

Chapter 3

Multiple Linear Regression

Chapter 3a

Multiple linear regression models – examples (pages 3-5)

Multiple linear regression model (page 6)

Data for multiple linear regression model (page 7)

Example – Delivery time data (pages 8-12)

Least-squares function and least-squares regression (page 13)

Least-squares normal equations and estimates of regression coefficients (pages 14-15)

Example – Delivery time data (page 16)

Least-squares estimation – matrix approach (pages 17-21)

Example – Delivery time data (pages 22-24)

Example – Cholesterol age data (pages 25-26)

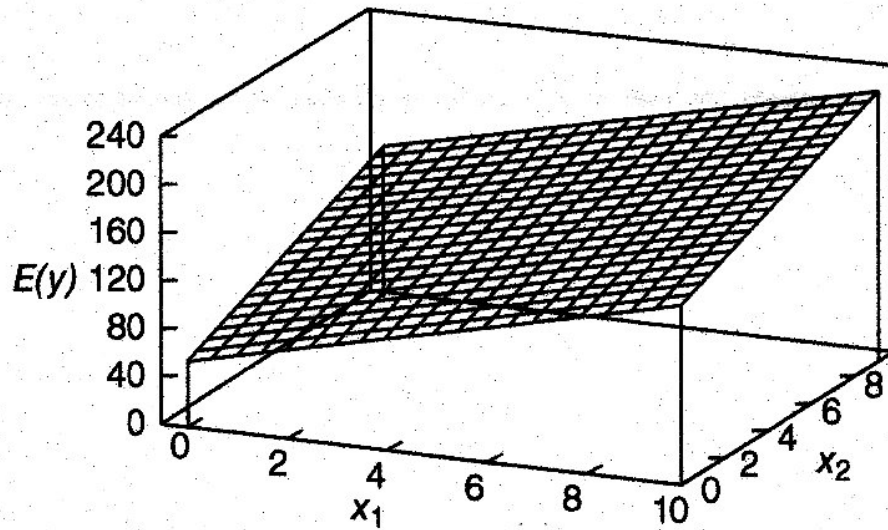
Fitting straight line and quadratic models (pages 27-30)

2 regressor variable?

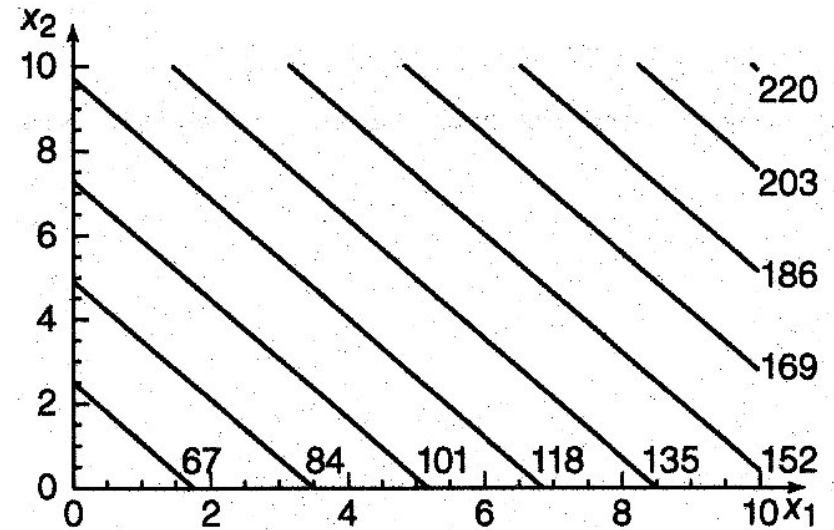
Multiple linear regression models

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

$$E(y) = 50 + 10x_1 + 7x_2$$



regression plane

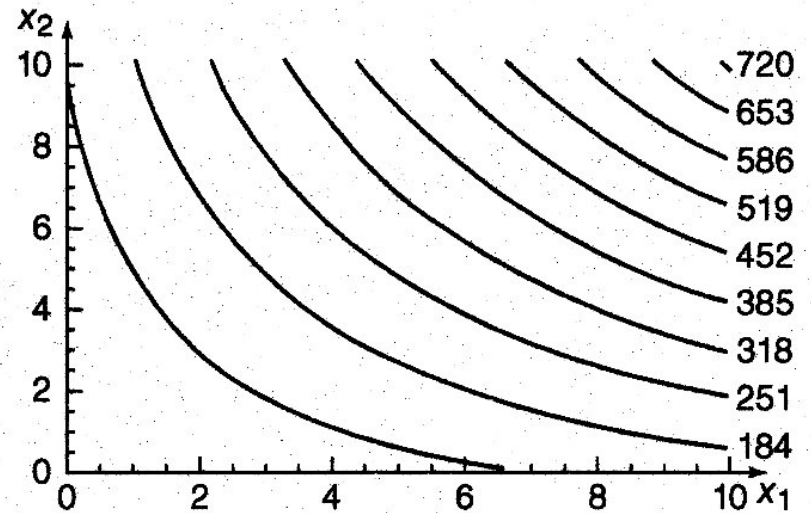
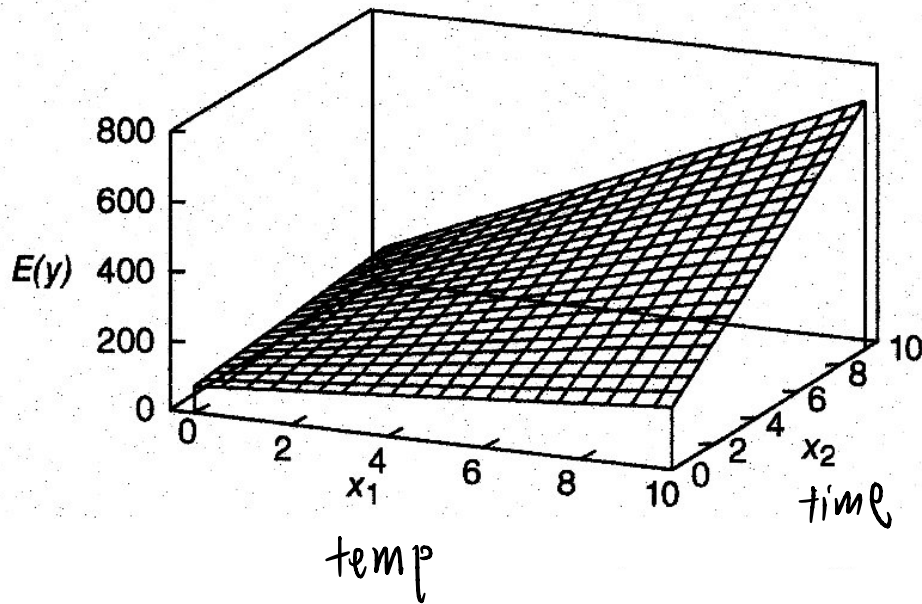


contour plot

interaction term

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$$

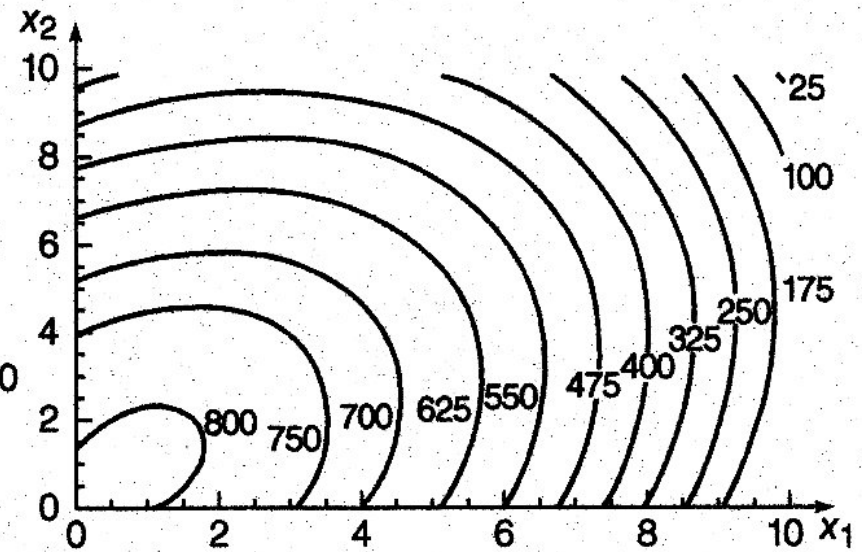
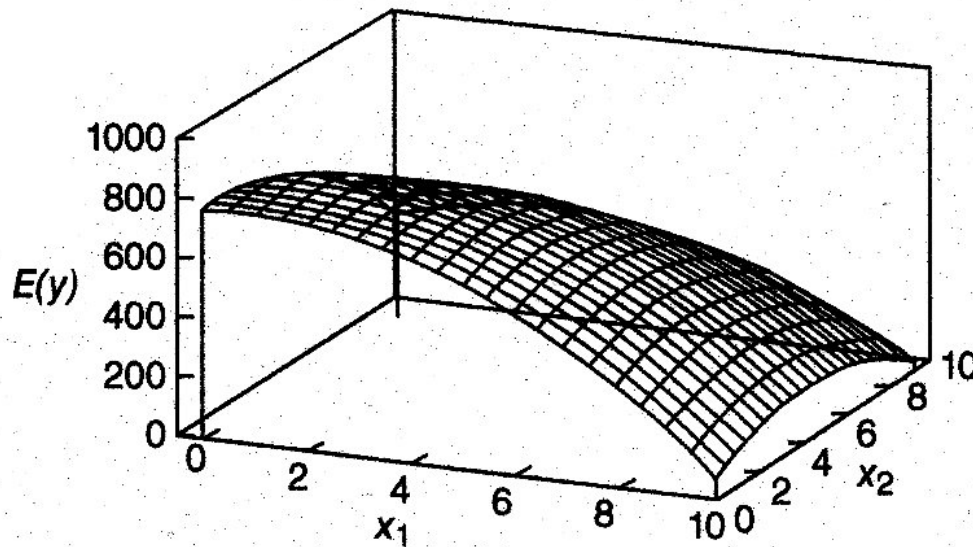
$$E(y) = 50 + 10x_1 + 7x_2 + 5x_1x_2$$



quadratic component

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$

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



Multiple linear regression model

The multiple linear regression model for a response variable y and regressor variables x_1, x_2, \dots, x_k can be written as

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} + \epsilon_i, \quad i = 1, 2, \dots, n,$$
$$= \beta_0 + \sum_{j=1}^k \beta_j x_{ij} + \epsilon_i, \quad i = 1, 2, \dots, n, \quad k \text{ regressor variable}$$

where $E(\epsilon_i) = 0$, $Var(\epsilon_i) = \sigma^2$, $i = 1, 2, \dots, n$ and ϵ_i 's are independent. Note that the number of regressor variables is k and the number of regression coefficients is $p = k + 1$.

The coefficients $\beta_j, j = 1, 2, \dots, k$ are called partial regression coefficients. The parameter β_j represents the expected change in the response per unit change in x_j when all the remaining regressor variables are held constant.

Data for Multiple Linear Regression

Observation, i	Response, y	Regressors			
		x_1	x_2	\dots	x_k
1	y_1	x_{11}	x_{12}	\dots	x_{1k}
2	y_2	x_{21}	x_{22}	\dots	x_{2k}
\vdots	\vdots	\vdots	\vdots		\vdots
n	y_n	x_{n1}	x_{n2}	\dots	x_{nk}

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

$$\xi_i = y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik})$$

least square function
(in terms of $k+1$ variable) $= \sum \xi_i^2$

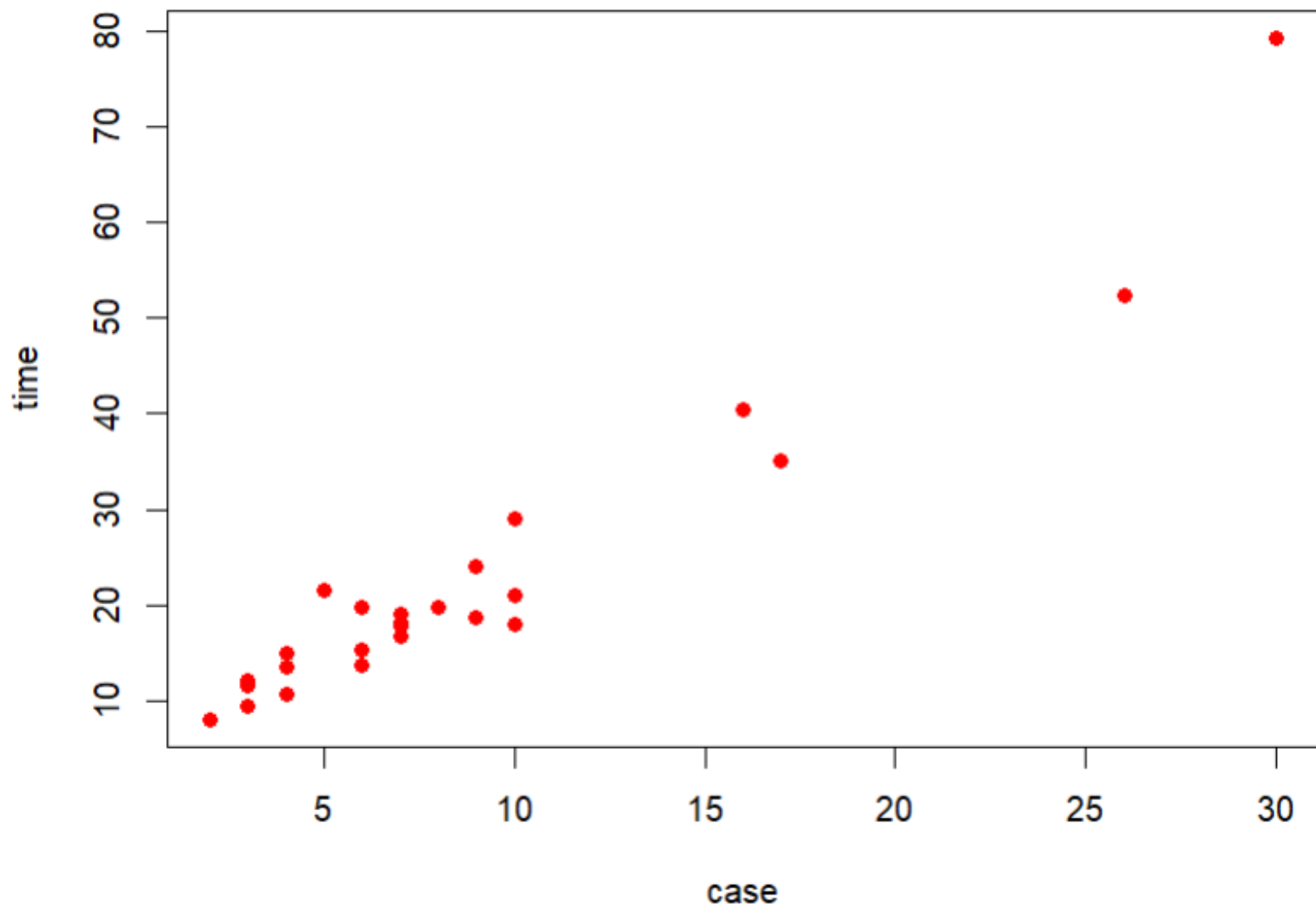
$$\left. \begin{array}{l} \frac{\partial S}{\partial \beta_0} = 0, \quad \frac{\partial S}{\partial \beta_1} = 0, \quad \dots, \quad \frac{\partial S}{\partial \beta_k} = 0 \\ \underbrace{\hspace{10em}}_{k+1 \text{ equations}} \end{array} \right\}$$

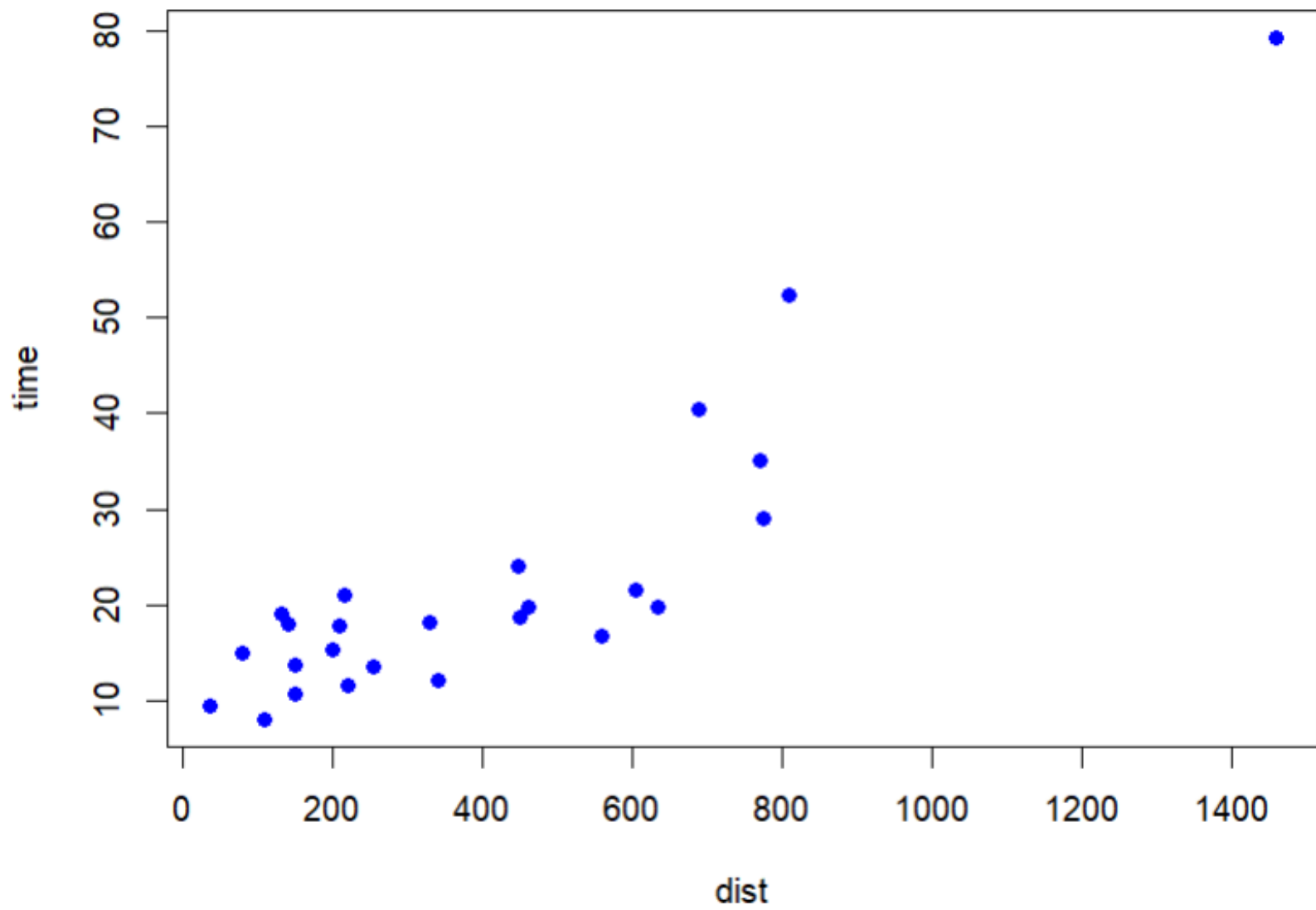
The delivery time data

The response y is the amount of time in minutes required by a route driver to stock the vending machines with beverage products and do minor maintenance of the machines in an outlet. The two regressor variables are (i) number of cases of products stocked (x_1), and (ii) the distance walked in feet (x_2). The data set is displayed below.

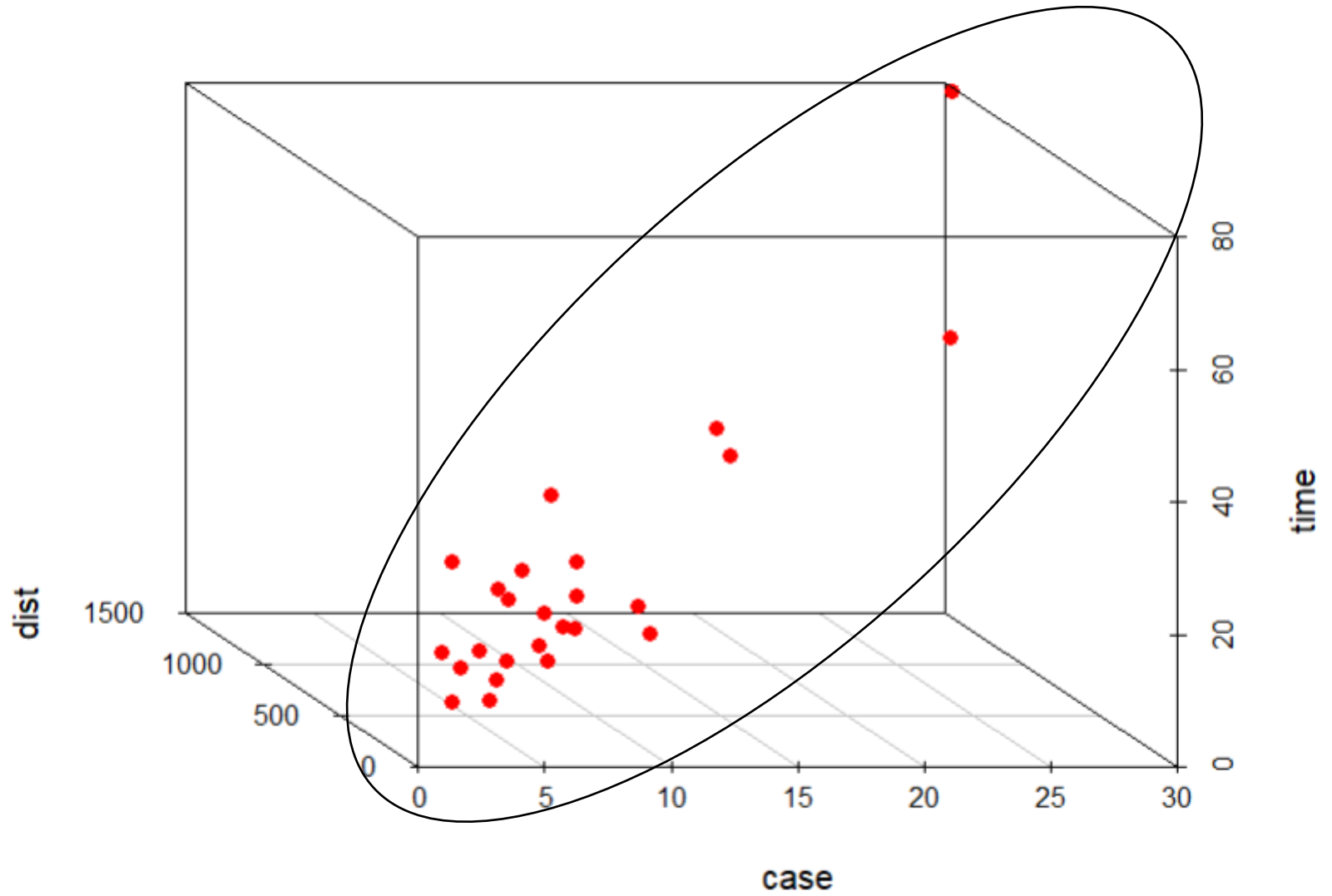
	time	case	dist
1	16.68	7	560
2	11.50	3	220
3	12.03	3	340
4	14.88	4	80
5	13.75	6	150
6	18.11	7	330
7	8.00	2	110
8	17.83	7	210
9	79.24	30	1460
10	21.50	5	605
11	40.33	16	688
12	21.00	10	215
13	13.50	4	255
14	19.75	6	462
15	24.00	9	448
16	29.00	10	776
17	15.35	6	200
18	19.00	7	132
19	9.50	3	36
20	35.10	17	770
21	17.90	10	140
22	52.32	26	810
23	18.75	9	450
24	19.83	8	635
25	10.75	4	150


```
1 #install.packages("scatterplot3d") # install package
2 library(scatterplot3d)
3 library(MASS)
4 rm(list = ls())
5 dat <- read.csv("D:\\nus_teaching\\st3131\\data\\Delivery_Time.csv",
6               header = T, sep=",")
7 dat
8 obs <- dat[,1]
9 time <- dat[,2]
10 case <- dat[,3]
11 dist <- dat[,4]
12
13 # 2d scatter plots
14 plot(case,time,pch=16,col="red")
15 plot(dist,time,pch=16,col="blue")
16
17 # 3d scatter plot
18 scatterplot3d(case,dist,time,main="3D Scatterplot",
19               pch=16,color="red",angle=145)
```





3D Scatterplot



Least-squares function and least-squares regression

The least-squares function is the error sum of squares

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

Least-squares regression means fitting a model that minimizes the error sum of squares.

$$S \quad \frac{\partial S}{\partial \beta_0} = \sum_{i=1}^n 2 \left\{ y_i - \beta_0 - \sum_{j=1}^k \beta_j x_{ij} \right\} (-1)$$

Least-squares normal equations and estimates of regression coefficients

The least-squares estimates $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$ of $\beta_0, \beta_1, \dots, \beta_k$ are obtained by minimizing the error sum of squares with respect to $\beta_0, \beta_1, \dots, \beta_k$. This is done by (i) Differentiate S with respect to $\beta_0, \beta_1, \dots, \beta_k$ to obtain $\frac{\partial S}{\partial \beta_0}, \frac{\partial S}{\partial \beta_1}, \dots, \frac{\partial S}{\partial \beta_k}$, and (ii) Set $\frac{\partial S}{\partial \beta_0}, \frac{\partial S}{\partial \beta_1}, \dots, \frac{\partial S}{\partial \beta_k}$ equal to zero to find $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$.

(i) Differentiate S with respect to $\beta_0, \beta_1, \dots, \beta_k$,

$$\begin{aligned}\frac{\partial S}{\partial \beta_0} &= \sum_{i=1}^n 2 \left(y_i - \beta_0 - \sum_{j=1}^k \beta_j x_{ij} \right) (-1), \\ \frac{\partial S}{\partial \beta_j} &= \sum_{i=1}^n 2 \left(y_i - \beta_0 - \sum_{j=1}^k \beta_j x_{ij} \right) (-x_{ij}), \quad j = 1, 2, \dots, k.\end{aligned}$$

(ii) Set $\frac{\partial S}{\partial \beta_0}, \frac{\partial S}{\partial \beta_1}, \dots, \frac{\partial S}{\partial \beta_k}$ equal to zero:

$$\begin{aligned}0 &= -2 \sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \sum_{j=1}^k \hat{\beta}_j x_{ij} \right), \\ 0 &= -2 \left[\sum_{i=1}^n x_{ij} y_i - \hat{\beta}_0 \sum_{i=1}^n x_{ij} - \sum_{i=1}^n x_{ij} \left(\sum_{j=1}^k \hat{\beta}_j x_{ij} \right) \right], \quad j = 1, 2, \dots, k.\end{aligned}$$

we have as it is now an estimate

The $k + 1$ equations can be simplified to obtain

$$n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^n x_{i1} + \hat{\beta}_2 \sum_{i=1}^n x_{i2} + \dots + \hat{\beta}_k \sum_{i=1}^n x_{ik} = \sum_{i=1}^n y_i$$

$$\hat{\beta}_0 \sum_{i=1}^n x_{i1} + \hat{\beta}_1 \sum_{i=1}^n x_{i1}^2 + \hat{\beta}_2 \sum_{i=1}^n x_{i1}x_{i2} + \dots + \hat{\beta}_k \sum_{i=1}^n x_{i1}x_{ik} = \sum_{i=1}^n x_{i1}y_i$$

$$\hat{\beta}_0 \sum_{i=1}^n x_{i2} + \hat{\beta}_1 \sum_{i=1}^n x_{i2}x_{i1} + \hat{\beta}_2 \sum_{i=1}^n x_{i2}^2 + \dots + \hat{\beta}_k \sum_{i=1}^n x_{i2}x_{ik} = \sum_{i=1}^n x_{i2}y_i$$

⋮

$$\hat{\beta}_0 \sum_{i=1}^n x_{ik} + \hat{\beta}_1 \sum_{i=1}^n x_{ik}x_{i1} + \hat{\beta}_2 \sum_{i=1}^n x_{ik}x_{i2} + \dots + \hat{\beta}_k \sum_{i=1}^n x_{ik}^2 = \sum_{i=1}^n x_{ik}y_i$$

The $k + 1$ equations can then be solved to find $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k$.

Delivery time data

Fitting multiple linear regression model

```
--  
22 # fit multiple linear regression model  
23 fitted.model <- lm(time ~ case + dist)  
24 summary(fitted.model)  
25  
26
```

19:4 (Top Level) ↕

Console

Background Jobs x

R 3.4.1 · ↗

```
> # fit multiple linear regression model  
> fitted.model <- lm(time ~ case + dist)  
> summary(fitted.model)
```

Call:

```
lm(formula = time ~ case + dist)
```

Residuals:

Min	1Q	Median	3Q	Max
-5.7880	-0.6629	0.4364	1.1566	7.4197

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	2.341231	1.096730	2.135	0.044170	*
case	1.615907	0.170735	9.464	3.25e-09	***
dist	0.014385	0.003613	3.981	0.000631	***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.259 on 22 degrees of freedom

Multiple R-squared: 0.9596, Adjusted R-squared: 0.9559

F-statistic: 261.2 on 2 and 22 DF, p-value: 4.687e-16

Least-squares estimation - matrix approach

1. Multiple linear regression model in terms of the n observations:

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \dots + \beta_k x_{1k} + \epsilon_1$$
$$\begin{pmatrix} y_2 \\ \vdots \\ y_n \end{pmatrix} = \beta_0 + \beta_1 x_{21} + \beta_2 x_{22} + \dots + \beta_k x_{2k} + \epsilon_2$$
$$\begin{pmatrix} y_n \end{pmatrix} = \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \dots + \beta_k x_{nk} + \epsilon_n$$

vector
 y

2. Multiple linear regression model in matrix notation:

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

regressor variable

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1k} \\ 1 & x_{21} & x_{22} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nk} \end{bmatrix}_{n \times (k+1)}$$

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}_{(k+1) \times 1} \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}_{n \times 1} \quad (\epsilon_1 \ \epsilon_2 \ \dots \ \epsilon_n) \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

3. Least-squares function

$$y = X\beta + \xi$$

$$\Rightarrow \xi = y - X\beta$$

$$S = \sum_{i=1}^n \epsilon_i^2$$

$$= \epsilon' \epsilon$$

$$= (y - X\beta)'(y - X\beta)$$

$$= (y' - \beta' X')(y - X\beta)$$

$$= y'y - y'X\beta - \beta'X'y + \beta'X'X\beta$$

$$= y'y - 2y'X\beta + \beta'X'X\beta \quad \because y'X\beta = \beta'X'y$$

4. Least-squares normal equations

$$\frac{\partial \mathcal{S}}{\partial \beta} = -2X'y + 2X'X\beta \quad \because \frac{\partial(a'\beta)}{\partial \beta} = a, \quad \frac{\partial(\beta'A\beta)}{\partial \beta} = 2A\beta$$

Annotations: "scalar quantity" points to \mathcal{S} ; "vector" points to β .

$$0 = -2X'y + 2X'X\hat{\beta}$$

$$X'X\hat{\beta} = X'y$$

Annotation: "same" points to the boxed equation.

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

$$\begin{bmatrix} n & \sum_{i=1}^n x_{i1} & \sum_{i=1}^n x_{i2} & \dots & \sum_{i=1}^n x_{ik} \\ \sum_{i=1}^n x_{i1} & \sum_{i=1}^n x_{i1}^2 & \sum_{i=1}^n x_{i1}x_{i2} & \dots & \sum_{i=1}^n x_{i1}x_{ik} \\ \sum_{i=1}^n x_{i2} & \sum_{i=1}^n x_{i2}x_{i1} & \sum_{i=1}^n x_{i2}^2 & \dots & \sum_{i=1}^n x_{i2}x_{ik} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n x_{ik} & \sum_{i=1}^n x_{ik}x_{i1} & \sum_{i=1}^n x_{ik}x_{i2} & \dots & \sum_{i=1}^n x_{ik}^2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_{i1}y_i \\ \sum_{i=1}^n x_{i2}y_i \\ \vdots \\ \sum_{i=1}^n x_{ik}y_i \end{bmatrix}$$

5. Least-squares estimates of $\hat{\beta}$

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

6. Predicted response \hat{y} and residual e

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

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

$$= \boxed{X(X'X)^{-1}X'}y$$

$$= Hy \quad \text{where } H \text{ is called the hat matrix.}$$

$$\text{residual } e = y - \hat{y} \quad (\text{observed} - \text{predicted})$$

$$= y - X\hat{\beta}$$

$$= y - Hy$$

$$= (I_n - H)y$$

Delivery time data

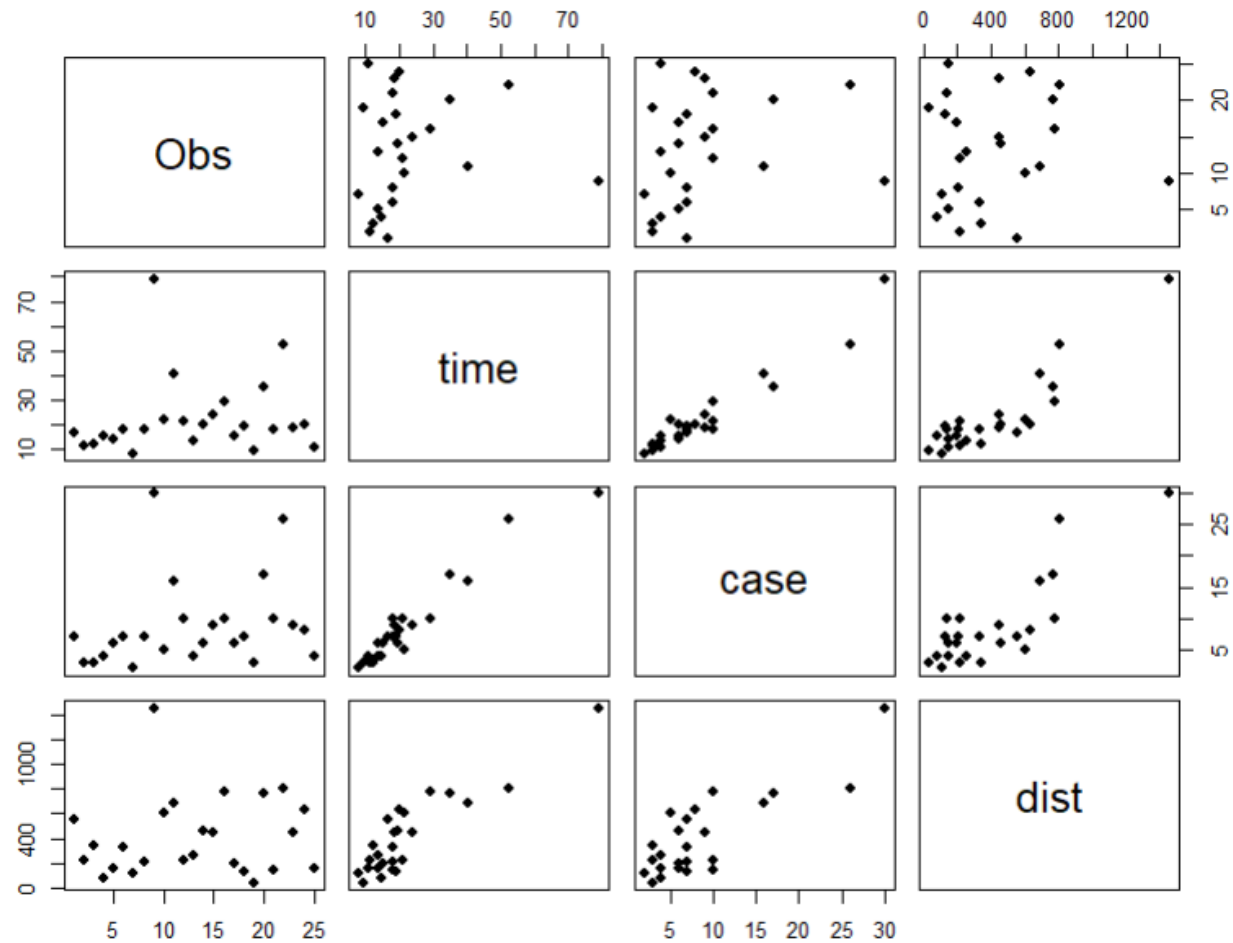
29

```
30 # scatter matrix plot
```

```
31 pairs(dat, pch=16)
```

32

30:1 (Top Level) ↕



Journal of Management Education 36(7)p.809-824

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ 7 & 3 & \dots & 4 \\ 560 & 220 & \dots & 150 \end{bmatrix} \begin{matrix} 1 \times 3 \\ 1 \times 3 \\ \vdots \\ 1 \times 3 \end{matrix} = \begin{bmatrix} 25 & 219 & 10,232 \\ 219 & 3,055 & 133,899 \\ 10,232 & 133,899 & 6,725,688 \end{bmatrix} \begin{matrix} 3 \times 3 \\ 3 \times 3 \\ 3 \times 3 \end{matrix}$$

$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ 7 & 3 & \dots & 4 \\ 560 & 220 & \dots & 150 \end{bmatrix} \begin{bmatrix} 16.68 \\ 11.50 \\ \vdots \\ 10.75 \end{bmatrix} = \begin{bmatrix} 559.60 \\ 7,375.44 \\ 337,072.00 \end{bmatrix}$$

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

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix} = \begin{bmatrix} 25 & 219 & 10,232 \\ 219 & 3,055 & 133,899 \\ 10,232 & 133,899 & 6,725,688 \end{bmatrix}^{-1} \begin{bmatrix} 559.60 \\ 7,375.44 \\ 337,072.00 \end{bmatrix}$$

$$= \begin{bmatrix} 0.11321518 & -0.00444859 & -0.00008367 \\ -0.00444859 & 0.00274378 & -0.00004786 \\ -0.00008367 & -0.00004786 & 0.00000123 \end{bmatrix} \begin{bmatrix} 559.60 \\ 7,375.44 \\ 337,072.00 \end{bmatrix}$$

$$= \begin{bmatrix} 2.34123115 \\ 1.61590712 \\ 0.01438483 \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} 1 & 7 & 560 \\ 1 & 3 & 220 \\ 1 & 3 & 340 \\ 1 & 4 & 80 \\ 1 & 6 & 150 \\ 1 & 7 & 330 \\ 1 & 2 & 110 \\ 1 & 7 & 210 \\ 1 & 30 & 1460 \\ 1 & 5 & 605 \\ 1 & 16 & 688 \\ 1 & 10 & 215 \\ 1 & 4 & 255 \\ 1 & 6 & 462 \\ 1 & 9 & 448 \\ 1 & 10 & 776 \\ 1 & 6 & 200 \\ 1 & 7 & 132 \\ 1 & 3 & 36 \\ 1 & 17 & 770 \\ 1 & 10 & 140 \\ 1 & 26 & 810 \\ 1 & 9 & 450 \\ 1 & 8 & 635 \\ 1 & 4 & 150 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 16.68 \\ 11.50 \\ 12.03 \\ 14.88 \\ 13.75 \\ 18.11 \\ 8.00 \\ 17.83 \\ 79.24 \\ 21.50 \\ 40.33 \\ 21.00 \\ 13.50 \\ 19.75 \\ 24.00 \\ 29.00 \\ 15.35 \\ 19.00 \\ 9.50 \\ 35.10 \\ 17.90 \\ 52.32 \\ 18.75 \\ 19.83 \\ 10.75 \end{bmatrix}$$

```

33 # matrices and finding betas
34 one <- rep(1,length(time))
35 X <- array(c(one,case,dist), dim=c(length(time),3))
36 y <- array(time, dim=c(length(time),1))
37 XPX <- t(X) %*% X
38 XPX
39 XPy <- t(X) %*% y
40 XPy
41 betahat <- solve(XPX, XPy)
42 betahat
43

```

33:1 (Top Level) ↕

Console

Background Jobs x

R 3.4.1 · ↗

```
> y <- array(time, dim=c(length(time),1))
```

```
> XPX <- t(X) %*% X
```

```
> XPX
```

```

      [,1] [,2] [,3]
[1,]    25  219 10232
[2,]   219 3055 133899
[3,] 10232 133899 6725688

```

```
> XPy <- t(X) %*% y
```

```
> XPy
```

```

      [,1]
[1,]  559.60
[2,] 7375.44
[3,] 337071.69

```

```
> betahat <- solve(XPX, XPy)
```

```
> betahat
```

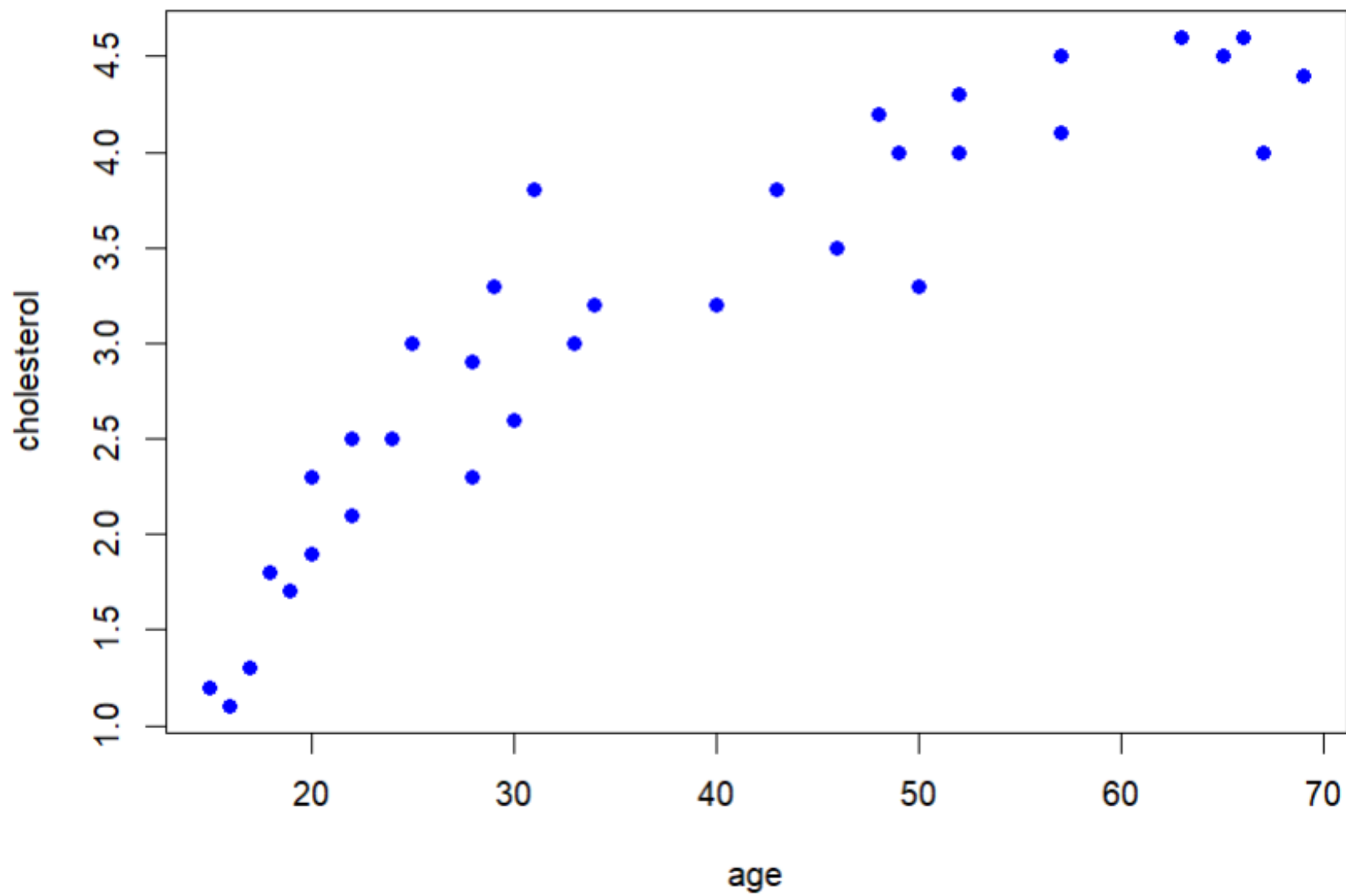
```

      [,1]
[1,] 2.34123115
[2,] 1.61590721
[3,] 0.01438483

```


Cholesterol age data

	age	cholesterol_level		age	cholesterol_level
1	15	1.2	18	31	3.8
2	17	1.3	19	40	3.2
3	16	1.1	20	43	3.8
4	19	1.7	21	46	3.5
5	18	1.8	22	48	4.2
6	20	2.3	23	49	4.0
7	20	1.9	24	50	3.3
8	22	2.1	25	52	4.0
9	22	2.5	26	52	4.3
10	24	2.5	27	57	4.1
11	25	3.0	28	57	4.5
12	28	2.3	29	63	4.6
13	28	2.9	30	65	4.5
14	29	3.3	31	66	4.6
15	30	2.6	32	67	4.0
16	33	3.0	33	69	4.4
17	34	3.2			



Cholesterol age data

Straight line model

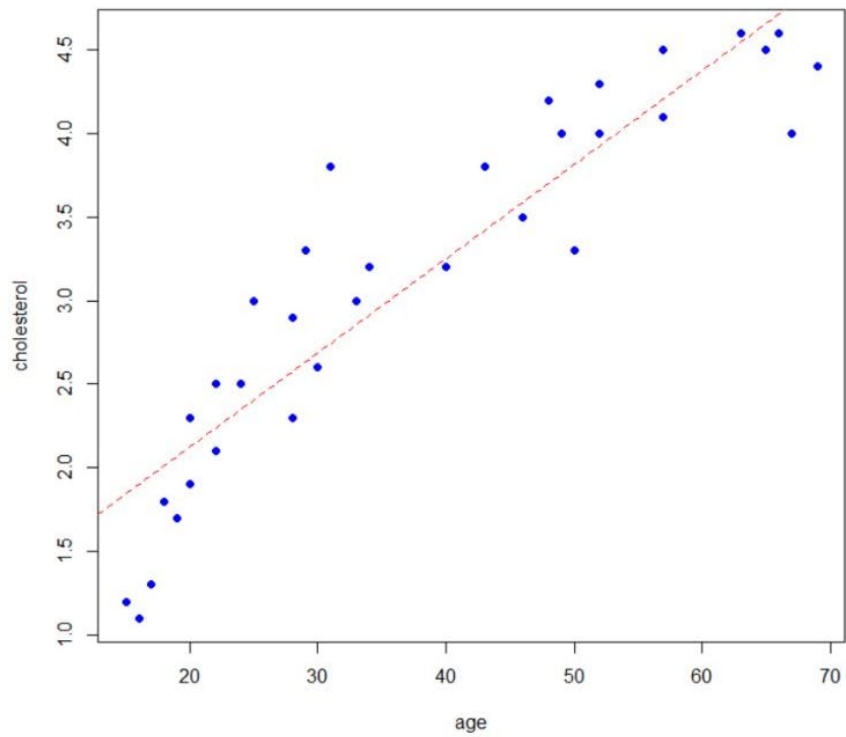
$$\textit{cholesterol} = \beta_0 + \beta_1 \textit{age} + \epsilon$$

Quadratic line model

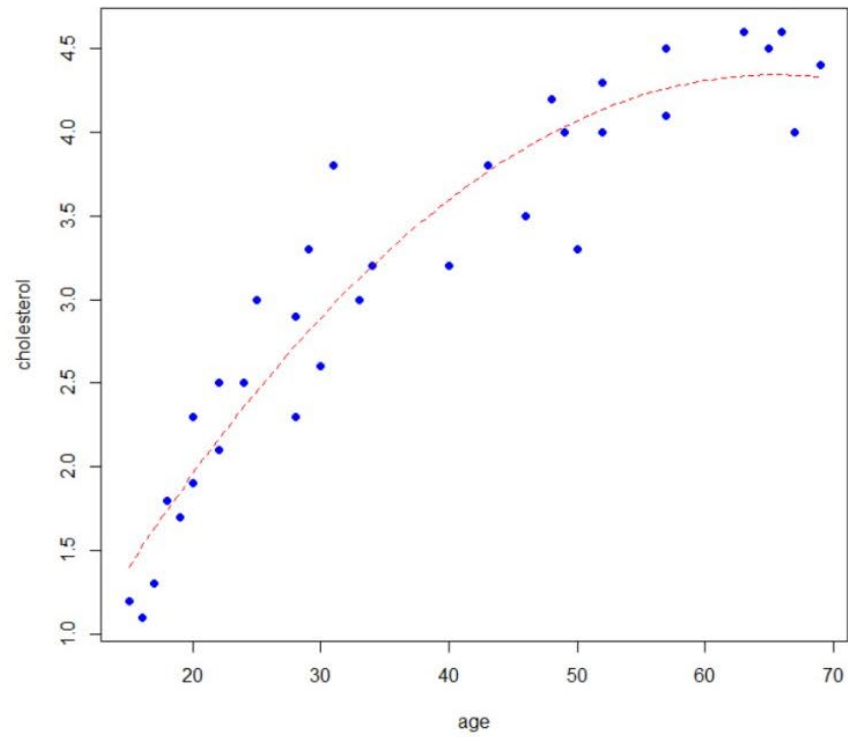
$$\textit{cholesterol} = \beta_0 + \beta_1 \textit{age} + \beta_2 \textit{age}^2 + \epsilon$$

Cholesterol age data

```
2 #install.packages("np")
3 library(MASS)
4 library(np)
5 rm(list=ls())
6
7 dat <- read.csv("D:\\nus_teaching\\st3131\\data\\cholesterol_age.csv",
8               header = T, sep=",")
9 age <- dat[,1]
10 cholesterol <- dat[,2]
11
12 #Fit straight line model
13 mod1 <- lm(cholesterol~age)
14 COEF <- coef(mod1)
15 names(COEF) <- NULL
16 beta0 <- COEF[1]
17 beta1 <- COEF[2]
18 plot(age,cholesterol,pch=16,col="blue")
19 abline(beta0,beta1,lty=1,col="red")
20 summary(mod1)
21
22 #Fit quadratic model
23 mod2 <-lm(cholesterol~age + I(age^2))
24 mod2
25 COEF2 <- coef(mod2)
26 names(COEF2) <- NULL
27 COEF2
28 beta2.0 <- COEF2[1]
29 beta2.1 <- COEF2[2]
30 beta2.2 <- COEF2[3]
31 beta2.0
32 beta2.1
33 beta2.2
34 summary(mod2)
35 plot(age,cholesterol,pch=16,col="blue")
36 curve(beta2.0+x*beta2.1+x*x*beta2.2, add=TRUE, lty=1,col="red")
```



Multiple R-squared: 0.839

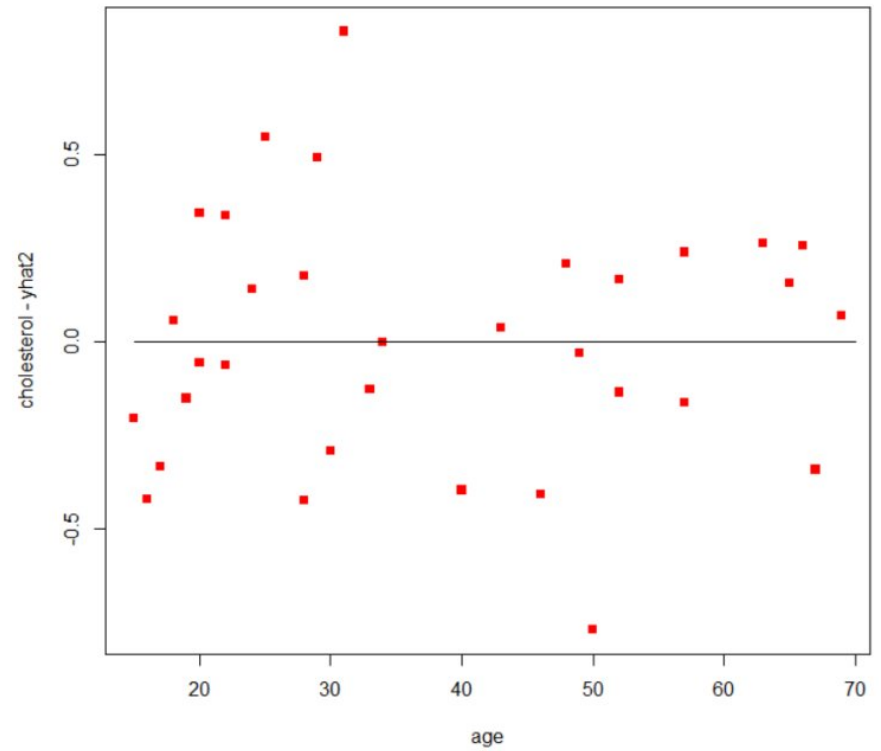
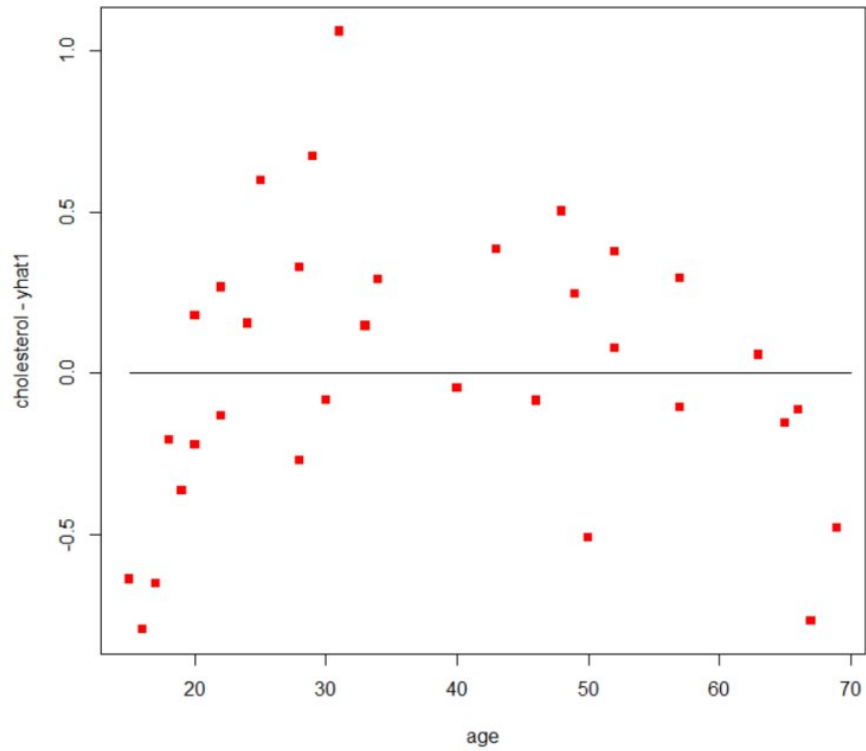


Multiple R-squared: 0.9041

straight line model

Residual plots

quadratic model



The End