

12

Multiple Linear Regression

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12-1 Multiple Linear Regression Models

12-1.1 Introduction

- Many applications of regression analysis involve situations in which there are more than one regressor variable.
- A regression model that contains more than one regressor variable is called a **multiple regression model**.

12-1 Multiple Linear Regression Models

12-1.1 Introduction

- For example, suppose that the effective life of a cutting tool depends on the cutting speed and the tool angle. A possible multiple regression model could be

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

where

Y – tool life

x_1 – cutting speed

x_2 – tool angle

12-1 Multiple Linear Regression Models

12-1.1 Introduction

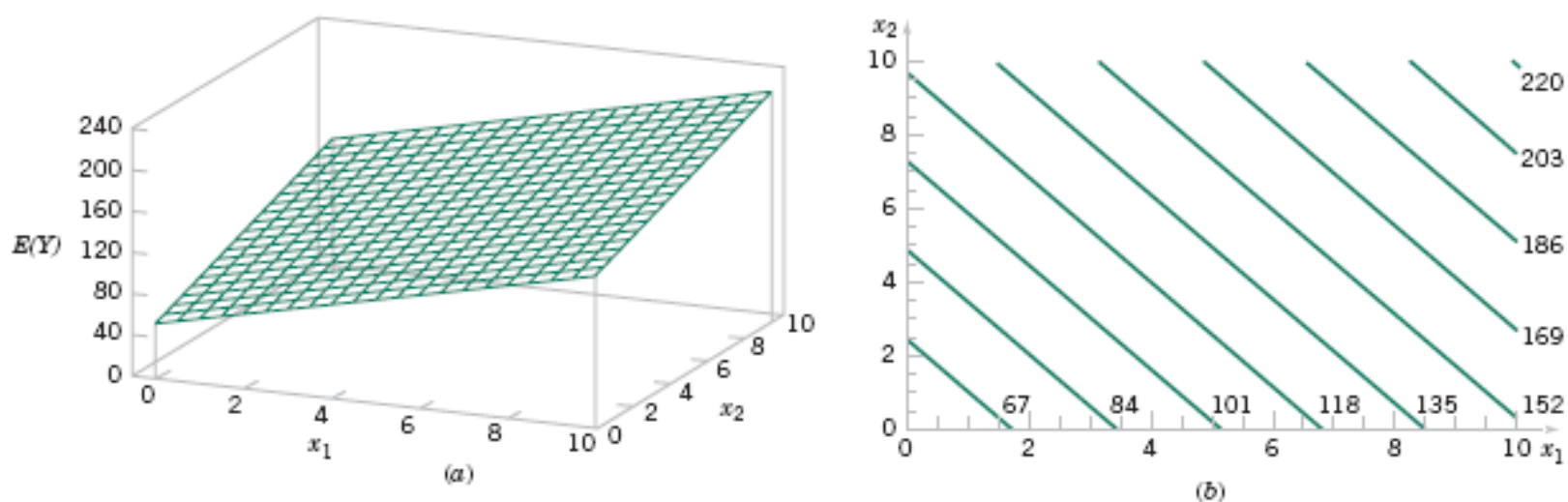


Figure 12-1 (a) The regression plane for the model $E(Y) = 50 + 10x_1 + 7x_2$. (b) The contour plot

12-1 Multiple Linear Regression Models

12-1.1 Introduction

In general, the **dependent variable** or **response** Y may be related to k **independent** or **regressor variables**. The model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon \quad (12-2)$$

is called a multiple linear regression model with k regressor variables. The parameters $\beta_j, j = 0, 1, \dots, k$, are called the regression coefficients. This model describes a hyperplane in the k -dimensional space of the regressor variables $\{x_j\}$. The parameter β_j represents the expected change in response Y per unit change in x_j when all the remaining regressors $x_i (i \neq j)$ are held constant.

12-1 Multiple Linear Regression Models

12-1.1 Introduction

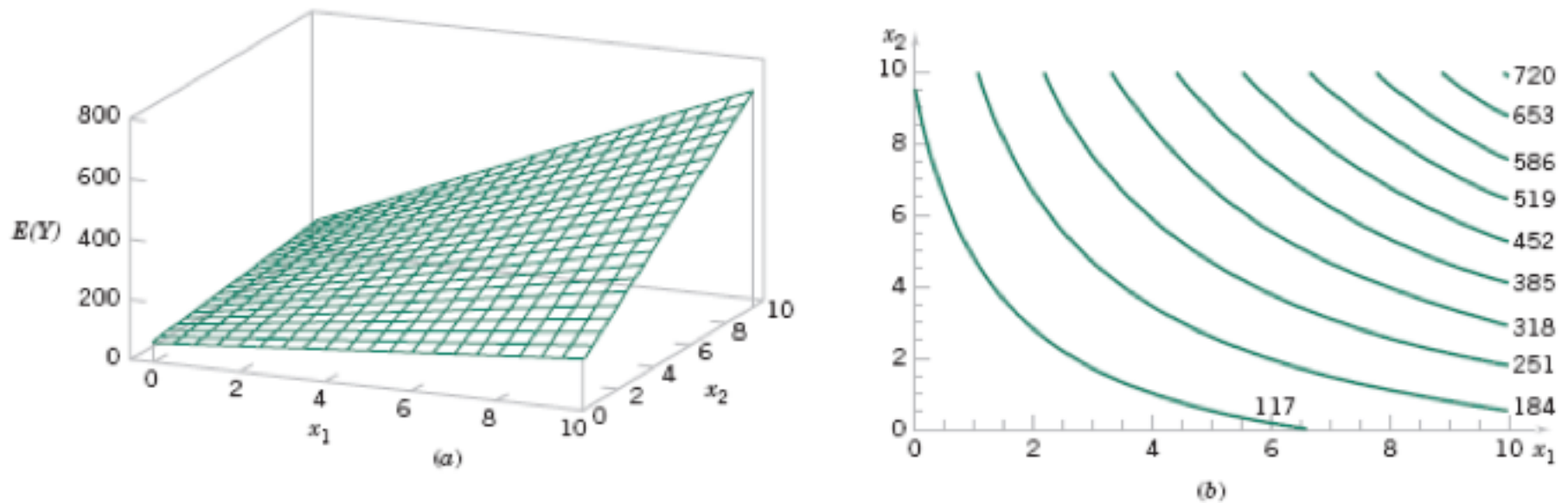


Figure 12-2 (a) Three-dimensional plot of the regression model $E(Y) = 50 + 10x_1 + 7x_2 + 5x_1x_2$.

(b) The contour plot

12-1 Multiple Linear Regression Models

12-1.1 Introduction

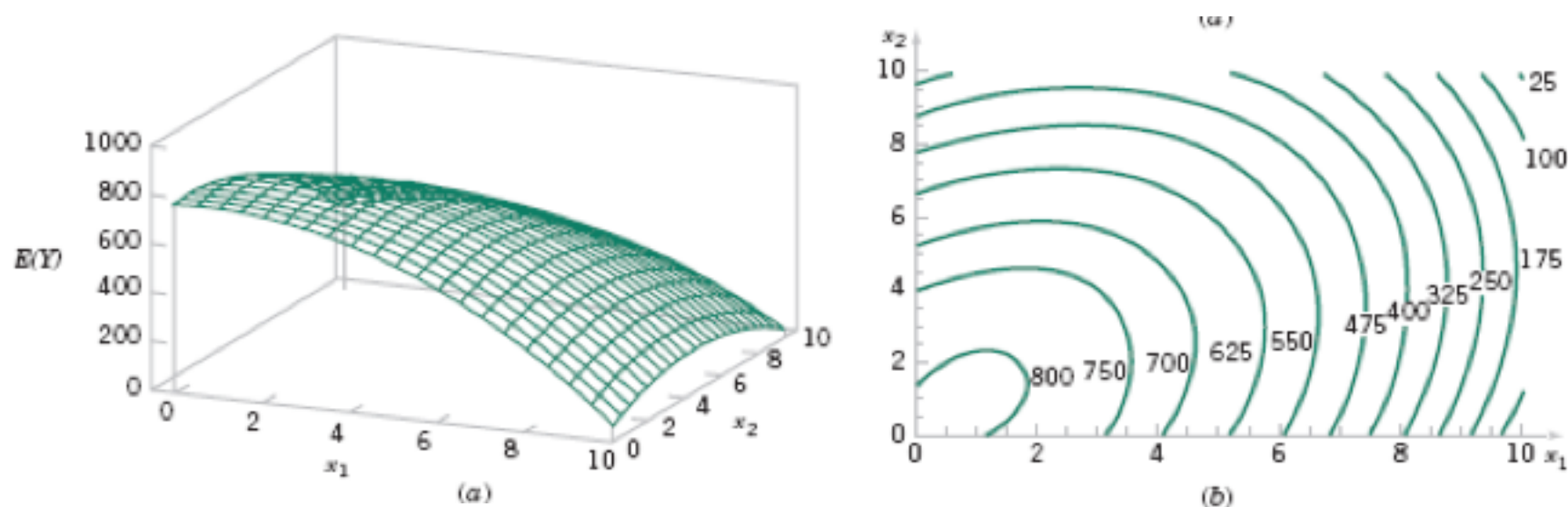


Figure 12-3 (a) 3-D plot of the regression model

$$E(Y) = 800 + 10x_1 + 7x_2 - 8.5x_1^2 - 5x_2^2 + 4x_1x_2.$$

(b) The contour plot

12-1 Multiple Linear Regression Models

12-1.2 Least Squares Estimation of the Parameters

The **method of least squares** may be used to estimate the regression coefficients in the multiple regression model, Equation 12-2. Suppose that $n > k$ observations are available, and let x_{ij} denote the i th observation or level of variable x_j . The observations are

$$(x_{i1}, x_{i2}, \dots, x_{ik}, y_i), \quad i = 1, 2, \dots, n \quad \text{and} \quad n > k$$

It is customary to present the data for multiple regression in a table such as Table 12-1.

Table 12-1 Data for Multiple Linear Regression

y	x_1	x_2	\dots	x_k
y_1	x_{11}	x_{12}	\dots	x_{1k}
y_2	x_{21}	x_{22}	\dots	x_{2k}
\vdots	\vdots	\vdots		\vdots
y_n	x_{n1}	x_{n2}	\dots	x_{nk}

12-1 Multiple Linear Regression Models

12-1.2 Least Squares Estimation of the Parameters

- The **least squares function** is given by

$$L = \sum_{i=1}^n \epsilon_i^2 = \sum_{i=1}^n \left(y_i - \beta_0 - \sum_{j=1}^k \beta_j x_{ij} \right)^2$$

- The **least squares estimates** must satisfy

$$\frac{\partial L}{\partial \beta_0} \Big|_{\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k} = -2 \sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \sum_{j=1}^k \hat{\beta}_j x_{ij} \right) = 0$$

and

$$\frac{\partial L}{\partial \beta_j} \Big|_{\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k} = -2 \sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \sum_{j=1}^k \hat{\beta}_j x_{ij} \right) x_{ij} = 0 \quad j = 1, 2, \dots, k$$

12-1 Multiple Linear Regression Models

12-1.2 Least Squares Estimation of the Parameters

- The **least squares normal Equations** are

$$\begin{array}{ccccccc} n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^n x_{i1} & + \hat{\beta}_2 \sum_{i=1}^n x_{i2} & + \cdots + \hat{\beta}_k \sum_{i=1}^n x_{ik} & = & \sum_{i=1}^n y_i \\ \hat{\beta}_0 \sum_{i=1}^n x_{i1} + \hat{\beta}_1 \sum_{i=1}^n x_{i1}^2 & + \hat{\beta}_2 \sum_{i=1}^n x_{i1} x_{i2} & + \cdots + \hat{\beta}_k \sum_{i=1}^n x_{i1} x_{ik} & = & \sum_{i=1}^n x_{i1} y_i \\ \vdots & \vdots & \vdots & & \vdots \\ \hat{\beta}_0 \sum_{i=1}^n x_{ik} + \hat{\beta}_1 \sum_{i=1}^n x_{ik} x_{i1} & + \hat{\beta}_2 \sum_{i=1}^n x_{ik} x_{i2} & + \cdots + \hat{\beta}_k \sum_{i=1}^n x_{ik}^2 & = & \sum_{i=1}^n x_{ik} y_i \end{array}$$

- The solution to the normal Equations are the **least squares estimators** of the regression coefficients.

12-1 Multiple Linear Regression Models

12-1.3 Matrix Approach to Multiple Linear Regression

Suppose the model relating the regressors to the response is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i \quad i = 1, 2, \dots, n$$

In matrix notation this model can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

12-1 Multiple Linear Regression Models

12-1.3 Matrix Approach to Multiple Linear Regression

$$y = X\beta + \epsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} \\ 1 & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nk} \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \quad \text{and} \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

12-1 Multiple Linear Regression Models

12-1.3 Matrix Approach to Multiple Linear Regression

We wish to find the vector of least squares estimators that minimizes:

$$L = \sum_{i=1}^n \epsilon_i^2 = \epsilon' \epsilon = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

The resulting least squares estimate is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y} \quad (12-13)$$

12-1 Multiple Linear Regression Models

12-1.3 Matrix Approach to Multiple Linear Regression

The fitted regression model is

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^k \hat{\beta}_j x_{ij} \quad i = 1, 2, \dots, n \quad (12-14)$$

In matrix notation, the fitted model is

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

The difference between the observation y_i and the fitted value \hat{y}_i is a **residual**, say, $e_i = y_i - \hat{y}_i$. The $(n \times 1)$ vector of residuals is denoted by

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} \quad (12-15)$$

12-1 Multiple Linear Regression Models

Example 12-2

Table 12-2 Wire Bond Data for Example 11-1

Observation Number	Pull Strength y	Wire Length x_1	Die Height x_2	Observation Number	Pull Strength y	Wire Length x_1	Die Height x_2
1	9.95	2	50	14	11.66	2	360
2	24.45	8	110	15	21.65	4	205
3	31.75	11	120	16	17.89	4	400
4	35.00	10	550	17	69.00	20	600
5	25.02	8	295	18	10.30	1	585
6	16.86	4	200	19	34.93	10	540
7	14.38	2	375	20	46.59	15	250
8	9.60	2	52	21	44.88	15	290
9	24.35	9	100	22	54.12	16	510
10	27.50	8	300	23	56.63	17	590
11	17.08	4	412	24	22.13	6	100
12	37.00	11	400	25	21.15	5	400
13	41.95	12	500				

12-1 Multiple Linear Regression Models

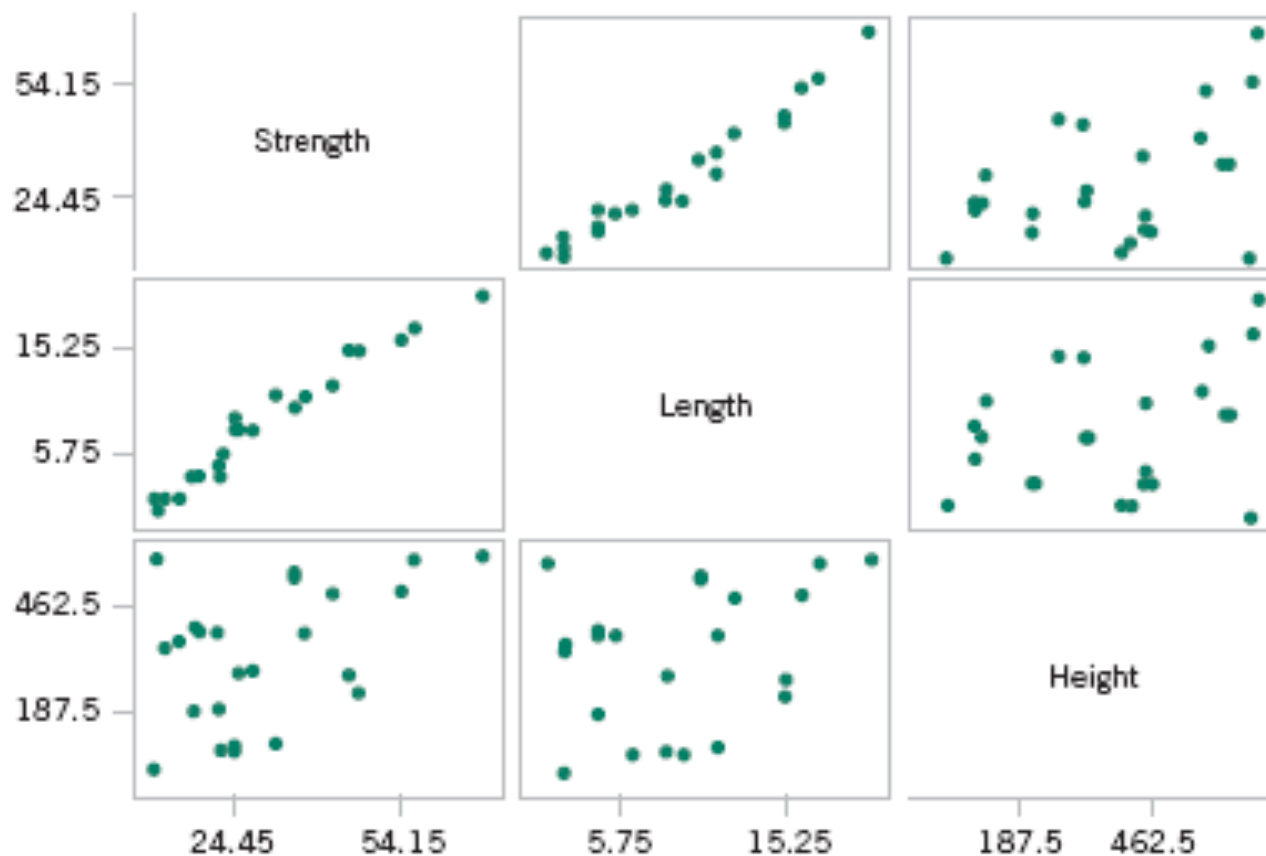


Figure 12-4 Matrix of scatter plots (from Minitab) for the wire bond pull strength data in Table 12-2.

Example 12-2

$\mathbf{X} =$	1	2	50	$\mathbf{y} =$	9.95
	1	8	110		24.45
	1	11	120		31.75
	1	10	550		35.00
	1	8	295		25.02
	1	4	200		16.86
	1	2	375		14.38
	1	2	52		9.60
	1	9	100		24.35
	1	8	300		27.50
	1	4	412		17.08
	1	11	400		37.00
	1	12	500		41.95
	1	2	360		11.66
	1	4	205		21.65
	1	4	400		17.89
	1	20	600		69.00
	1	1	585		10.30
	1	10	540		34.93
	1	15	250		46.59
	1	15	290		44.88
	1	16	510		54.12
	1	17	590		56.63
	1	6	100		22.13
	1	5	400		21.15

12-1 Multiple Linear Regression Models

Example 12-2

The $\mathbf{X}'\mathbf{X}$ matrix is

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 2 & 8 & \cdots & 5 \\ 50 & 110 & \cdots & 400 \end{bmatrix} \begin{bmatrix} 1 & 2 & 50 \\ 1 & 8 & 110 \\ \vdots & \vdots & \vdots \\ 1 & 5 & 400 \end{bmatrix} = \begin{bmatrix} 25 & 206 & 8,294 \\ 206 & 2,396 & 77,177 \\ 8,294 & 77,177 & 3,531,848 \end{bmatrix}$$

and the $\mathbf{X}'\mathbf{y}$ vector is

$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 2 & 8 & \cdots & 5 \\ 50 & 110 & \cdots & 400 \end{bmatrix} \begin{bmatrix} 9.95 \\ 24.45 \\ \vdots \\ 21.15 \end{bmatrix} = \begin{bmatrix} 725.82 \\ 8,008.37 \\ 274,811.31 \end{bmatrix}$$

The least squares estimates are found from Equation 12-13 as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

12-1 Multiple Linear Regression Models

Example 12-2

or

$$\begin{aligned} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix} &= \begin{bmatrix} 25 & 206 & 8,294 \\ 206 & 2,396 & 77,177 \\ 8,294 & 77,177 & 3,531,848 \end{bmatrix}^{-1} \begin{bmatrix} 725.82 \\ 8,008.37 \\ 274,811.31 \end{bmatrix} \\ &= \begin{bmatrix} 0.214653 & -0.007491 & -0.000340 \\ -0.007491 & 0.001671 & -0.000019 \\ -0.000340 & -0.000019 & +0.0000015 \end{bmatrix} \begin{bmatrix} 725.82 \\ 8,008.47 \\ 274,811.31 \end{bmatrix} = \begin{bmatrix} 2.26379143 \\ 2.74426964 \\ 0.01252781 \end{bmatrix} \end{aligned}$$

Therefore, the fitted regression model with the regression coefficients rounded to five decimal places is

$$\hat{y} = 2.26379 + 2.74427x_1 + 0.01253x_2$$

This is identical to the results obtained in Example 12-1.

12-1 Multiple Linear Regression Models

Example 12-2

This regression model can be used to predict values of pull strength for various values of wire length (x_1) and die height (x_2). We can also obtain the **fitted values** \hat{y}_i by substituting each observation (x_{i1}, x_{i2}) , $i = 1, 2, \dots, n$, into the equation. For example, the first observation has $x_{11} = 2$ and $x_{12} = 50$, and the fitted value is

$$\begin{aligned}\hat{y}_1 &= 2.26379 + 2.74427x_{11} + 0.01253x_{12} \\ &= 2.26379 + 2.74427(2) + 0.01253(50) \\ &= 8.38\end{aligned}$$

The corresponding observed value is $y_1 = 9.95$. The *residual* corresponding to the first observation is

$$\begin{aligned}e_1 &= y_1 - \hat{y}_1 \\ &= 9.95 - 8.38 \\ &= 1.57\end{aligned}$$

Table 12-3 displays all 25 fitted values \hat{y}_i and the corresponding residuals. The fitted values and residuals are calculated to the same accuracy as the original data.

12-1 Multiple Linear Regression Models

Example 12-2

Table 12-3 Observations, Fitted Values, and Residuals for Example 12-2

Observation Number	y_t	\hat{y}_t	$e_t = y_t - \hat{y}_t$	Observation Number	y_t	\hat{y}_t	$e_t = y_t - \hat{y}_t$
1	9.95	8.38	1.57	14	11.66	12.26	-0.60
2	24.45	25.60	-1.15	15	21.65	15.81	5.84
3	31.75	33.95	-2.20	16	17.89	18.25	-0.36
4	35.00	36.60	-1.60	17	69.00	64.67	4.33
5	25.02	27.91	-2.89	18	10.30	12.34	-2.04
6	16.86	15.75	1.11	19	34.93	36.47	-1.54
7	14.38	12.45	1.93	20	46.59	46.56	-0.03
8	9.60	8.40	1.20	21	44.88	47.06	-2.18
9	24.35	28.21	-3.86	22	54.12	52.56	1.56
10	27.50	27.98	-0.48	23	56.63	56.31	0.32
11	17.08	18.40	-1.32	24	22.13	19.98	2.15
12	37.00	37.46	-0.46	25	21.15	21.00	0.15
13	41.95	41.46	0.49				

Table 12-4 Minitab Multiple Regression Output for the Wire Bond Pull Strength Data

Regression Analysis: Strength versus Length, Height

The regression equation is

$$\text{Strength} = 2.26 + 2.74 \text{ Length} + 0.0125 \text{ Height}$$

Predictor	Coef	SE Coef	T	P	VIF
Constant	$\hat{\beta}_0 \rightarrow 2.264$	1.060	2.14	0.044	
Length	$\hat{\beta}_1 \rightarrow 2.74427$	0.09352	29.34	0.000	1.2
Height	$\hat{\beta}_2 \rightarrow 0.012528$	0.002798	4.48	0.000	1.2

S = 2.288

R-Sq = 98.1%

R-Sq (adj) = 97.9%

PRESS = 156.163

R-Sq (pred) = 97.44%

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	2	5990.8	2995.4	572.17	0.000
Residual Error	22	115.2	5.2 $\leftarrow \hat{\sigma}^2$		
Total	24	6105.9			

Source	DF	Seq SS
Length	1	5885.9
Height	1	104.9

Predicted Values for New Observations

New Obs	Fit	SE Fit	95.0% CI	95.0% PI
1	27.663	0.482	(26.663, 28.663)	(22.814, 32.512)

Values of Predictors for New Observations

New Obs	Length	Height
1	8.00	275

12-1 Multiple Linear Regression Models

Estimating σ^2

An unbiased estimator of σ^2 is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n e_i^2}{n - p} = \frac{SS_E}{n - p} \quad (12-16)$$

12-1 Multiple Linear Regression Models

12-1.4 Properties of the Least Squares Estimators

Unbiased estimators:

$$\begin{aligned} E(\hat{\boldsymbol{\beta}}) &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}] \\ &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon})] \\ &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\epsilon}] \\ &= \boldsymbol{\beta} \end{aligned}$$

Covariance Matrix:

$$\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} C_{00} & C_{01} & C_{02} \\ C_{10} & C_{11} & C_{12} \\ C_{20} & C_{21} & C_{22} \end{bmatrix}$$

12-1 Multiple Linear Regression Models

12-1.4 Properties of the Least Squares Estimators

Individual variances and covariances:

$$V(\hat{\beta}_j) = \sigma^2 C_{jj}, \quad j = 0, 1, 2$$
$$\text{cov}(\hat{\beta}_i, \hat{\beta}_j) = \sigma^2 C_{ij}, \quad i \neq j$$

In general,

$$\text{cov}(\hat{\beta}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1} = \sigma^2 \mathbf{C}$$

12-2 Hypothesis Tests in Multiple Linear Regression

12-2.1 Test for Significance of Regression

The appropriate hypotheses are

$$\begin{aligned} H_0: \beta_1 = \beta_2 = \dots = \beta_k = 0 \\ H_1: \beta_j \neq 0 \quad \text{for at least one } j \end{aligned} \quad (12-17)$$

The test statistic is

$$F_0 = \frac{SS_R/k}{SS_E/(n-p)} = \frac{MS_R}{MS_E} \quad (12-18)$$

12-2 Hypothesis Tests in Multiple Linear Regression

12-2.1 Test for Significance of Regression

Table 12-9 Analysis of Variance for Testing Significance of Regression in Multiple Regression

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Regression	SS_R	k	MS_R	MS_R/MS_E
Error or residual	SS_E	$n - p$	MS_E	
Total	SS_T	$n - 1$		

12-2 Hypothesis Tests in Multiple Linear Regression

Example 12-3

Table 12-10 Test for Significance of Regression for Example 12-3

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	f_0	P -value
Regression	5990.7712	2	2995.3856	572.17	1.08E-19
Error or residual	115.1735	22	5.2352		
Total	6105.9447	24			

The analysis of variance is shown in Table 12-10. To test $H_0: \beta_1 = \beta_2 = 0$, we calculate the statistic

$$f_0 = \frac{MS_R}{MS_E} = \frac{2995.3856}{5.2352} = 572.17$$

Since $f_0 > f_{0.05,2,22} = 3.44$ (or since the P -value is considerably smaller than $\alpha = 0.05$), we reject the null hypothesis and conclude that pull strength is linearly related to either wire length or die height, or both. However, we note that this does not necessarily imply that the

12-2 Hypothesis Tests in Multiple Linear Regression

R^2 and Adjusted R^2

The **coefficient of multiple determination**

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

- For the wire bond pull strength data, we find that $R^2 = SS_R/SS_T = 5990.7712/6105.9447 = 0.9811$.
- Thus, the model accounts for about 98% of the variability in the pull strength response.

12-2 Hypothesis Tests in Multiple Linear Regression

R² and Adjusted R²

The **adjusted R²** is

$$R_{\text{adj}}^2 = 1 - \frac{SS_E/(n - p)}{SS_T/(n - 1)} \quad (12-22)$$

- The adjusted R² statistic penalizes the analyst for adding terms to the model.
- It can help guard against **overfitting** (including regressors that are not really useful)

12-2 Hypothesis Tests in Multiple Linear Regression

12-2.2 Tests on Individual Regression Coefficients and Subsets of Coefficients

$$\begin{aligned}H_0: \beta_j &= \beta_{j0} \\H_1: \beta_j &\neq \beta_{j0}\end{aligned}\tag{12-23}$$

The test statistic for this hypothesis is

$$T_0 = \frac{\beta_{j0} - \beta_j}{\sqrt{\sigma^2 C_{jj}}} = \frac{\hat{\beta}_j - \beta_{j0}}{se(\hat{\beta}_j)}\tag{12-24}$$

- Reject H_0 if $|t_0| > t_{\alpha/2, n-p}$.
- This is called a **partial** or **marginal test**

12-2 Hypothesis Tests in Multiple Linear Regression

Example 12-4

Consider the wire bond pull strength data, and suppose that we want to test the hypothesis that the regression coefficient for x_2 (die height) is zero. The hypotheses are

$$H_0: \beta_2 = 0$$

$$H_1: \beta_2 \neq 0$$

The main diagonal element of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix corresponding to $\hat{\beta}_2$ is $C_{22} = 0.0000015$, so the t -statistic in Equation 12-24 is

$$t_0 = \frac{\hat{\beta}_2}{\sqrt{\hat{\sigma}^2 C_{22}}} = \frac{0.01253}{\sqrt{(5.2352)(0.0000015)}} = 4.4767$$

Note that we have used the estimate of σ^2 reported to four decimal places in Table 12-10. Since $t_{0.025,22} = 2.074$, we reject $H_0: \beta_2 = 0$ and conclude that the variable x_2 (die height) contributes significantly to the model. We could also have used a P -value to draw conclusions.

12-2 Hypothesis Tests in Multiple Linear Regression

Example 12-4

The P -value for $t_0 = 4.4767$ is $P = 0.0002$, so with $\alpha = 0.05$ we would reject the null hypothesis. Note that this test measures the marginal or partial contribution of x_2 given that x_1 is in the model. That is, the t -test measures the contribution of adding the variable $x_2 =$ die height to a model that already contains $x_1 =$ wire length. Table 12-4 shows the value of the t -test computed by Minitab. The Minitab t -test statistic is reported to two decimal places. Note that the computer produces a t -test for each regression coefficient in the model. These t -tests indicate that both regressors contribute to the model.

R commands and outputs

```
> dat=read.table("http://www.stat.ucla.edu/~hqxu/stat105/
data/table12_2.txt", h=T)
```

```
> g=lm(Strength~Length+Height, dat)
```

```
> summary(g)
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	2.263791	1.060066	2.136	0.044099	*
Length	2.744270	0.093524	29.343	< 2e-16	***
Height	0.012528	0.002798	4.477	0.000188	***

Residual standard error: 2.288 on 22 degrees of freedom

Multiple R-Squared: 0.9811, Adjusted R-squared: 0.9794

F-statistic: 572.2 on 2 and 22 DF, p-value: < 2.2e-16