1 Simple Linear Regression

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1.1 Least Squares Estimate

1 Simple Linear Regression

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad i = 1 \dots n$$

If assumptions hold true,

• Y_i is normally distributed

$$E(Y_i) = \beta_0 + \beta_1 x_i$$
$$Var(Y_i) = \sigma^2$$

• Mean: $\beta_0 + \beta_1 x_i$

Variance: σ²

Assumptions

- $\epsilon_1 \dots \epsilon_n$
- $E(\epsilon_i) = 0, var(\epsilon_i) = 0$, where σ^2 is an unknown constant
- ϵ_i is normal. (normality assumption)

1.1 Least Squares Estimate

$$\sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 x_i)^2 \tag{4}$$

Take the first order derivative with respect to β_0, β_1 to minimize equation (4) to find optimal β_0, β_1 .

LS estimators

$$\hat{\beta}_{1} = \frac{\sum_{i=1}^{n} (x_{i} - \bar{x})(Y_{i} - \bar{Y})}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}}$$

$$\hat{\beta}_{0} = \bar{Y} - \hat{\beta}_{1}\bar{x}$$
(6)

$$q = \bar{Y} - \hat{\beta}_1 \bar{x}$$
 (6)

- $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ (sample mean of the x_i 's)
- $\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$ (sample mean of the Y_i 's)
- Regression Line: $y = \hat{\beta}_0 + \hat{\beta}_1 x$

Properties of LS Estimators

• $E(\hat{\beta}_0) = \beta_0$, $E(\hat{\beta}_1) = \beta_1$. The average of many sample beta values will approach the true beta values.

Fitted (or predicted) values are estimates. The fitted value for Y_i is $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$

 \hat{Y} is an unbiased estimator of $E(Y) = \beta_0 + \beta_1 x$ so (1) $E(\hat{Y}) = E(Y)$

1.2 Residuals

Residuals : $\hat{\epsilon}_i = Y_i - \hat{Y}_i, i = 1 \dots n$ Properties of Residuals

- $\Sigma_{i=1}^n \hat{\epsilon}_i = 0$
 - The residuals are not independent.
 - If one residual is positive, another residual has to compensate.

1.3 Variance

Estimation of σ^2 , the variance of the errors (which is the same as the variance of Y_i)

$$s^{2} = \frac{1}{n-2} \sum_{i=1}^{n} (Y_{i} - \hat{Y}_{i})^{2}$$
 (7)

where \hat{Y}_i is the estimate of $E(Y_i)$.

Notes

- \hat{Y}_i is an estimator of $E(Y_i)=\beta_0+\beta_1x_i$ in which two parameters are estimated $(\beta_0$ and $\beta_1)\implies 2$ degrees of freedoms are subtracted.
- $E(s^2) = \sigma^2$

When errors are normally distributed, the LS estimators of β_0, β_1 is equal to the MLEs (Maximum Likelihood Estimators) of β_0 , β_1 , but the MLE of σ^2 , $\hat{\sigma}^2$, is different from

$$s^2$$
 is just (7)

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \hat{\epsilon}_i^2 \qquad (8)$$

Inference in regression and correlation analysis

2.1 Inference about β_1

For testing β_1

 $H_0: \beta_1 = \beta_{10}, \beta_{10}$ is a given value such as 0.

 $H_a: \beta_1 \neq \beta_{10}, \beta_1 > \beta_{10},$ or $\beta_1 < \beta_{10}$ Test statistic: A statistic whose distribution is known under the null hypothesis.

$$t = \frac{\hat{\beta}_1 - \beta_{10}}{s.e.(\hat{\beta}_1)} \tag{9}$$

where $\hat{\beta}_1$ is the LS estimate of β_1 , and

$$s.e.(\hat{\beta}_1) = \sqrt{\frac{MSE}{\sum_i (x_i - \bar{x})^2}}$$

$$(10)$$

$$MSE = s^2$$

If normal, $T \sim t_{n-1}$

$$T = \frac{\hat{\beta}_1 - \beta_1}{s.e.(\hat{\beta}_1)} \tag{12}$$

Therefore under the $H_0: \beta_1 = \beta_{10}, t \sim t_{n-2}$ Decision Rules

$$\begin{split} H_1: \beta_1 &\neq \beta_{10}, reject \ H_0 \ if \ |t| > t_{n-2,\alpha/2} \\ H_1: \beta_1 &> \beta_{10}, reject \ H_0 \ if \ |t| > t_{n-2;\alpha} \\ H_1: \beta_1 &< \beta_{10}, reject \ H_0 \ if \ |t| < -t_{n-2;\alpha} \end{split}$$

Alternatively, Reject H_0 if the p-value of t is $\leq \alpha$

- Type I : Reject H₀ when it is true.
- Type II : Fail to reject H_0 when it is false.

Level of Significance α

 α is the upper bound for the probability of Type I error. P-value

probability that the test statistic is as extreme as observed given H_0 is true.

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Power

Power is the probability of rejecting H_0 when the alternative holds at a given value.

If $\beta_{10} = 0, \beta_1 = 1, s.d.(\hat{\beta}_1) = 0.5$, we have $\delta = \frac{1}{0.5} = 2$ Let $\alpha = 0.05$. From table B.5 we find the power is 0.48.

Confidence interval for β_k

Assuming normality, a $100(1-\alpha)\%$ c.i. for β_k is

$$\hat{\beta}_k \pm t_{n-2} (1 - \frac{alpha}{2} * s.e.(\hat{\beta}_1)$$
 (13)
 $k = 0, 1$ (14)

$$k = 0, 1$$
 (14)

where $s.e.(\hat{\beta}_1)$ can be found with eq(10) and $s.e.(\hat{\beta}_0)$ can be found with eq(15).

2.2 Inference about β_0

$$s.e.(\beta_0) = \sqrt{mse(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2})}$$
 (15)

Confidence intervals for β_0 can be found with (13)

2.3 Inference about \hat{Y}

Confidence Interval for $E(Y) = \beta_0 + \beta_1 x$

$$\hat{Y} \pm t_{n-2} (1 - \frac{alpha}{2}) * s.e.(\hat{Y})$$
 (16)
$$s.e.(\hat{Y}) = \sqrt{MSE(\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2})}$$
 (17)

2.4 Prediction interval for \hat{Y}

A
$$100(1-\alpha)\%$$
 prediction interval for $Y=E(Y)+\epsilon=\beta_0+\beta_1x+\epsilon$, where Y is the future observation and ϵ is the new error:

$$\hat{Y} \pm t_{n-2}(1 - \frac{\alpha}{2}) * p.s.e.(\hat{Y})$$
 (18)

$$\hat{Y} \pm t_{n-2} (1 - \frac{\alpha}{2}) * p.s.e.(\hat{Y})$$
 (18)
$$p.s.e.(\hat{Y}) = \sqrt{MSE(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2})}$$
 (19)

Where p.s.e. is the percent standard error. The 1 in the p.s.e is because the variance of $\epsilon=\sigma^2$. If $var(\epsilon) = \frac{\sigma^2}{2}$ change the 1 to $\frac{1}{2}$.

2.5 ANOVA and F-test

$$SSTO = SSR + SSE$$
 (20)

$$= \sum_{i=1}^{n} (Y_i - \bar{Y})^2 \tag{21}$$

$$SSR = \sum_{i=1}^{n} (\hat{Y}_{i} - \bar{Y})^{2}$$
 (22)

$$SSE = \sum_{i=1}^{n} (Y_i - \hat{Y})^2$$
(23)

Sum of Squares of Regression (SSR) explains the variability in Y due to the regression model compared to the baseline model. Sum of Squares of Errors (SSE) is the remaining unexplained variability of Y found from SSTO

Degrees of Freedom

$$\begin{split} SSRdf &= 1\\ SSEdf &= n-2\\ SSTOdf &= n-2+1 = n-1 \end{split}$$

Mean Squares

Mean squares is SS divided by its degrees of freedom.

$$MSR = \frac{SSR}{1}$$
(25)

$$MSE = \frac{\overrightarrow{SSE}}{n-2} \tag{26}$$

(27)

F-Statistic

$$F = \frac{MSR}{MSE} = \frac{SSR * (n-2)}{SSE}$$
 (28)

ANOVA table: Analysis of variance.

The distribution of F under the null hypothesis $H_0: \beta_1 =$

Source	SS	df	$_{ m MS}$	F
Regression	SSR	1	MSR	F
Error	SSE	n-2	MSE	
Total	SSTO	n-1		

2.6 Inference about ρ

 \mathbb{R}^2 : a measure of goodness of fit, which is the proportion of variation in Y explained by the regression (i.e. by x).

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO} \tag{29}$$

Coefficient of correlation:

$$r = \pm \sqrt{R^2} = \begin{cases} +\sqrt{R^2} & if \ \hat{\beta}_1 > 0\\ -\sqrt{R^2} & if \ \hat{\beta}_1 < 0 \end{cases}$$

$$r = \frac{\sum_i (Y_i - \bar{Y})(x_i - \bar{x})}{\sqrt{\sum_i (Y_i - \bar{Y})^2 \sum_i (x_i - \bar{x})^2}}$$
(31)

$$r = \frac{\sum_{i} (Y_{i} - \bar{Y})(x_{i} - \bar{x})}{\sqrt{\sum_{i} (Y_{i} - \bar{Y})^{2} \sum_{i} (x_{i} - \bar{x})^{2}}}$$
(31)

Properties of \mathbb{R}^2 and

- $\bullet \ \ 0 \leq R^2 \leq 1 \quad \ -1 \leq r \leq 1$
- $R^2 \approx 1$ or $r \approx \pm 1$, if there is a strong linear association between x and Y.
- $R^2 \approx 0$, or $r \approx 0$, if there is a weak or no linear association between x and Y.
- \bullet Both R^2 and r are measures of linear association

Covariance and correlation between two random variables

$$cov(X,Y) = E\{(X - \mu_X)(Y - \mu_Y)\}$$

$$= E(XY) - E(X)E(Y)$$
(32)

$$cor(X,Y) = \frac{cov(X,Y)}{sd(X)sd(Y)}$$
(34)

where $\mu_X = E(X), sd(X) = \sqrt{var(X)}$, etc.

Special case: (X, Y) has a bivariate normal distribution.

Testing for ρ

Assume that the bivariate normal distribution holds for (X,Y).

 $H_0 : \rho = 0$

 $H_a: \rho \neq 0 (or \rho > 0 or \rho < 0)$

$$t^* = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} \sim t_{n-2} \text{ under } H_0$$
 (35)

3 Diagnostics

The goal of diagnostics is to examine the departures from the simple linear regression model with normal er-Typical departures and corresponding diagnostic plots/tests are:

- The regression is not linear residual plots(residual against the predictor variable, or against the fitted values), lack of fit test.
- The error terms are not normally distributed histogram, boxplot/dot plot of residuals, normal probability plot (aka QQ plot), Shapiro-Wilk's test, correlation test for normality.
- The error terms do not have constant variance residual plots, Brown - Forsythe (BF) test,
- The error terms are not independent residual against time.
- The model fits all but one or a few outlier observations - (semistudentized) residual plots, box plots, dot plots, stem and leaf plots.
- Some important predictors are missing residual plots (residual against other possibly important predictors).

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3.2 Diagnostic Tests

Shapiro Wilk's test

 $H_0 \ data \ \sim N()$

 H_a : data not normal.

 $p-val \leq \alpha$ reject normality assumption.

Correlation test for normality

Step 1. Compute the coefficient of correlation between the ordered residuals and their expected values. The latter are

$$\sqrt{MSE}z(\frac{k-0.375}{n+0.25}), \quad k=1,\dots,n$$
 (36)

where z(p) is the pth quantile of the standard normal distribution, that is, $P[Z \le z(p)] = p$, where Z has the standard normal distribution.

Step 2. Compare the coefficient of correlation on I with the critical value from Table B.6, if the coefficient of correlation exceeds the critical value, accept the normality assumption.

BF test for constant variance

 $1.\,$ Divide the residuals into two parts according to residual pattern (or no pattern)

Let $\hat{\epsilon}_{i1} = 1, \dots, n_1$ be the residuals for the first part, and $\hat{\epsilon}_{i2}, i = 1, \dots, n_2$ be the residuals for the second part, where $n_1 + n_2 = n$.

Compute $m(\hat{\epsilon}_1) = median \ of \ \hat{\epsilon}_{i1}, i = 1, ..., n_1$ and

2. Compute $d_{i1} = |\hat{\epsilon}_{i1} - m(\hat{\epsilon}_1)|, i = 1...n_1 \text{ and } d_{i2} =$ $|\hat{\epsilon}_{i2} - m(\hat{\epsilon}_2)|, i = 1 \dots n_2$

3. Compute t score.

$$t_{BF} = \frac{\bar{d}_1 - \bar{d}_2}{s\sqrt{n_1^{-1} + n_2^{-1}}} \tag{37}$$

$$s^{2} = \frac{\sum_{i=1}^{n_{1}} (d_{i1} - \bar{d}_{1})^{2} + \sum_{i=1}^{n_{2}} (d_{i2} - \bar{d}_{2})^{2}}{n - 2}$$
(38)

4. Test $H_0: \sigma_1^2 = \sigma_2^2$ vs $H_a: \sigma_1^2 \neq \sigma_2^2$

 $t_{BF} \sim t_{n-2}$ under H_0 . Given α , use the critical value (or p-value) to test H_0 .

F-test for lack of fit

Regression model: $Y_{ij} = \beta_0 + \beta_1 x_j + \epsilon_{ij}, j = 1 \dots c, i =$ $1 \dots n_j$ where x_j is the *jth* value of x, c is the number of different x values, and Y_{ij} , $i = 1 \dots n_j$ are the Y values corresponding to the same x_j . Full model: $Y_{ij} = \mu_j + \epsilon_{ij}, j = 1 \dots c, i = 1 \dots n_j$

F-statistic:

$$F = \frac{SSE(R) - SSE(F)}{df_R - df_F} \{ \frac{SSE(F)}{df_F} \}^{-1}$$
 (39)

where

3.1 Residual Plots

Residuals can be used to check whether

- The regression function is not linear
- The variance of the errors is not constant.
- The errors are not independent.
- Outliers
- The errors are not normal.
- Some important predictors are missing.

Scatter Plot

- Check linearity residuals normally disributed.
- Check constant variance residuals are random and dont follow a cone pattern.

Box Plot and Dot Plot

• Normality - residuals should be centered and symmetric about 0.

Normality probability plot - QQ Plot

- OO plot is linear ⇒ normal residuals.
- ullet QQ plot is nonlinear \Longrightarrow non normal residuals.

$$SSE(R) = \Sigma_j \Sigma_i (Y_{ij} - \hat{Y}_{ij})^2$$
 (40)

$$SSE(F) = \sum_{i} \sum_{i} (Y_{ij} - \hat{\mu}_{i})^{2} \tag{41}$$

with $\hat{Y}_{ij} = \hat{\beta}_0 + \hat{\beta}_1 x_j$ and $\hat{\mu}_j = \bar{Y}_j - n_j^{-1} \Sigma_{i=1}^{n_j} Y_{ij}$, $df_R = n-2$ with $n = \Sigma_{j=1}^c n_j$ and $df_F = n-c$. Under H_0 : The assumed model is correct, $F \sim F_{c-2,n-c}$.

3.3 Remedial Measures

Transformation of x: for nonlinear association.

Transformation of Y: for nonnormality/unequal vari-

Box Cox transformation

This is a collection of transformations depending on a "tuning parameter", λ .

$$Y_i' = \begin{cases} K_1(Y_i^{\lambda} - 1), & \lambda \neq 0 \\ K_2 log(Y_i), & \lambda = 0 \end{cases}$$

$$(42)$$

where K_1, K_2 are two numbers computed from the data.

$$K_2 = (Y_1 Y_2 \dots Y_n)^{\frac{1}{n}} = e^{\overline{\log Y}}$$

$$\tag{43}$$

$$K_2 = (Y_1 Y_2 \dots Y_n)^{\frac{1}{n}} = e^{\overline{\log Y}}$$
 (43)
 $K_1 = \frac{1}{\lambda K_2^{\lambda - 1}}$ (44)