 : E(y_i) = \beta_0 + \beta_1 x_i, H_1 : E(y_i) \neq \beta_0 + \beta_1 x_i$$

Reject the null hypothesis when $F^* > F_{\alpha, m-2, n-m}$.

Anova Table for Lack of Fit

Source	Sum of Squares	DF
Regression	$SSR = \sum_{i=1}^m \sum_{j=1}^{n_i} (y_{ij} - \hat{y}_i)^2$	1
Residuals	$SSE(R) = \sum_{i=1}^m \sum_{j=1}^{n_i} (y_{ij} - \hat{y}_i)^2$	$n - 2$
Lack of Fit	$SS_{LOF} = \sum_{i=1}^m n_i (\bar{y}_i - \hat{y}_i)^2$	$m - 2$
Pure Error	$SS_{PE} = \sum_{i=1}^m \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2$	$n - m$
Total	$\sum_{i=1}^m \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2$	$n - 1$

Source	Mean Square = SS/df	F-Statistic
Regression	$SSR/1$	MSR/MSE
Residuals	$SSE(R)/n - 2$	
Lack of Fit	$SS_{LOF}/m - 2$	MS_{LOF}/MS_{PE}
Pure Error	$SS_{PE}/n - m$	

Model Adequacy

Normality

- **Using a boxplot:** Box plot of residuals should be symmetric around a median of 0.
- **Histogram:** Should be of the shape of a normal distribution.
- **QQ-Plot:** Plot $E_k = \sqrt{MSE} \cdot \Phi^{-1} \left(\frac{k-0.375}{n+0.25} \right)$ vs the residuals $e_{(k)}$, should be a straight line.

Constant Variance

Studentize the residuals, and plot $\sqrt{e_i^*}$ vs \hat{Y}_i .

$$e_i^* = \frac{e_i}{\sqrt{MSE(1 - h_{ii})}}$$

- Plot should show a random distribution of points. Otherwise, signs of non-constant variance.
- Residuals lie in a narrow band around 0 \Rightarrow no need of correction.
- Residuals are increasing or decreasing \Rightarrow variance is non constant.
- Double-bow pattern \Rightarrow variance in the middle is larger than the variance at the extremes.
- Quadratic relationship (parabola shape) \Rightarrow maybe a nonlinear relationship

Confidence Intervals

Confidence Intervals on Regression Coefficients

To construct a confidence interval on β_j , use the statistic

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 C_{jj}}} \sim t_{n-p}$$

The CI is then

$$\hat{\beta}_j - t_{\alpha/2, n-p} \sqrt{\hat{\sigma}^2 C_{jj}} \leq \beta_j \leq \hat{\beta}_j + t_{\alpha/2, n-p} \sqrt{\hat{\sigma}^2 C_{jj}}$$

Recall C_{jj} is the j th diagonal entry of $(X'X)^{-1}$ the standard error is

$$se(\hat{\beta}_j) = \sqrt{\hat{\sigma}^2 C_{jj}}$$

Confidence Interval on Mean Response

To construct confidence intervals at points $x_{01}, x_{02}, \dots, x_{0k}$, define

$$x_0 = [1 \quad x_{01} \quad x_{02} \quad \dots \quad x_{0k}]^T$$

The fitting value is then

$$\hat{y}_0 = x_0' \hat{\beta}$$

This is an unbiased estimator, $E(y|x_0) = x_0' \beta = E(\hat{y}_0)$, and $\text{Var}(\hat{y}_0) = \sigma^2 x_0' (X'X)^{-1} x_0$. The CI is then

$$[\hat{y}_0 \pm t_{\alpha/2, n-p} \sqrt{\hat{\sigma}^2 x_0' (X'X)^{-1} x_0}]$$

Simultaneous Confidence Interval

Theorem (Bonferroni Inequality). For two events A_1, A_2 , we have that

$$P(A_1 \cup A_2) \leq P(A_1) + P(A_2)$$

From DeMorgan's identity, we also have

$$P(A_1^c \cap A_2^c) = 1 - P(A_1 \cup A_2) \geq 1 - P(A_1) - P(A_2)$$

If we define the events

$$A_1^c: \hat{\beta}_0 \pm t_{1-\alpha/2, n-2} s(\hat{\beta}_0)$$

$$A_2^c: \hat{\beta}_1 \pm t_{1-\alpha/2, n-2} s(\hat{\beta}_1)$$

From Bonferroni's Inequality, if we have $P(A_1) = P(A_2) = \alpha$, then

$$P(A_1^c \cap A_2^c) \geq 1 - P(A_1) - P(A_2) = 1 - 2\alpha$$

In general, if we have p parameters and each confidence interval has confidence, $1 - \frac{\alpha}{p}$, then

$$P\left(\bigcap_{i=1}^p A_i^c\right) \geq 1 - p \frac{\alpha}{p} = 1 - \alpha$$

Transformations and Weighting

Variance Stabilizing Transformations

- **Poisson** ($\mu = \sigma^2$): $y \sim \text{Poisson}(\lambda) \Rightarrow \sqrt{y}$ is nearly normal and has variance 1/4 if λ is large.
- **Binomial**: $y \sim \text{Bin}(n, p)$ with mean $m = np$, then

$$y' = \sin^{-1} \left(\sqrt{\frac{y+c}{n+2c}} \right)$$

The optimal value of c is 3/8 when m and $n-m$ are large. The variance is approximately $\frac{1}{4} (n + \frac{1}{2})^{-1}$.

Transformations to Linearize Models.

- **Exponential**: $\beta'_0 = \ln \beta_0$, $\epsilon' = \ln \epsilon$,
 $y = \beta_0 e^{\beta_1 x} \epsilon \rightarrow y' = \ln y = \beta'_0 + \beta_1 x + \epsilon'$
- **Reciprocal**: $x' = \frac{1}{x}$,
 $y = \beta_0 + \beta_1 \frac{1}{x} + \epsilon \rightarrow y = \beta_0 + \beta_1 x' + \epsilon$
 $\frac{1}{y} = \beta_0 + \beta_1 x + \epsilon \rightarrow y' = \frac{1}{y}$
- **Two Step Reciprocal**: $y' = \frac{1}{y}$, $x' = \frac{1}{x}$,
 $y = \frac{x}{\beta_0 + \beta_1 x} \rightarrow y' = \beta_0 x' + \beta_1$

Box-Cox Transformations

When data is not normally distributed, can apply a power transformation

$$y^{(\lambda)} = \begin{cases} \frac{y^{\lambda}-1}{\lambda y^{\lambda-1}} & \lambda \neq 0 \\ \ln y & \lambda = 0 \end{cases}, \quad \hat{y} = \ln^{-1} \left(\frac{1}{n} \sum_{i=1}^n \ln y_i \right)$$

We want a value for λ that minimizes SSE , this value is found by trial and error.

Weighted Least Squares

$$W = \begin{bmatrix} w_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & w_n \end{bmatrix}$$

$$X_W = \begin{bmatrix} 1\sqrt{w_1} & \dots & x_{1k}\sqrt{w_1} \\ 1\sqrt{w_2} & \dots & x_{2k}\sqrt{w_2} \\ \vdots & \ddots & \vdots \\ 1\sqrt{w_n} & \dots & x_{nk}\sqrt{w_n} \end{bmatrix}, \quad Y_W = \begin{bmatrix} y_1\sqrt{w_1} \\ y_2\sqrt{w_2} \\ \vdots \\ y_n\sqrt{w_n} \end{bmatrix}$$

New Weighted Model: $Y_w = X_w \beta + \epsilon_w$, estimate becomes

$$\hat{\beta} = (X_W' X_W)^{-1} X_W' Y_W = (X' W X)^{-1} X' W Y$$

Weighted mean square error is

$$MSE_W = \frac{\sum_{i=1}^n w_i (y_i - \hat{y}_i)^2}{n - p} = \frac{\sum_{i=1}^n w_i e_i^2}{n - p}$$