CHAPTER 14

14.1 The data can be tabulated and the sums computed as

i	*x*	*y*	x^2	x^3	x^4	*xy*	x^2y
1	10	25	100	1000	10000	250	2500
2	20	70	400	8000	160000	1400	28000
3	30	380	900	27000	810000	11400	342000
4	40	550	1600	64000	2560000	22000	880000
5	50	610	2500	125000	6250000	30500	1525000
6	60	1220	3600	216000	12960000	73200	4392000
7	70	830	4900	343000	24010000	58100	4067000
8	80	1450	6400	512000	40960000	116000	9280000
Σ	360	5135	20400	1296000	87720000	312850	20516500

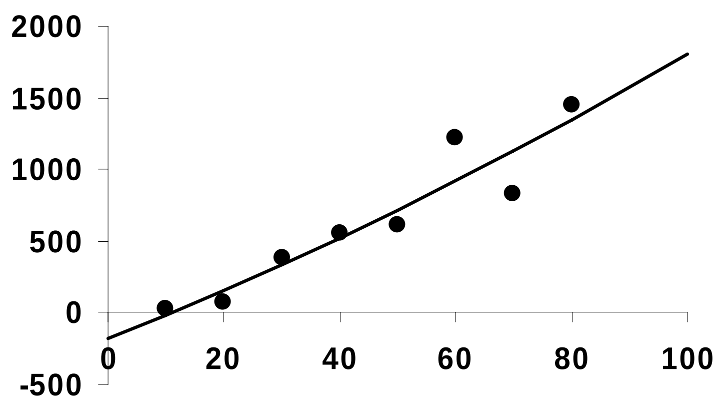
Normal equations:

$$\begin{bmatrix} 8 & 360 & 20400 \\ 360 & 20400 & 1296000 \\ 20400 & 1296000 & 87720000 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 5135 \\ 312850 \\ 20516500 \end{Bmatrix}$$

which can be solved for the coefficients yielding the following best-fit polynomial

$$F = -178.4821 + 16.12202v + 0.037202v^2$$

Here is the resulting fit:



The predicted values can be used to determined the sum of the squares. Note that the mean of the *y* values is 641.875.

i	*x*	*y*	y_{pred}	$(y_i - \bar{y})^2$	$(y - y_{\text{pred}})^2$
1	10	25	-13.5417	380535	1485
2	20	70	158.8393	327041	7892
3	30	380	338.6607	68579	1709

4	40	550	525.9226	8441	580
5	50	610	720.625	1016	12238
6	60	1220	922.7679	334229	88347
7	70	830	1132.351	35391	91416
8	80	1450	1349.375	653066	10125
Σ				1808297	213793

The coefficient of determination can be computed as

$$r^2 = \frac{1808297 - 213793}{1808297} = 0.88177$$

The model fits the trend of the data nicely, but it has the deficiency that it yields physically unrealistic negative forces at low velocities.

14.2 The sum of the squares of the residuals for this case can be written as

$$S_r = \sum_{i=1}^{n} \left(y_i - a_1 x_i - a_2 x_i^2 \right)^2$$

The partial derivatives of this function with respect to the unknown parameters can be determined as

$$\frac{\partial S_r}{\partial a_1} = -2 \sum \left[(y_i - a_1 x_i - a_2 x_i^2) x_i \right]$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum \left[(y_i - a_1 x_i - a_2 x_i^2) x_i^2 \right]$$

Setting the derivative equal to zero and evaluating the summations gives

$$\left(\sum x_i^2 \right) a_1 + \left(\sum x_i^3 \right) a_2 = \sum x_i y_i$$

$$\left(\sum x_i^3 \right) a_1 + \left(\sum x_i^4 \right) a_2 = \sum x_i^2 y_i$$

which can be solved for

$$a_1 = \frac{\sum x_i y_i \sum x_i^4 - \sum x_i^2 y_i \sum x_i^3}{\sum x_i^2 \sum x_i^4 - \left(\sum x_i^3 \right)^2}$$

$$a_2 = \frac{\sum x_i^2 \sum x_i^2 y_i - \sum x_i y_i \sum x_i^3}{\sum x_i^2 \sum x_i^4 - \left(\sum x_i^3 \right)^2}$$

The model can be tested for the data from Table 12.1.

x	y	x^2	x^3	x^4	xy	x^2y
10	25	100	1000	10000	250	2500
20	70	400	8000	160000	1400	28000
30	380	900	27000	810000	11400	342000
40	550	1600	64000	2560000	22000	880000
50	610	2500	125000	6250000	30500	1525000
60	1220	3600	216000	12960000	73200	4392000
70	830	4900	343000	24010000	58100	4067000
80	1450	6400	512000	40960000	116000	9280000
Σ		20400	1296000	87720000	312850	20516500

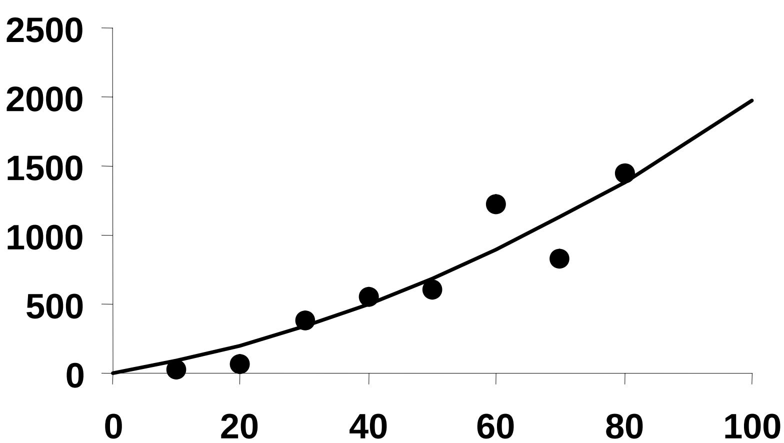
$$a_1 = \frac{312850(87720000) - 20516500(1296000)}{20400(87720000) - (1296000)^2} = 7.771024$$

$$a_2 = \frac{20400(20516500) - 312850(1296000)}{20400(87720000) - (1296000)} = 0.119075$$

Therefore, the best-fit model is

$$y = 7.771024x + 0.119075x^2$$

The fit, along with the original data can be plotted as



14.3 The data can be tabulated and the sums computed as

i	x	y	x^2	x^3	x^4	x^5	x^6	xy	x^2y	x^3y
1	3	1.6	9	27	81	243	729	4.8	14.4	43.2
2	4	3.6	16	64	256	1024	4096	14.4	57.6	230.4
3	5	4.4	25	125	625	3125	15625	22	110	550
4	7	3.4	49	343	2401	16807	117649	23.8	166.6	1166.2
5	8	2.2	64	512	4096	32768	262144	17.6	140.8	1126.4
6	9	2.8	81	729	6561	59049	531441	25.2	226.8	2041.2

7	11	3.8	121	1331	14641	161051	1771561	41.8	459.8	5057.8
8	12	4.6	144	1728	20736	248832	2985984	55.2	662.4	7948.8
Σ	59	26.4	509	4859	49397	522899	5689229	204.8	1838.4	18164

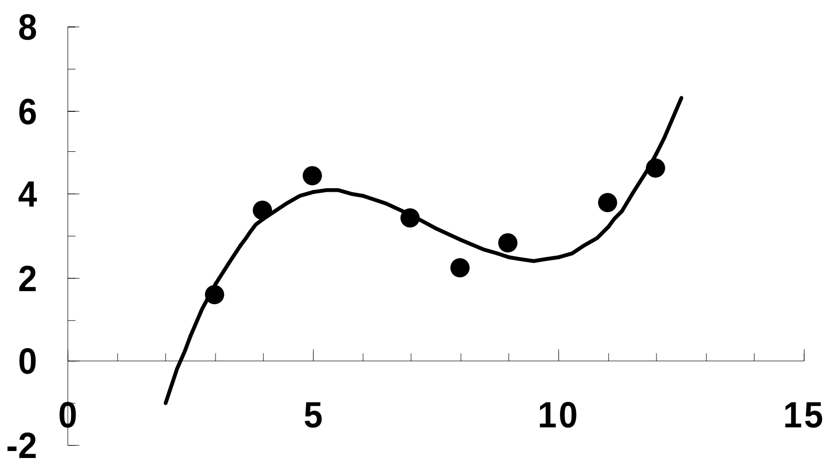
Normal equations:

$$\begin{bmatrix} 8 & 59 & 509 & 4859 \\ 59 & 509 & 4859 & 49397 \\ 509 & 4859 & 49397 & 522899 \\ 4859 & 49397 & 522899 & 5689229 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix} = \begin{Bmatrix} 26.4 \\ 204.8 \\ 1838.4 \\ 18164 \end{Bmatrix}$$

which can be solved for the coefficients yielding the following best-fit polynomial

$$y = -11.4887 + 7.143817x - 1.04121x^2 + 0.046676x^3$$

Here is the resulting fit:



The predicted values can be used to determined the sum of the squares. Note that the mean of the y values is 3.3.

i	x	y	y_{pred}	$(y_i - \bar{y})^2$	$(y - y_{\text{pred}})^2$
1	3	1.6	1.83213	2.8900	0.0539
2	4	3.6	3.41452	0.0900	0.0344
3	5	4.4	4.03471	1.2100	0.1334
4	7	3.4	3.50875	0.0100	0.0118
5	8	2.2	2.92271	1.2100	0.5223
6	9	2.8	2.4947	0.2500	0.0932
7	11	3.8	3.23302	0.2500	0.3215
8	12	4.6	4.95946	1.6900	0.1292
Σ				7.6000	1.2997

The coefficient of determination can be computed as

$$r^2 = \frac{7.6 - 1.2997}{7.6} = 0.829$$

14.4
```
function p = polyreg(x,y,m)
% polyreg(x,y,m):
%   Polynomial regression.
% input:
%   x = independent variable
%   y = dependent variable
%   m = order of polynomial
% output:
%   p = vector of coefficients

n = length(x);
if length(y)~=n, error('x and y must be same length'); end
for i = 1:m+1
  for j = 1:i
    k = i+j-2;
    s = 0;
    for l = 1:n
      s = s + x(l)^k;
    end
    A(i,j) = s;
    A(j,i) = s;
  end
  s = 0;
  for l = 1:n
    s = s + y(l)*x(l)^(i-1);
  end
  b(i) = s;
end
p = A\b';
```

<u>Test solving Prob. 14.3:</u>

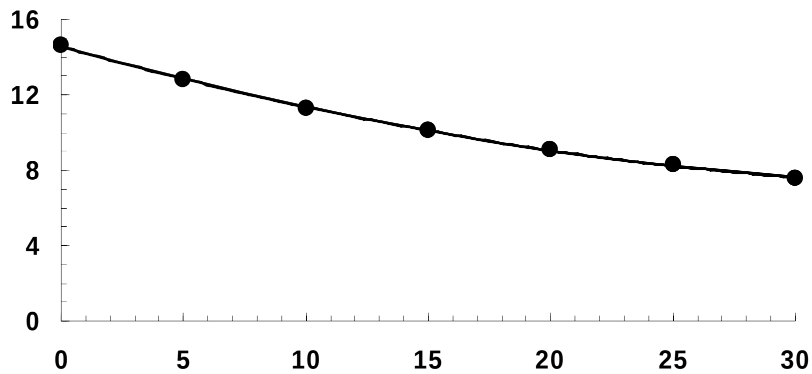
```
>> x = [3 4 5 7 8 9 11 12];
>> y = [1.6 3.6 4.4 3.4 2.2 2.8 3.8 4.6];
>> polyreg(x,y,3)

ans =

  -11.4887
    7.1438
   -1.0412
    0.0467
```

14.5 Because the data is curved, a linear regression will undoubtedly have too much error. Therefore, as a first try, fit a parabola,

```
>> format long
>> T = [0 5 10 15 20 25 30];
>> c = [14.6 12.8 11.3 10.1 9.09 8.26 7.56];
>> p = polyfit(T,c,2)

p =
   0.00439523809524  -0.36335714285714  14.55190476190477
```

Thus, the best-fit parabola would be

$$c = 14.55190476 - 0.36335714T + 0.0043952381T^2$$



We can use this equation to generate predictions corresponding to the data. When these values are rounded to the same number of significant digits the results are

T	*c*-data	*c*-pred	rounded
0	14.6	14.55190	14.6
5	12.8	12.84500	12.8
10	11.3	11.35786	11.4
15	10.1	10.09048	10.1
20	9.09	9.04286	9.04
25	8.26	8.21500	8.22
30	7.56	7.60690	7.61

Thus, although the plot looks good, discrepancies occur in the third significant digit.

We can, therefore, fit a third-order polynomial

```
>> p = polyfit(T,c,3)

p =
  -0.00006444444444   0.00729523809524  -0.39557936507936  14.60023809523810
```

Thus, the best-fit cubic would be

$$c = 14.600238095 - 0.3955793651T + 0.0072952381T^2 - 0.0000644444T^3$$

We can use this equation to generate predictions corresponding to the data. When these values are rounded to the same number of significant digits the results are

T	c-data	c-pred	rounded
0	14.6	14.60020	14.6
5	12.8	12.79663	12.8
10	11.3	11.30949	11.3
15	10.1	10.09044	10.1
20	9.09	9.09116	9.09
25	8.26	8.26331	8.26
30	7.56	7.55855	7.56

Thus, the predictions and data agree to three significant digits.

14.6 The multiple linear regression model to evaluate is

$$o = a_0 + a_1 T + a_2 c$$

The [Z] and y matrices can be set up using MATLAB commands in a fashion similar to Example 14.4,

```
>> format long
>> t = [0 5 10 15 20 25 30];
>> T = [t t t]';
>> c = [zeros(size(t)) 10*ones(size(t)) 20*ones(size(t))]';
>> Z = [ones(size(T)) T c];
>> y = [14.6 12.8 11.3 10.1 9.09 8.26 7.56 12.9 11.3 10.1 9.03 8.17
7.46 6.85 11.4 10.3 8.96 8.08 7.35 6.73 6.2]';
```

The coefficients can be evaluated as

```
>> a = Z\y

a =
  13.52214285714286
  -0.20123809523810
  -0.10492857142857
```

Thus, the best-fit multiple regression model is

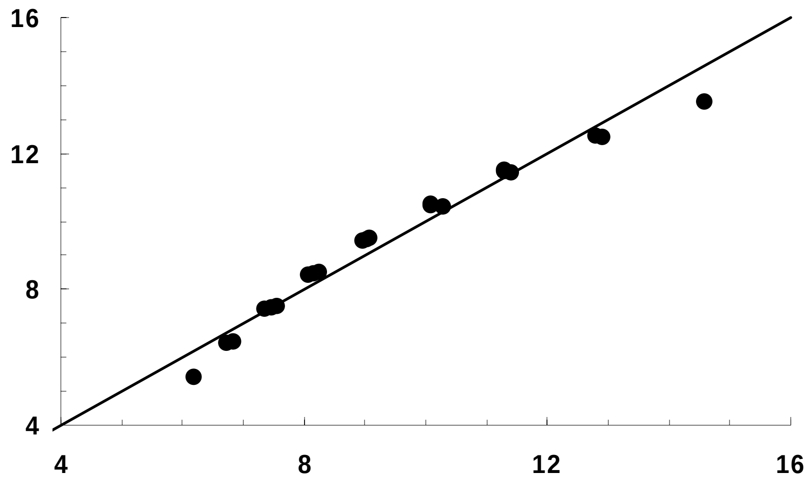
$$o = 13.52214285714286 - 0.20123809523810T - 0.10492857142857c$$

We can evaluate the prediction at T = 12 and c = 15 and evaluate the percent relative error as

```
>> cp = a(1)+a(2)*12+a(3)*15

cp =
   9.53335714285714

>> ea = abs((9.09-cp)/9.09)*100
```

```
ea =
   4.87741631305987
```

Thus, the error is considerable. This can be seen even better by generating predictions for all the data and then generating a plot of the predictions versus the data. A one-to-one line is included to show how the predictions diverge from a perfect fit.



The cause for the discrepancy is because the dependence of oxygen concentration on the unknowns is significantly nonlinear. It should be noted that this is particularly the case for the dependency on temperature.

14.7 The multiple linear regression model to evaluate is

$$y = a_0 + a_1T + a_2T^2 + a_3T^3 + a_4c$$

The [Z] matrix can be set up as in

```
>> T = 0:5:30;
>> T = [T T T]';
>> c = [0 0 0  0 0 0 0 10 10 10 10 10 10 10 20 20 20 20 20 20 20]';
>> o = [1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1]';
>> y = [14.6 12.8 11.3 10.1 9.09 8.26 7.56 12.9 11.3 10.1 9.03 8.17
7.46 6.85 11.4 10.3 8.96 8.08 7.35 6.73 6.2]';
>> Z = [o T T.^2 T.^3 c];
```

Then, the coefficients can be generated by solving Eq.(14.10)

```
>> format long
>> a = (Z'*Z)\[Z'*y]

a =
  14.02714285714287
  -0.33642328042328
   0.00574444444444
```

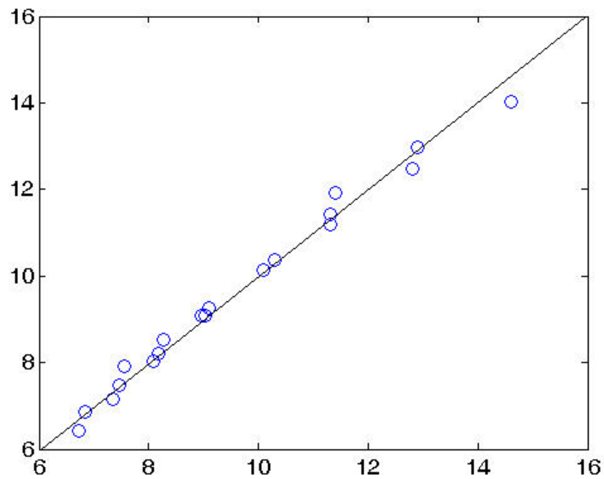
```
  -0.00004370370370
  -0.10492857142857
```

Thus, the least-squares fit is

$$y = 14.027143 - 0.336423T + 0.00574444T^2 - 0.000043704T^3 - 0.10492857c$$

The model can then be used to predict values of oxygen at the same values as the data. These predictions can be plotted against the data to depict the goodness of fit.

```
>> yp = Z*a
>> plot(y,yp,'o')
```



Finally, the prediction can be made at T = 12 and c = 15,

```
>> a(1)+a(2)*12+a(3)*12^2+a(4)*12^3+a(5)*15
ans =
   9.16781492063485
```

which compares favorably with the true value of 9.09 mg/L.

14.8 The multiple linear regression model to evaluate is

$$y = a_0 + a_1 x_1 + a_2 x_2$$

The [Z] matrix can be set up as in

```
>> x1 = [0 1 1 2 2 3 3 4 4]';
>> x2 = [0 1 2 1 2 1 2 1 2]';
>> y = [15.1 17.9 12.7 25.6 20.5 35.1 29.7 45.4 40.2]';
>> o = [1 1 1 1 1 1 1 1 1]';
>> Z = [o x1 x2 y];
```

Then, the coefficients can be generated by solving Eq.(14.10)

```
>> a = (Z'*Z)\[Z'*y]

a =
   14.4609
    9.0252
   -5.7043
```

Thus, the least-squares fit is

$$y = 14.4609 + 9.0252x_1 - 5.7043x_2$$

The model can then be used to predict values of the unknown at the same values as the data. These predictions can be used to determine the correlation coefficient and the standard error of the estimate.

```
>> yp = Z*a

>> SSR = sum((yp - y).^2)
SSR =
    4.7397

>> SST = sum((y - mean(y)).^2)
SST =
  1.0587e+003

>> r2 = (SST - SSR)/SST
r2 =
    0.9955

>> r = sqrt(r2)
r =
    0.9978

>> syx = sqrt(SSR/(length(y)-3))
syx =
    0.8888
```

14.9 The multiple linear regression model to evaluate is

$$\log Q = \log \alpha_0 + \alpha_1 \log(D) + \alpha_2 \log(S)$$

The [Z] matrix can be set up as in

```
>> D = [.3 .6 .9 .3 .6 .9 .3 .6 .9]';
>> S = [.001 .001 .001 .01 .01 .01 .05 .05 .05]';
>> Q = [.04 .24 .69 .13 .82 2.38 .31 1.95 5.66]';
>> o = [1 1 1 1 1 1 1 1 1]';
>> Z = [o log10(D) log10(S)]
```

Then, the coefficients can be generated by solving Eq.(14.10)

```
>> a = (Z'*Z)\[Z'*log10(Q)]
```

```
a =
    1.5609
    2.6279
    0.5320
```

Thus, the least-squares fit is

$$\log Q = 1.5609 + 2.6279\log(D) + 0.5320\log(S)$$

Taking the inverse logarithm gives

$$Q = 10^{1.5609} D^{2.6279} S^{0.5320} = 36.3813 D^{2.6279} S^{0.5320}$$

14.10 The linear regression model to evaluate is

$$p(t) = Ae^{-1.5t} + Be^{-0.3t} + Ce^{-0.05t}$$

The unknowns can be entered and the [Z] matrix can be set up as in

```
>> p = [6 4.4 3.2 2.7 2 1.9 1.7 1.4 1.1]';
>> t = [0.5 1 2 3 4 5 6 7 9]';
>> Z = [exp(-1.5*t) exp(-0.3*t) exp(-0.05*t)];
```

Then, the coefficients can be generated by solving Eq.(14.10)

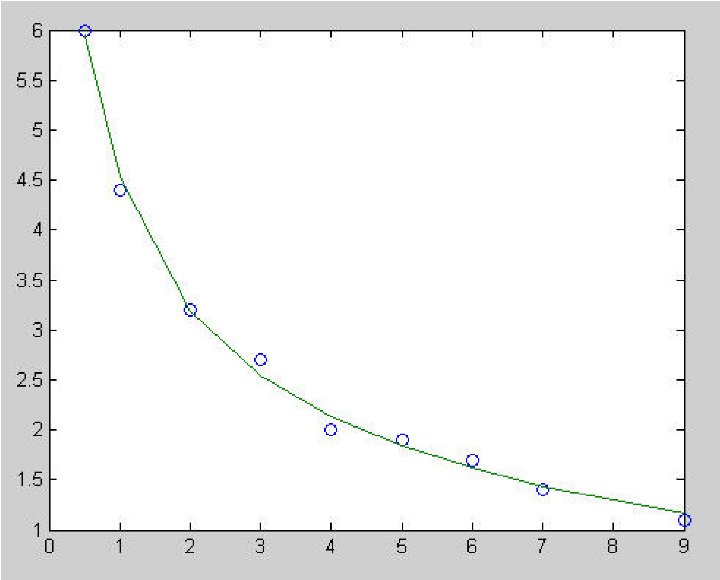
```
>> a = (Z'*Z)\[Z'*p]

a =
    4.1375
    2.8959
    1.5349
```

Thus, the least-squares fit is

$$p(t) = 4.1375e^{-1.5t} + 2.8959e^{-0.3t} + 1.5349e^{-0.05t}$$

The fit and the data can be plotted as

```
>> pp = Z*a;
>> plot(t,p,'o',t,pp)
```



14.11 First, an M-file function must be created to compute the sum of the squares,

```
function f = fSSR(a,Im,Pm)
Pp = a(1)*Im/a(2).*exp(-Im/a(2)+1);
f = sum((Pm-Pp).^2);
```

The data can then be entered as

```
>> I = [50 80 130 200 250 350 450 550 700];
>> P = [99 177 202 248 229 219 173 142 72];
```

The minimization of the function is then implemented by

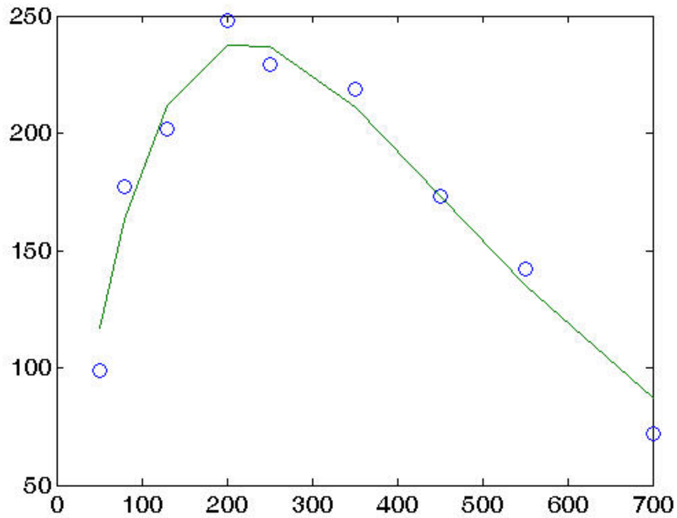
```
>> a = fminsearch(@fSSR, [200, 200], [], I, P)

a =
  238.7124  221.8239
```

The best-fit model is therefore

$$P = 238.7124 \frac{I}{221.8239} e^{-\frac{I}{221.8239}+1}$$

The fit along with the data can be displayed graphically.

```
>> Pp = a(1)*I/a(2).*exp(-I/a(2)+1);
>> plot(I,P,'o',I,Pp)
```



14.12 First, an M-file function must be created to compute the sum of the squares,

```
function f = fSSR(a,xm,ym)
yp = a(1)*xm.*exp(a(2)*xm);
f = sum((ym-yp).^2);
```

The data can then be entered as

```
>> x = [.1 .2 .4 .6 .9 1.3 1.5 1.7 1.9];
>> y = [0.75 1.25 1.45 1.25 0.85 0.55 0.35 0.28 0.18];
```

The minimization of the function is then implemented by

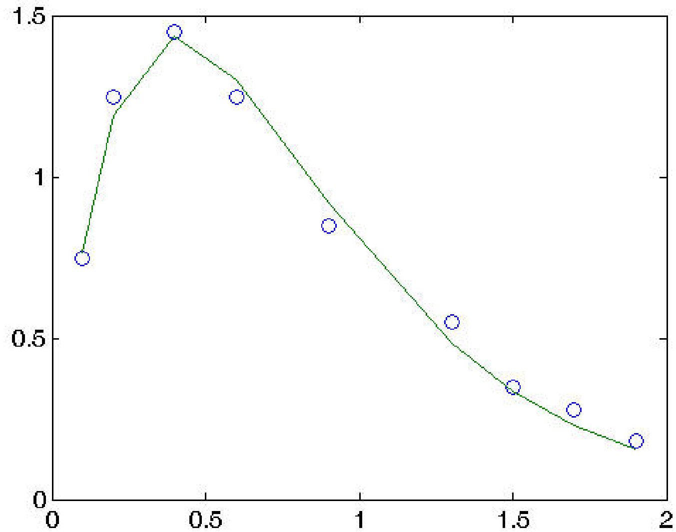
```
>> a = fminsearch(@fSSR, [1, 1], [], x, y)

a =
    9.8545   -2.5217
```

The best-fit model is therefore

$$y = 9.8545xe^{-2.5217x}$$

The fit along with the data can be displayed graphically.

```
>> yp = a(1)*x.*exp(a(2)*x);
>> plot(x,y,'o',x,yp)
```



14.13 (a) The model can be linearized by inverting it,

$$\frac{1}{v_0} = \frac{K}{k_m}\frac{1}{[S]^3} + \frac{1}{k_m}$$

If this model is valid, a plot of $1/v_0$ versus $1/[S]^3$ should yield a straight line with a slope of K/k_m and an intercept of $1/k_m$. The slope and intercept can be implemented in MATLAB using the M-file function `linregr` (Fig. 12.12),

```
>> S = [.01 .05 .1 .5 1 5 10 50 100];
>> v0 = [6.078e-11 7.595e-9 6.063e-8 5.788e-6 1.737e-5 2.423e-5 2.43e-5
2.431e-5 2.431e-5];
>> a = linregr(1./S.^3,1./v0)

a =
  1.0e+004 *
   1.64527391375701   4.13997346408367
```

These results can then be used to compute k_m and K,

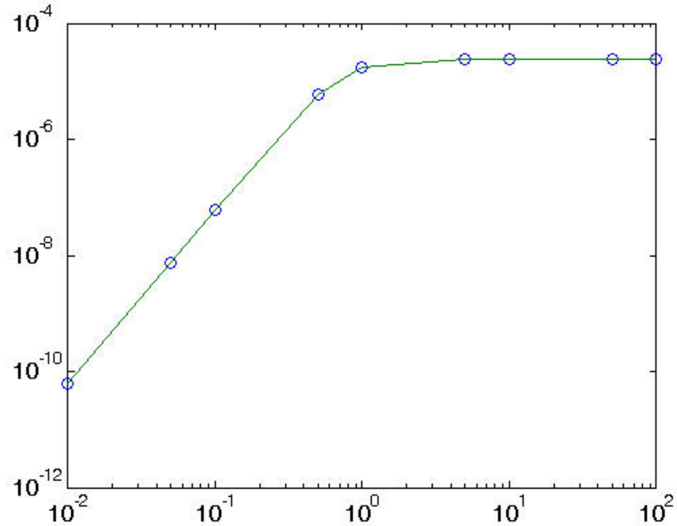
```
>> km=1/a(2)
km =
    2.415474419523452e-005

>> K=km*a(1)
K =
   0.39741170517893
```

Thus, the best-fit model is

$$v_0 = \frac{2.415474 \times 10^{-5}[S]^3}{0.39741 + [S]^3}$$

The fit along with the data can be displayed graphically. We will use a log-log plot because of the wide variation of the magnitudes of the values being displayed,

```
>> v0p = km*S.^3./(K+S.^3);
>> loglog(S,v0,'o',S,v0p)
```



(b) An M-file function must be created to compute the sum of the squares,

```
function f = fSSR(a,Sm,v0m)
v0p = a(1)*Sm.^3./(a(2)+Sm.^3);
f = sum((v0m-v0p).^2);
```

The data can then be entered as

```
>> S = [.01 .05 .1 .5 1 5 10 50 100];
>> v0 = [6.078e-11 7.595e-9 6.063e-8 5.788e-6 1.737e-5 2.423e-5 2.43e-5
2.431e-5 2.431e-5];
```

The minimization of the function is then implemented by

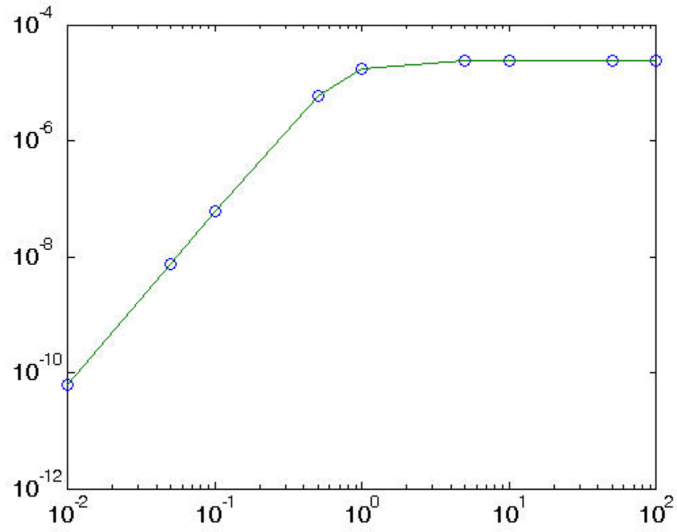
```
>> format long
>> a = fminsearch(@fSSR, [2e-5, 1], [], S, v0)

a =
   0.00002430998303   0.39976314533880
```

The best-fit model is therefore

$$v_0 = \frac{2.431 \times 10^{-5}[S]^3}{0.399763 + [S]^3}$$

The fit along with the data can be displayed graphically. We will use a log-log plot because of the wide variation of the magnitudes of the values being displayed,

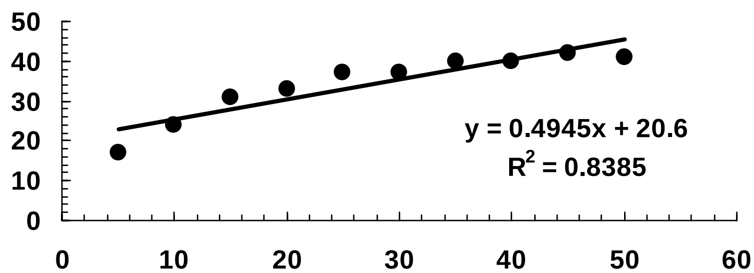
```
>> v0p = a(1)*S.^3./(a(2)+S.^3);
>> loglog(S,v0,'o',S,v0p)
```



14.14 (a) We regress y versus x to give

$$y = 20.6 + 0.494545x$$

The model and the data can be plotted as



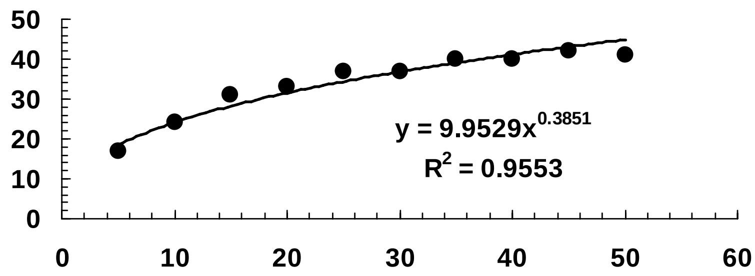
(b) We regress $\log_{10}y$ versus $\log_{10}x$ to give

$$\log_{10} y = 0.99795 + 0.385077 \log_{10} x$$

Therefore, $\alpha_2 = 10^{0.99795} = 9.952915$ and $\beta_2 = 0.385077$, and the power model is

$$y = 9.952915x^{0.385077}$$

The model and the data can be plotted as



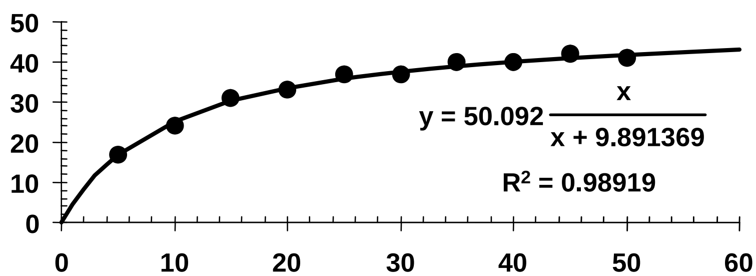
(c) We regress 1/*y* versus 1/*x* to give

$$\frac{1}{y} = 0.019963 + 0.197464\frac{1}{x}$$

Therefore, α_3 = 1/0.01996322 = 50.09212 and β_3 = 0.19746357(50.09212) = 9.89137, and the saturation-growth-rate model is

$$y = 50.09212\frac{x}{9.89137 + x}$$

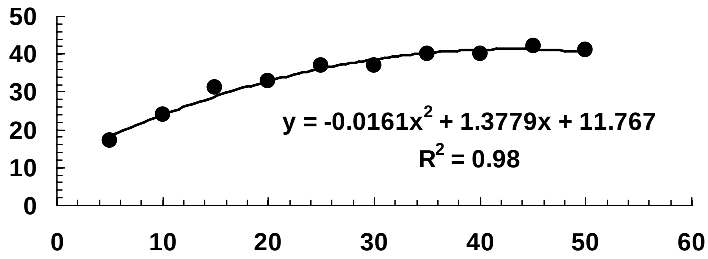
The model and the data can be plotted as



(d) We employ polynomial regression to fit a parabola

$$y = -0.01606x^2 + 1.377879x + 11.76667$$

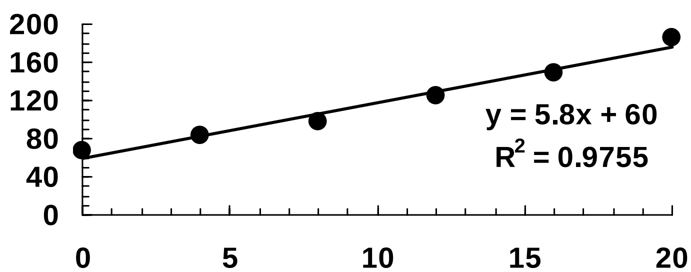
The model and the data can be plotted as



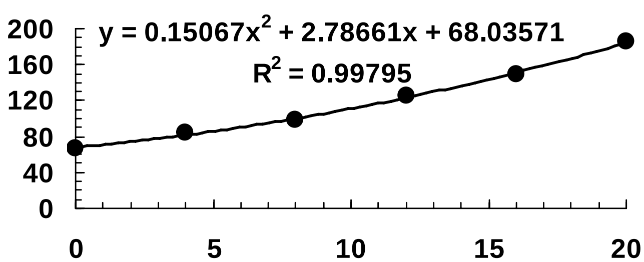
Comparison of fits: The linear fit is obviously inadequate. Although the power fit follows the general trend of the data, it is also inadequate because (1) the residuals do not appear to be randomly distributed around the best fit line and (2) it has a lower r^2 than the saturation and parabolic models.

The best fits are for the saturation-growth-rate and the parabolic models. They both have randomly distributed residuals and they have similar high coefficients of determination. The saturation model has a slightly higher r^2. Although the difference is probably not statistically significant, in the absence of additional information, we can conclude that the saturation model represents the best fit.

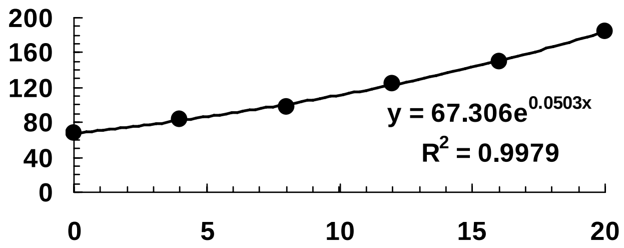
14.15 Linear regression gives



Polynomial regression yields a best-fit parabola



Exponential model:



The linear model is inadequate since it does not capture the curving trend of the data. At face value, the parabolic and exponential models appear to be equally good. However, knowledge of bacterial growth might lead you to choose the exponential model as it is commonly used to simulate the growth of microorganism populations. Interestingly, the choice matters when the models are used for prediction. If the exponential model is used, the result is

$$B = 67.306e^{0.0503(40)} = 503.3317$$

For the parabolic model, the prediction is

$$B = 0.15067t^2 + 2.78661t + 68.03571 = 420.5721$$

Thus, even though the models would yield very similar results within the data range, they yield dramatically different results for extrapolation outside the range.

14.16 The sum of the squares of the residuals for this case can be written as

$$S_r = \sum_{i=1}^{n} \left(y_i - a_1 x_i - a_2 x_i^2\right)^2$$

The partial derivatives of this function with respect to the unknown parameters can be determined as

$$\frac{\partial S_r}{\partial a_1} = -2\sum \left[(y_i - a_1 x_i - a_2 x_i^2) x_i\right]$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum \left[(y_i - a_1 x_i - a_2 x_i^2) x_i^2\right]$$

Setting the derivative equal to zero and evaluating the summations gives

$$\left(\sum x_i^2\right) a_1 + \left(\sum x_i^3\right) a_2 = \sum x_i y_i$$

$$\left(\sum x_i^3\right) a_1 + \left(\sum x_i^4\right) a_2 = \sum x_i^2 y_i$$

which can be solved for

$$a_1 = \frac{\sum x_i y_i \sum x_i^4 - \sum x_i^2 y_i \sum x_i^3}{\sum x_i^2 \sum x_i^4 - \left(\sum x_i^3\right)^2}$$

$$a_2 = \frac{\sum x_i^2 \sum x_i^2 y_i - \sum x_i y_i \sum x_i^3}{\sum x_i^2 \sum x_i^4 - \left(\sum x_i^3\right)^2}$$

The model can be tested for the data from Table 13.1.

x	y	x^2	x^3	x^4	xy	x^2y
10	25	100	1000	10000	250	2500
20	70	400	8000	160000	1400	28000
30	380	900	27000	810000	11400	342000
40	550	1600	64000	2560000	22000	880000
50	610	2500	125000	6250000	30500	1525000
60	1220	3600	216000	12960000	73200	4392000
70	830	4900	343000	24010000	58100	4067000
80	1450	6400	512000	40960000	116000	9280000
Σ		20400	1296000	87720000	312850	20516500

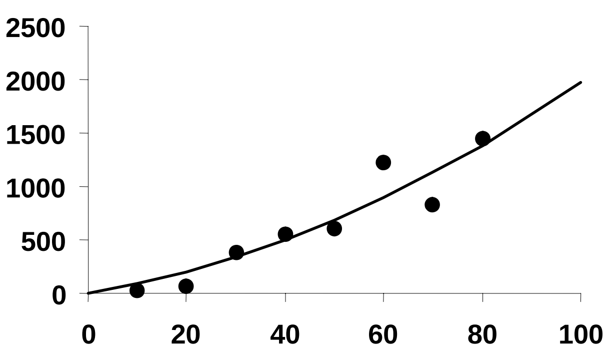
$$a_1 = \frac{312850(87720000) - 20516500(1296000)}{20400(87720000) - (1296000)^2} = 7.771024$$

$$a_2 = \frac{20400(20516500) - 312850(1296000)}{20400(87720000) - (1296000)} = 0.119075$$

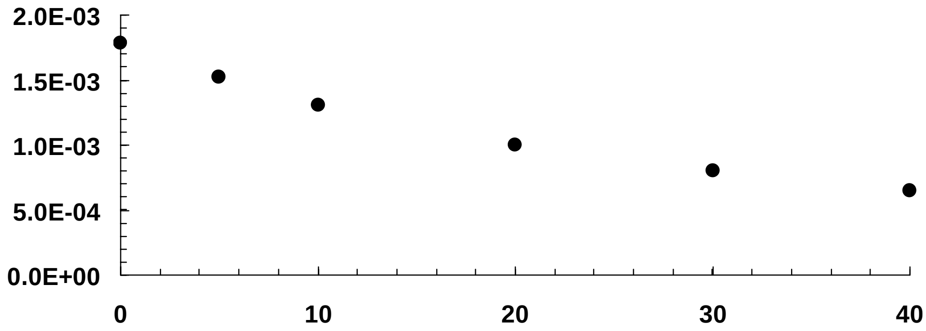
Therefore, the best-fit model is

$$y = 7.771024x + 0.119075x^2$$

The fit, along with the original data can be plotted as



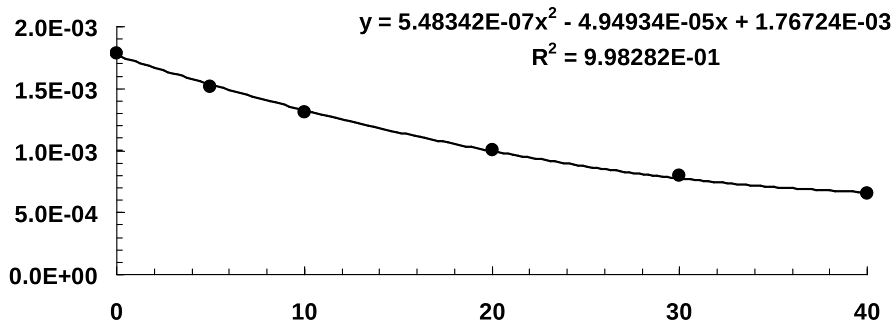
14.17 (a) The data can be plotted as



(b) Linear interpolation yields.

$$\mu = 1.519 \times 10^{-3} + \frac{1.307 \times 10^{-3} - 1.519 \times 10^{-3}}{10 - 5}(7.5 - 5) = 1.413 \times 10^{-3}$$

(b) Polynomial regression yields



This leads to a prediction of

$$\mu = 5.48342 \times 10^{-7}(7.5)^2 - 4.94934 \times 10^{-5}(7.5) + 1.76724 \times 10^{-3} = 1.4269 \times 10^{-3}$$

14.18 The equation can be expressed in the form of the general linear least-squares model,.

$$\frac{PV}{RT} - 1 = A_1 \frac{1}{V} + A_2 \frac{1}{V^2}$$

```
>> R=82.05;T=303;
>> P=[0.985 1.108 1.363 1.631]';
>> V=[25000 22200 18000 15000]';
>> y=P.*V/R/T-1;
>> Z=[1./V 1./V.^2];
>> a=(Z'*Z)\(Z'*y)

a =
     -231.67
 -1.0499e+005
```

Alternatively, nonlinear regression can also be used to evaluate the coefficients. First, a function can be set up to compute the sum of the squares of the residuals,

```
function f = fSSR1418(a,V,ym)
yp=1+a(1)./V+a(2)./V.^2;
f = sum((ym-yp).^2);
```

Then, the `fminsearch` function can be employed to determine the coefficients,

```
>> fminsearch(@fSSR1418,[-200 1],[],V,y)

ans =
      -231.67 -1.0499e+005
```

14.19 We can use general linear least squares to generate the best-fit equation. The $[Z]$ and y matrices can be set up using MATLAB commands as

```
>> format long
>> x = [273.15 283.15 293.15 303.15 313.15]';
>> Kw = [1.164e-15 2.950e-15 6.846e-15 1.467e-14 2.929e-14]';
>> y=-log10(Kw);
>> Z = [(1./x) log10(x) x ones(size(x))];
```

The coefficients can be evaluated as

```
>> a=inv(Z'*Z)*(Z'*y)
Warning: Matrix is close to singular or badly scaled.
         Results may be inaccurate. RCOND = 6.457873e-020.

a =
  1.0e+003 *
   5.18067187500000
   0.01342456054688
   0.00000562858582
  -0.03827636718750
```

Note the warning that the results are ill-conditioned. According to this calculation, the best-fit model is

$$-\log_{10} K_w = \frac{5180.67}{T_a} + 13.42456 \log_{10} T_a + 0.00562859 T_a - 38.276367$$

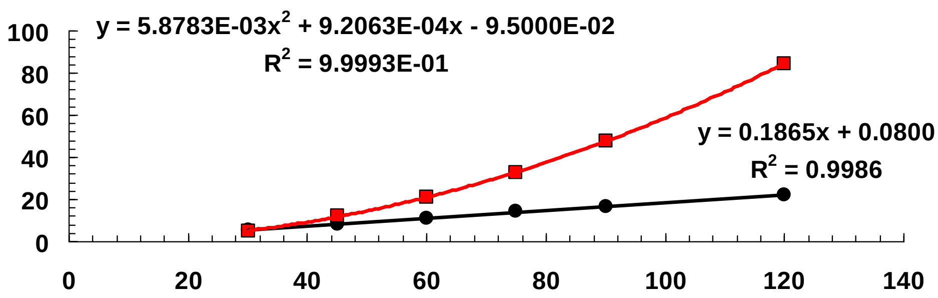
We can check the results by using the model to make predictions at the values of the original data

```
>> yp=10.^-(a(1)./x+a(2)*log10(x)+a(3)*x+a(4))

yp =
  1.0e-013 *
   0.01161193308242
   0.02943235714551
   0.06828461729494
```

```
0.14636330575049
0.29218444886852
```

These results agree to about 2 or 3 significant digits with the original data.

14.20 The “Thinking” curve can be fit with a linear model whereas the “Braking” curve can be fit with a quadratic model as in the following plot.



A prediction of the total stopping distance for a car traveling at 110 km/hr can be computed as

$$d = 0.1865(110) + 0.0800 + 5.8783 \times 10^{-3}(110)^2 + 9.2063 \times 10^{-4}(110) - 9.5000 \times 10^{-2} = 91.726 \text{ m}$$

14.21 The angular frequency can be computed as $\omega_0 = 2\pi/24 = 0.261799$. The various summations required for the normal equations can be set up as

t	*y*	cos($\omega_0 t$)	sin($\omega_0 t$)	sin($\omega_0 t$)cos($\omega_0 t$)	cos^2($\omega_0 t$)	sin^2($\omega_0 t$)	*y*cos($\omega_0 t$)	*y*sin($\omega_0 t$)
0	7.6	1.00000	0.00000	0.00000	1.00000	0.00000	7.60000	0.00000
2	7.2	0.86603	0.50000	0.43301	0.75000	0.25000	6.23538	3.60000
4	7.0	0.50000	0.86603	0.43301	0.25000	0.75000	3.50000	6.06218
5	6.5	0.25882	0.96593	0.25000	0.06699	0.93301	1.68232	6.27852
7	7.5	-0.25882	0.96593	-0.25000	0.06699	0.93301	-1.94114	7.24444
9	7.2	-0.70711	0.70711	-0.50000	0.50000	0.50000	-5.09117	5.09117
12	8.9	-1.00000	0.00000	0.00000	1.00000	0.00000	-8.90000	0.00000
15	9.1	-0.70711	-0.70711	0.50000	0.50000	0.50000	-6.43467	-6.43467
20	8.9	0.50000	-0.86603	-0.43301	0.25000	0.75000	4.45000	-7.70763
22	7.9	0.86603	-0.50000	-0.43301	0.75000	0.25000	6.84160	-3.95000
24	7.0	1.00000	0.00000	0.00000	1.00000	0.00000	7.00000	0.00000
Sum→	84.8	2.31784	1.93185	0.00000	6.13397	4.86603	14.94232	10.18401

The normal equations can be assembled as

$$\begin{bmatrix} 11 & 2.317837 & 1.931852 \\ 2.3178 & 6.133975 & 0 \\ 1.931852 & 0 & 4.866025 \end{bmatrix} \begin{Bmatrix} A_0 \\ A_1 \\ B_1 \end{Bmatrix} = \begin{Bmatrix} 84.8 \\ 14.94232 \\ 10.18401 \end{Bmatrix}$$

This system can be solved for $A_0 = 8.02704$, $A_1 = -0.59717$, and $B_1 = -1.09392$. Therefore, the best-fit sinusoid is

$$pH = 8.02704 - 0.59717\cos(\omega_0 t) - 1.09392\sin(\omega_0 t)$$

The result can also be expressed in the alternate form of Eq. 14.14 by computing the amplitude,

$$C_1 = \sqrt{0.59717^2 + 1.09392^2} = 1.246305$$

and the phase shift

$$\theta = \arctan\left(-\frac{-1.09392}{-0.59717}\right) = 2.070488$$

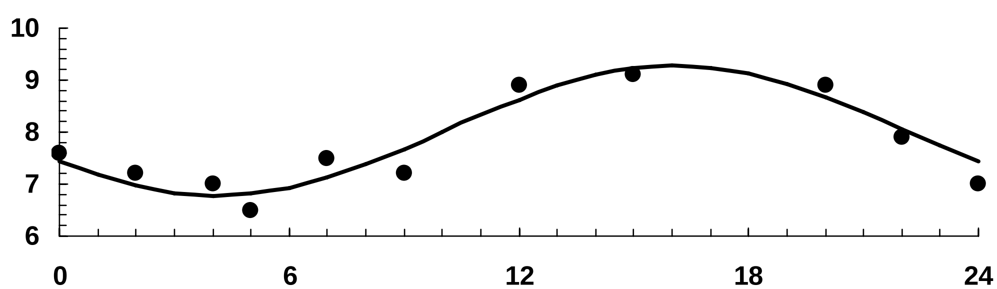
Therefore, the fit can also be expressed as

$$pH = 8.02704 + 1.246305\cos(\omega_0 t + 2.070488)$$

Consequently, the mean is 8.02704 and the amplitude is 1.246305. The time of the maximum can be computed as

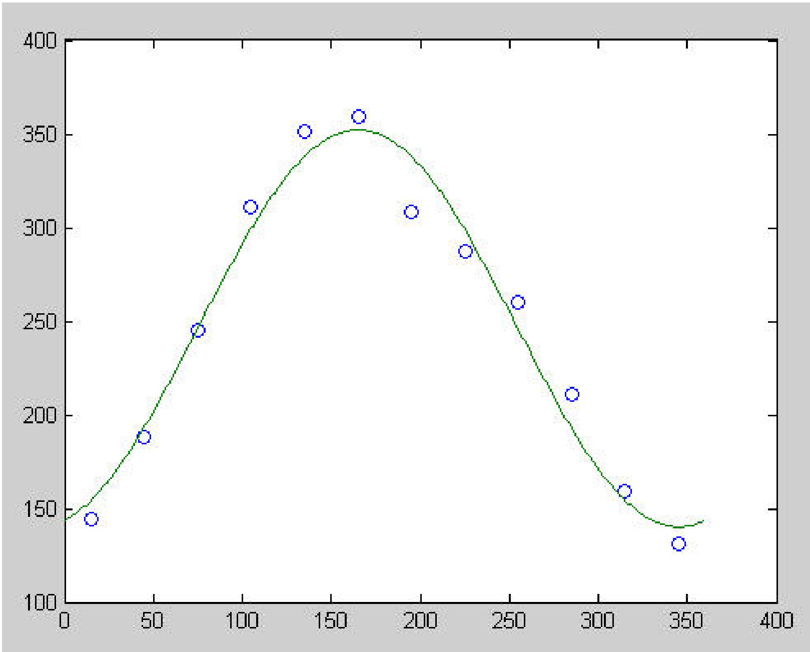
$$t_{\max} = 24 - 2.070488 \times \frac{24\text{ hr}}{2\pi} = 16.09132\text{ hrs}$$

This is equal to about 16:05:29 or 4:05:29 PM. The data and the model can be plotted as



14.22 The coefficients can be determined as

```
>> t=[15 45 75 105 135 165 195 225 255 285 315 345]';
>> R=[144 188 245 311 351 359 308 287 260 211 159 131]';
>> Z=[ones(size(t)) cos(w0*t) sin(w0*t)];
>> a=(Z'*Z)\(Z'*R)

a =
       246.17
      -102.36
       27.405

>> tp=[0:360];
>> Rp=a(1)+a(2)*cos(w0*tp)+a(3)*sin(w0*tp);
>> plot(t,T,'o',tp,Rp)
```



The value for mid-August can be computed as

```
>> a(1)+a(2)*cos(w0*225)+a(3)*sin(w0*225)

ans =
       299.17
```